# Activities & Scientific Reports


cecam
Centre Européen de Calcul Atomique et Moléculaire

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# Table of Contents

# INTRODUCTION

The 2024 CECAM Flagship program showcased 77 events hosted at the Headquarters (HQ) and the Nodes.

Of these, the CECAM HQ at EPFL hosted 21 events (19 workshops and 2 schools), accounting for 25% of the total program. The remaining 56 events (39 workshops and 17 schools) were held at the various Nodes (Fig.1).

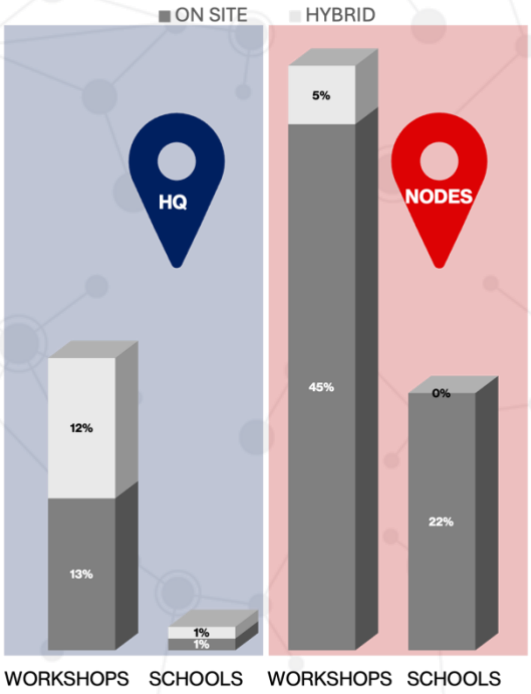


*Fig.1: CECAM Flagship program 2024. On site and hybrid part of workshop and schools in the Headquaters and the Nodes.*

335 scientists based in 24 different countries organized these events, 91 for the HQ events and 244 for the Nodes events.

The total number of participants reached 4374 people in 2024, with 48% attending HQ events and 52% attending Node events. A similar gender ratio was maintained across both HQ and Node activities (Fig.2).

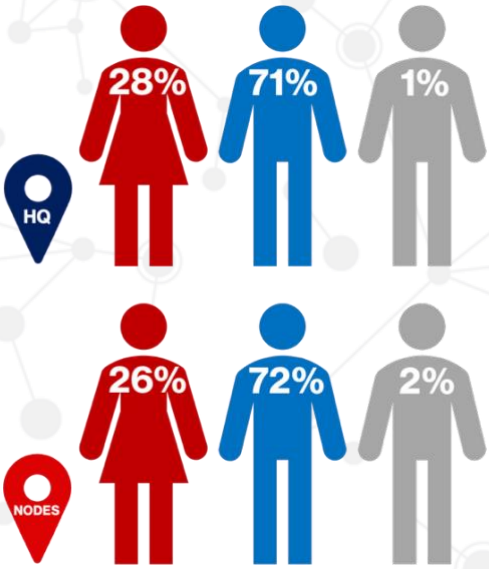


*Fig.2: CECAM Flagship program 2024. Women, men and gender-neutral participation to Headquaters and Node events.*

Analysis of event data indicates a strong community preference for in-person events, which constituted 81% of all activities. Indeed, on site participation amounted to 70% of the total.

Based on informal interviews and post-event surveys, participants and organizers favor the in-person format for its ability to enhance scientific exchange, facilitate networking, and simplify the planning of future

collaborations. This preference is even more pronounced at the Node events than at the HQ (Fig.3).

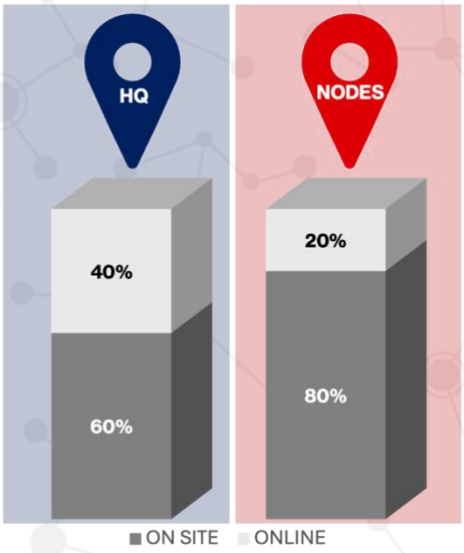


*Fig.3: CECAM Flagship program 2024. Onsite and online participation to events in the Headquaters and the Nodes.*

However, remote participation remains highly valued for its role in reducing the program's carbon footprint and increasing accessibility for individuals in developing countries. Data confirms that about 10% of online participants, at CECAM activities, have affiliations in developing countries, as detailed below (Tab.1) for HQ and Nodes.

| HQ / NODES | ON SITE | ONLINE |
|---|---|---|
| DEVELOPED COUNTRIES | 46%<br>74% | 24%<br>15% |
| DEVELOPING COUNTRIES | 14%<br>6% | 16%<br>5% |

*Tab.1: CECAM Flagship program 2024. Developed countries and developing countries participation to on site and online Headquarters and Node events.*

In addition to the activities carried out within the Flagship program, several other initiatives were carried out in the year.

The *Mary Ann Mansigh conversation series* consisted of a single lecture about *science writing and science editing*. Science editors and writers are vital to the scientific ecosystem, ensuring research is accessible and accurate. While journal editors manage the publication and peer review of scientific papers, science journalists translate complex findings into newsworthy stories for the public. Understanding their roles and how to communicate with them is a crucial skill for young scientists, and it also opens potential career paths in publishing and communication. The event was received very well, with about 50 in person participants and more than 80 following the streaming.

*Classics in Molecular and materials modelling* also consisted in a single lecture about *methods for computational biology and drug discovery*. Shoshana Wodak and Bill Jorgensen shared with us their contributions to the birth of docking methods and the adoption and development of free energy methods, focusing on pharmacological applications. Participation was similar to the

one for the Mary Ann Mansigh event, consolidating these initiatives as an appreciated on and off campus activity.

In 2024, CECAM continued to expand its outreach strategy with six *CECAM webinars*. These focused on dissemination activities for projects within the scope of CECAM: the EuroHPC MultiXscale and TREX Centers of Excellence for Computing Applications, the EU Horizon funded Molecular Dynamics Data Base initiative, the CO2112 path finder project, and the Lhumos web portal for educational material. The webinars enable to share groundbreaking scientific results, facilitate the dissemination of cutting-edge research, make our activities more accessible globally, and engage with the scientific community. The lighter logistical workload for CECAM staff and the organizers is well adapted for focused, timely, and efficient dissemination. The webinars then serve as a strategic and complementary component to our dynamic, in-person environment of workshops and schools, providing an additional format within the CECAM program, enhancing its overall scope and enabling us to connect with a wider community.

The reports and descriptions of activities hereafter show that CECAM serves as a central point for the scientific community, delivering a highly valued platform for scientific exchange, collaboration, and training. The program's diverse and vibrant nature is a result of a rigorous selection process of bottom-up proposals. This process ensures a balance between cutting-edge topics, foundational subjects, and applications with clear societal benefits, ultimately fostering a unique environment for progress and global dissemination of knowledge and reaching a worldwide and diverse audience.

# Atomistic modelling of solid-liquid interfaces in electrocatalysis

**Location: Lorentz Center, Leiden, the Netherlands**
**Webpage : https://www.cecam.org/workshop-details/atomistic-modelling-of-solid-liquid-interfaces-in-electrocatalysis-1254**
**Dates: Jan 8, 2024 - Jan 12, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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Electrocatalytic reactions are nowadays of paramount importance to realize the green energy transition and meet the goals of the Paris agreement, since many of the technological solutions which are considered key to achieve carbon neutrality are based on the use of electrochemical devices. In all electrochemical devices, catalysts are required to speed up the reaction kinetics while increasing the selectivity of the desired products. Efficiency and selectivity of an electrocatalytic process are key features to make electrocatalysis economically competitive and industrially relevant. Therefore, in recent years, much effort has been devoted to gain understanding of what occurs at the catalyst surface with the aim to control and improve electrochemical processes. In this context, computational electrocatalysis has emerged as an important field since it can provide fundamental mechanistic understanding of complex reactions occurring at an electrode surface. This field not only provides support for interpreting experimental observation but can be used to guide the design of new materials and predict the activity of electrocatalysts which have not been yet synthesized in the laboratory. Hence, computer simulations have the power to shed light on chemical processes at the nanometric and sub-nanometric scale, and as such represents a unique tool to boost the understanding and the optimization of electrochemical systems.
This workshop aimed to tackle the complexity of electrode-electrolyte interfaces for relevant applications in electrocatalysis by bringing together physicists, chemists, electrochemists, materials scientists, and engineers with complementary expertise in computational modelling of: (i) solid surfaces and solid-liquid interfaces; (ii) complex liquid phases (dielectric solutions); (iii) electrocatalysis and (iv) machine learning. The focus of the event has been to discuss the state-of-the-art and beyond in the development of approaches and methods for the accurate modelling of electrochemical processes. Some of the biggest challenges in the field, that we addressed during the workshop are:
1) Improvement of implicit solvation models
2) The inclusion of the explicit liquid phase in the simulations
3) Study of the effect of the electrolyte solution on the catalysis

4) The inclusion of an external applied potential
These aspects are important to achieve an accurate, quantitative description of electrochemical processes which can be directly correlated with experimental investigations. A methodological development would have important implications for the development of energy storage and conversion devices, including fuel cells, batteries, supercapacitors, and electrolyzers for green $H_2$ production, and $CO_2$/$N_2$ conversion into value-added chemicals.

### Key References

*[1] R. Urrego-Ortiz, S. Builes, F. Illas, F. Calle-Vallejo, EES. Catal.,* ***2****, 157 (2024)*
*[2] B. Kirchhoff, E. Jónsson, T. Jacob, H. Jónsson, Top. Catal.,* ***66****, 1244 (2023)*
*[3] J. Nørskov, J. Rossmeisl, A. Logadottir, L. Lindqvist, J. Kitchin, T. Bligaard, H. Jónsson, J. Phys. Chem. B,* ***108****, 17886 (2004)*

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The meeting facilitated in-depth discussions on various aspects, including implicit and explicit solvent models, the role of an external applied potential, and the integration of machine learning in electrocatalysis simulations.
Implicit Solvent Models:
One major scientific focus of the workshop was the improvement of implicit solvation models. Participants discussed the challenges associated with these models, such as extensive parametrization requirements, the lack of benchmark data, and the need for more accurate descriptions of microsolvation and competitive adsorption. The limitations of current implicit solvent models, including the unphysical presence of the solution in certain regions, were acknowledged. Additionally, questions arose regarding the coupling between electrolyte and adsorbate dynamics and the potential role of machine learning algorithms in defining implicit solvent models.
Explicit Solvent Models:
Explicit solvent models, examined during the workshop, raised critical challenges in classical molecular dynamics (MD), ab initio MD, and hybrid methods. Challenges in classical MD included defining force fields for the interface and accurately describing polarization effects. Ab initio MD faced issues related to sampling for meaningful statistical averages, realistic electrolyte concentrations, and accurate descriptions of transition states. The hybrid methods raised questions about treating the boundary conditions when combining implicit and explicit solvent structures.
External Applied Potential:
Understanding the influence of an external applied potential emerged as a key topic. Challenges identified included benchmarking, incorporating electrode potential effects in the calculations of mechanism and rate of the various elementary steps of the reactions, and the impact of the chosen method on predicted electrode/electrolyte interface behavior. The need for improvement in

existing methods, such as utilizing sawtooth potentials or Barry phase methods, was highlighted. Concerns were raised about treating semiconductor electrodes, inhomogeneities in electric fields at non-flat electrodes, and calculating accurate differential double-layer capacitances.
Tangible Outcomes: Participants collaboratively generated proposed solutions to the identified challenges during focused brainstorming sessions. Notably, the participants committed to writing a commentary paper on the topic, intending to submit it to a high-impact factor journal. This commitment underscores the need to disseminating the workshop's findings to the broader scientific community.
The workshop facilitated an understanding of the complexities of electrocatalytic processes at solid-liquid interfaces. The realization that a community approach is essential to address the challenges and advance the field was an important point. Participants recognized the need for collaboration, knowledge exchange and the creation of a scientific community to collectively address the limitations of current simulation methodologies.
While the workshop made significant strides, participants acknowledged the existing limitations in current methodologies. Challenges persist in improving implicit solvation models, enhancing hybrid approaches, benchmarking modeling approaches, and achieving better integration between theoretical and experimental studies.

## 3. What was the take-home message for the participants?

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High-Performance Computing (HPC) Resources: The resource-intensive nature of simulations demands access to high-performance computing facilities. The community emphasized the importance of fostering collaborations with HPC centers and securing adequate computational resources for large-scale simulations.
Networking: Effective collaboration between computational and experimental researchers is crucial. The community expressed the need for organized initiatives to bridge the gap between these two domains. Workshops and collaborative projects were identified as means to facilitate communication and understanding between computational and experimental electrocatalysis researchers. Beyond computational researchers, engaging experts from diverse disciplines such as materials science, chemistry, physics, and engineering are essential. Establishing networks with researchers from related fields ensures a comprehensive approach to addressing the challenges in electrocatalysis.
Standardized Benchmarking Protocols: Benchmarking emerged as a critical need for the community. Establishing standardized benchmarking protocols for electrochemical interfaces will ensure consistent evaluation of computational methods. This initiative could be led by collaborative efforts involving researcher groups from different institutions.
The community also expressed the need for dedicated platforms or repositories to share benchmarking data and results. Online, open access repositories would serve as a valuable resource for researchers to compare their methods against

established benchmarks. Recognizing the importance of data sharing, the community emphasized the need for a culture of openness and collaboration. Encouraging researchers to share simulation data, methodologies, and results will contribute to transparency, reproducibility, and the overall advancement of the field. Establishing data-sharing standards and platforms was identified as a key step in promoting collaboration and accelerating progress in computational electrocatalysis.
The community would surely benefit from organizing a series of CECAM workshops dedicated to atomistic modeling of solid-liquid interfaces in electrocatalysis. A series would provide continuity, allowing for an in-depth exploration of specific challenges and fostering ongoing collaboration.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The participants engaged in explicit discussions regarding the prospect of writing a proposal for a COST (European Cooperation in Science and Technology) Action during the workshop. The COST framework emerged as a particularly attractive funding scheme due to its emphasis on fostering collaboration, building networks, and creating scientific communities across European countries.
Recognizing the interdisciplinary nature of the workshop and the need for sustained interaction among researchers, the idea of submitting a COST Action proposal gained prominence. Participants discussed how a COST Action could serve as an ideal platform for community building. It was recognized that such an initiative could facilitate continuous collaboration, knowledge exchange, and resource-sharing among researchers working on atomistic modeling of solid-liquid interfaces in electrocatalysis.
The COST framework's inclusive nature, allowing participation from researchers across European countries, is in line with the workshop's aim to bring together experts from diverse backgrounds.
The discussions emphasized that a COST Action could provide a structured framework for organizing workshops, training schools, and short-term scientific missions, fostering sustained interactions among the community members. Participants highlighted the potential for a COST Action to extend the impact of the workshop beyond its immediate outcomes. Establishing a COST network would offer a platform for continuous collaboration, addressing the identified challenges, and further advancing the field.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The research topic of the workshop, "Atomistic Modeling of Solid-Liquid Interfaces in Electrocatalysis," holds significant potential for various societal benefits, spanning economic and environmental domains. The outcomes of the workshop

have direct implications for industries focused on green energy, catalysis, and electrochemical devices. Improved understanding and optimization of electrocatalytic processes can enhance the efficiency and selectivity of energy conversion devices such as fuel cells, batteries, and electrolyzers. This, in turn, can lead to the development of more cost-effective and commercially viable technologies for energy storage, production, and conversion.
The workshop's focus on electrocatalysis aligns with global efforts towards environmental sustainability. By advancing the fundamental understanding of electrochemical processes, particularly those related to green hydrogen production, carbon dioxide reduction, and nitrogen conversion, the research contributes to the development of environmentally friendly technologies. The societal benefit lies in the potential to replace or supplement existing processes with more sustainable alternatives, thereby reducing carbon emissions and fostering a transition towards cleaner energy sources. This aligns with the broader goals of achieving carbon neutrality and mitigating climate change.

## 6. Organiser list

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**Cicero, Giancarlo**
Politecnico di Torino, Italy
**García-Melchor, Max**
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**Jónsson, Hannes**
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**Koper, Marc**
Leiden Institute of Chemistry, Leiden University, Netherlands
**López, Núria**
Institute of Chemical Research of Catalonia ICIQ, Spain


# MolSim-2024

**Location: CECAM-NL**
**Webpage : https://www.cecam.org/workshop-details/molsim-2024-1236**
**Dates: Jan 8, 2024 - Jan 19, 2024**

## 1. What were the major topics presented in the School?

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The MolSim-2024 school took place over a period of two weeks in January 2024. It offered a program focusing on basic and advanced molecular simulation methods. The program has an integrated and balanced structure of lectures (10 full morning plenary sessions) and hands-on exercises (9 full afternoon sessions, in two groups).
The school is organized on a yearly basis, and targets PhD candidates and postdoctoral researchers who want to enhance their understanding and skills of employing molecular simulation to study topics in physics, chemistry or biology. The setting - learning and working together for a more extended period - provides the participants ample time to interact with their peers (also socially), allowing them to build and/or enhance their scientific network.
The structure of the school's content was as follows:
- Basic theory and methods: statistical thermodynamics, Monte Carlo, molecular dynamics
- Advanced topics (theory and methods): free energy, enhanced sampling, rare events, machine learning
- Topical items: biological systems, (nanoporous) materials, soft matter
- Group activities: poster session, common daily meals/breaks, outing and school's dinner (weekend)

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

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Given the type of the event, providing a detailed report on items (questions/remarks/...) that were brought up would be outside of the scope of this report.
Participants are made aware (from the start) that "live interaction" is an important aspect of the lecture and lab sessions. The participant group was in this respect rather active while in session. An additional important observation is that "out of session" moments (breaks/lunch time) were typically fully used (to continue) discussions with the lecturer.

The lab-course session (carrying out calculations on participants laptops using prepared problems with minor coding / proper parameter setting) is by nature very interactive.
The lab-course session is carried out in a sectioned (3-5) setting, consisting of a "plenary introduction / individual work on a specific problem (in pairs) / plenary guide-to-answers". A (rather natural) aspect is that fully completing a problem is not always reached, as not all participants are on equal level. The provided guide-to-answers allows for post-school completion of most of the problems.
On the practical side, having the participant's laptops well is essential. Regarding this, the participants are provided detailed instructions a few weeks prior to the school's start. Remaining issues are resolved during the first lab course session.
Questions and remarks brought forward during the lecture/labcourse sessions were on a level and intensity typical for a postgraduate class, ranging from the basic to the (very) advanced level. The range of the level indicates that knowledge/understanding/skills among the group is substantial. The school is well aware of this and the content of lectures and lab-course is built such that if serves the whole group, as much as possible.

### 3. What was the take-home message for the participants?

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- use acquired understanding, knowledge and skills in the current (and future) research
- spend to some time to further understand the lecture topics
- look at the non-completed/non-covered problems in lab-course manual
- keep interactions and contacts alive
- notify potential future participants of next MolSim

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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The hard-copy and digital (compchem.nl/molsim) trace of the school :
- lecture slides (digital)
- lab course manual (paper & digital)
- lab course software packages
- lab course guide to solutions (digital)

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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**Participants** Here we aim for an evenly distributed diversity (match of research interest with school's focus / country of residence / research group / gender / underrepresented groups / nationality). This is reasonably well achieved.
Gender balance (F/M) applicants (110) / participants (70) was 0.35|0.65 / 0.33|0.66. Note, that almost all of the eligible female applicants were admitted.

Teaching Although aimed for, the composition of the team is not truly evenly diverse, though some broadness in the distribution lecturers: 5 countries/ mixed seniority / 2 female labcourse team: > 6 countries/well mixed gender

## 6. Participant list

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### Organisers

**Dubbeldam, David**
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**Alhanash, Mirna** - Chalmers University of Technology, Sweden
**Alizadeh, Vahideh** - University of Bonn, Germany
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**Berger, Esmée** - Chalmers University of Technology, Sweden
**Carbajo De La Guerra, Irene** - BCMaterials, Spain
**Castagnede, Antoine** - Laboratoire de Physique des Solides, France
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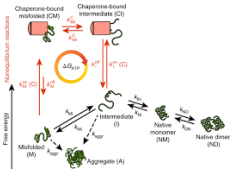

# Modeling energy-consuming biomolecular processes

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/modeling-energy-consuming-biomolecular-processes-1209**
**Dates: Jan 22, 2024 - Jan 25, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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The workshop addressed the role of active, energy-consuming processes in biomolecular systems, with a clear focus on protein quality control, DNA organization, cytoskeletal dynamics, membrane remodeling, and phase separation. Each session exposed a convergence between experimental findings and theoretical models grounded in non-equilibrium statistical physics. Notably, chaperone dynamics (Hsp70, Hsp90, ClpB) were discussed as paradigms of ATP-powered molecular machines that reshape folding landscapes and operate as unfoldases, confirmed by single-molecule and simulation studies. This adds quantitative support to the idea that energy consumption enables these systems to bypass equilibrium constraints and extend proteostasis.
In the domain of nuclear architecture, talks on SMC complexes and condensin-based loop extrusion clarified how ATP hydrolysis drives long-range chromosomal interactions. These models align with non-equilibrium polymer physics and suggest active selection mechanisms in genome folding and surveillance.
A central theme was the active regulation of biomolecular condensates, where enzymatic activity and ATPases tune material properties, composition, and phase behavior. This was supported by data on spatial fluxes, bridging condensate physics with catalysis.
Filament dynamics, including FtsZ treadmilling and actomyosin remodeling, were reframed in terms of entropy production, dynamic ordering, and feedback between chemical and mechanical signals. Lipid membrane modeling further extended non-equilibrium ideas to bilayer remodeling and vesicle formation, areas where direct experimental access remains limited.
By comparing diverse biological systems, the event highlighted how active processes reshape energy landscapes and make otherwise rare or inaccessible states dynamically stable. Theoretical contributions on evolutionary modeling and biochemical proofreading provided mechanistic depth and pushed conceptual boundaries of what constitutes a molecular machine.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop successfully brought together theorists and experimentalists around a shared interest in the energetics of cellular machinery. Several new modeling frameworks were presented and actively discussed, ranging from nonequilibrium polymer simulations and protein mechanics to mesoscopic descriptions of active phase separation and biochemical regulation. These methods offer tractable routes to quantify energy flux, entropy production, and work extraction in biological systems.

Participants aligned around the view that energy consumption plays a decisive role in controlling specificity, spatial localization, and reversibility – properties that are otherwise hard to reconcile with equilibrium physics. There was notable convergence in the way theoretical models and experimental setups now seek to quantify the energetic cost and benefits of processes like protein disaggregation, condensate modulation, and filament dynamics.

New conceptual tools were introduced, such as non-equilibrium binding affinities, local force generation from entropic confinement, and adaptive cycling in active enzymes. These tools pave the way for integrating data across scales and for interpreting complex dynamical behaviors.

Some open questions remain. For instance, the mapping between energy dissipation at the molecular level and measurable cellular consequences is still poorly understood. There are also gaps in connecting atomistic details of ATPase conformational cycles to system-level behavior, and in bridging timescales between fast biochemical transitions and slower emergent organization.

Nevertheless, the workshop produced a shared language and an informal roadmap for integrating active matter physics into biomolecular modeling. Several follow-ups are already underway and reflect a productive outcome beyond the event itself.

## 3. What was the take-home message for the participants?

Energy consumption enables control, specificity, and dynamical stability in biomolecular systems: nonequilibrium modeling is essential to understand them.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Understanding energy-consuming processes in cells has implications for treating protein misfolding diseases, modulating chromatin structure in cancer, and designing synthetic biological systems. Insights into chaperone-assisted folding and condensate regulation inform approaches to neurodegeneration and stress

response, while models of cytoskeletal and membrane remodeling can guide bioengineering applications.
More broadly, the workshop promoted interdisciplinary methods that may translate to the design of smart materials, programmable molecular systems, and synthetic compartments. Concepts such as entropic forces, active feedback, and non-equilibrium specificity can inform material science and nanotechnology. The educational benefit is also significant: by encouraging convergence between physics, biology, and computation, the event contributes to training a generation of researchers better equipped to tackle complex, real-world problems.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop led to the initiation of several new collaborations, particularly on active filament modeling, condensate-membrane interactions, and data-driven simulations of chaperone dynamics. Participants agreed to follow up with joint grant applications and manuscript drafts. Data sharing agreements and plans for shared modeling platforms were discussed, laying the groundwork for concrete joint outcomes.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The event featured a balanced mix of senior and early-career researchers, with substantial representation from PhD students and postdocs. Speakers were selected with attention to gender diversity and institutional breadth, with participants from across Europe, North America, and beyond, including smaller or underrepresented institutions. Remote access options were offered to include participants facing financial or logistical barriers.

## 7. Participant list

### Organisers

**Barducci, Alessandro**
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**De Los Rios, Paolo**
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**Cois, Davide** - EPFL, Switzerland

**Donini, Giacomo** - La Sapienza, Italy
**Forte, Giada** - University of Edinburgh, United Kingdom
**Frey, Erwin** - Ludwig-Maximilians-Universität-Müncher, Germany
**Goloubinoff, Pierre** - Unil / EPFL, Switzerland
**Gruber, Stephan** - Unil, Switzerland
**Hugel, Thorsten** - University of Freiburg, Germany
**Kruse, Karsten** - Université de Genève, Switzerland
**Kumar, Ashutosh** - University of Fribourg, Switzerland
**Lavagna, Enrico** - University of Genoa, Italy
**Leduc, Cecile** - Institut Jacques Monod, France
**Liang, Shiling** - MPI-PKS, Germany
**Liberati, Diego** - National Research Council of Italy, Italy
**Manley, Suliana** - EPFL, Switzerland
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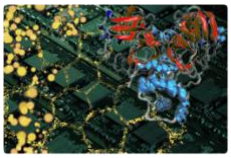

# Perspectives and challenges of future HPC installations for atomistic and molecular simulations

**Location: CECAM-DE-MMS**
**Webpage : https://www.cecam.org/workshop-details/perspectives-and-challenges-of-future-hpc-installations-for-atomistic-and-molecular-simulations-1227**
**Dates: Feb 19, 2024 - Feb 21, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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HPC and custom hardware play a major role in state-of-the-art classical and quantum mechanical atomistic simulations. Besides conventional massively-parallel HPC systems, heterogenous accelerators such as GPUs and FPGAs and even ASIC designs are becoming more and more widespread. Concurrent multiscale methods, such as QM/MM approaches, and enhanced sampling methods facilitate the study of functional mechanisms of increasingly complex biomolecular systems, from CRISPR-Cas9 genome editing to realistic models of cellular membranes.
Furthermore, machine learning techniques to represent the potential energy surface in molecular simulations is an emerging trend that comes in various flavors. Where some researchers employ these techniques as a novel approach to optimize conventional physics-based force fields, others using these techniques to learn a priori or on-the-fly neural network based potential energy surfaces from accurate quantum mechanical electronic structure methods. A most impressive demonstration of the power of such approaches was provided by a foundation model that was designed to map the whole periodic table, bypassing the computation of total energies and forces altogether.
Research code development and code performance improvement are moving more and more into focus so as to efficiently use modern architectures. Tools for automated parallelisation and porting codes from e.g. CPU to GPUs exist and are being developed further. Moreover, libraries for recurring tasks, such as matrix-vector multiplications, are being improved with hardware specific details, such as memory design, in mind.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The previously separate development of hardware and software is no longer appropriate in view of heterogeneous accelerators (GPUs, FPGAs, ASICs), and the rapidly emerging techniques of machine learning also place specific demands on hardware. The event fostered the exchange between stakeholders from all areas related to HPC for molecular simulation, namely hardware designers, architecture-specific software engineers, research code developers, and domain scientists, encouraging mutual awareness and knowledge sharing.
The previously disconnected design of novel hardware architectures and the development of atomistic simulations codes, is becoming more and more a hardware/software co-design effort. Data movement is often performance critical, which can be mitigated through the rational use of existing memory hierarchies. Novel distributed asynchronous object stores (DAOS), implemented in non-volatile memory (NVRAM), can boost data intensive workloads and high-throughput methods.

## 3. What was the take-home message for the participants?

The previously disconnected developments of hardware and software are no longer timely in view of heterogenous accelerators (GPUs, FPGAs, ASIC designs); also, the rapidly emerging machine learning techniques place specific demands on hardware. Efficient usage of HPC resources by informed users employing optimised code on suitable architecture will reduce energy consumption. To this end, stakeholders from all related areas must be made, and kept aware, of the respective other areas.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop contributes to the future viability and further development of simulation-based methods in the field of materials and molecular research. The previously separate development of hardware and software is no longer appropriate in view of heterogeneous accelerators (GPUs, FPGAs, ASICs), and the rapidly emerging techniques of machine learning also place specific demands on hardware. The event promoted exchange between hardware designers, software engineers, research code developers and scientists from the application areas. Participants discussed innovative hardware solutions for data-intensive workloads and emphasised the importance of co-design with regard to hardware and software, as well as the efficient use of HPC infrastructure to reduce energy consumption.
Improvement of methods/software/HPC-capabilities enables researchers in applied fields to tackle research questions related to health, e.g. in drug design, on relevant/more realistic scales in time and space. Improved force fields, moreover, increase the reliability of such research, eventually guiding experimental approaches and thus help sustainability.

Foundation models are often closed source and only made available as a service for pay. The open distribution of such machine learned and neural network-based potentials, similar to the OpenKIM initiative for conventional force fields, is essential.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

A key factor in this is effective communication between the various HPC-related disciplines and training users as early as the doctoral phase. Future workshops and schools on the topic "Computer science meets natural sciences" can make a valuable contribution to achieving these goals.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop gathered 38 participants from across Europe (including UK and Switzerland), the US, and Japan; in addition, there were ca. 20 online participants from all over the world. Four out of 15 invited talks were presented by women, and approximately 20% of all participants were female. These apparently low numbers are considerably higher than the average representation of women in research on HPC systems (10%).
Diversity aspects were taken into consideration when inviting speakers and selecting contributed talks. Two ASC Distinguished Lectures were selected from the submitted abstracts to promote early-career post-doctoral researchers. In addition, a poster prize was awarded at the doctorate level.

## 7. Participant list

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# Electronic structure software development: advancing the modular paradigm

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/electronic-structure-software-development-advancing-the-modular-paradigm-1194**
**Dates: Feb 19, 2024 - Feb 24, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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Shared computational libraries that provide key functionality are now firmly established parts of the electronic structure software ecosystem. As electronic structure methods and codes diversify and mature, the development of libraries strengthens collaborations and avoids reimplementing the same methods in the context of a different, monolithic code. Over the years, a modular paradigm has emerged in which central pieces can be shared and reused between different projects.
Many efforts carried out so far have focused on making this paradigm successful and sustainable, by building robust software components with stable interfaces, offering the best possible performance on a broad range of hardware architectures, and sharing development practices between developers with sometimes very different backgrounds. Among the most important ongoing challenges are (1) training and educating new developers to take advantage of existing developments where that is appropriate and (2) continuously evolving library software to be useful, current, and usable by end users in often complex environments like HPC systems.
The scientific reach of electronic structure theory continues to expand rapidly, including by generalisation of high-throughput calculations, creation of complex workflows, and rapid growth of data-driven methods and machine learning. All these developments now attract participants beyond academia. On the computational side, the involvement of industrial partners is growing steadily, bringing feedback and insights from engineers. Globally, several key collaborative efforts develop shared software, including the MaX and NOMAD Centers of Excellence (CoE), the UK ExCALIBUR exascale project, the Swiss THEOS and MARVEL projects, the U.S. based Molecular Sciences Software Institute, DoE's Exascale initiative, or DoE funded centers such as MiCCOM. Connections with other communities, like quantum chemistry, are getting stronger because of shared needs, as illustrated by the TREX CoE. The Swiss Scientific Computing Center (CSCS), the U.K.'s Daresbury Laboratory, and many other individual

institutions likewise act as lighthouses for shared developments within the broad electronic structure software ecosystem.
The CECAM Electronic Structure Library (ESL) initiative (https://esl.cecam.org) is a key venue that connects developers from electronic structure codes across the community (contributors represent, e.g., SIESTA, BigDFT, DFTB+, Quantum Espresso, Octopus, FHI-aims, and several others). It provides a space for coordination between developers, new library developments and enhancements of existing libraries, as well as interaction with the broader ecosystem of library developments for electronic structure theory. Especially through its workshops, the ESL also acts as a venue that brings together developers across the many broader centers and collaborative efforts (see above) providing a common ground to exchange information and coordinate developments.

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## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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**Summary**

Major outcomes:
- Unifying practices and tools to build software. We have agreed on using CMake in all ESL modules and created a repository to share good CMake recipes: https://gitlab.com/ElectronicStructureLibrary/esl-cmake-recipes.
- On top of this, we have agreed on further promoting the use of Spack and EasyBuild.
- Create a new section in the programme for early career colleagues to expose their research.

- Identified potential new partners for reviving the COST action, meetings are planned in the coming weeks.
- Increased participation from the US, with the help of a generous sponsorship from MOLSSI.
- A healthy intake of newcomers, around half of the 38 participants.
- Increased awareness of our Zulip channel to bring together the community
- Participants from other communities that made use of electronic structure libraries, e.g. Machine Learning and experimental materials

This workshop has identified a series of problems that can and should be addressed rapidly:
- Making use cases more accessible to newcomers. For this, we have started to upgrade the ESL Demonstrator.
- Improving the visibility of the Continuous Integration infrastructure. It now has its own dedicated repository: https://gitlab.com/ElectronicStructureLibrary/esl-ci.
- Sustain a collaborative chat channel (Zulip) where people can exchange ideas, and request feedback

**Discussions about the future of the ESL**

**Challenges**

It is more and more difficult to keep momentum within the community and important sustainability issues are now emerging, e.g. LibXC is used by around 80 different codes but is maintained by a single person who has to deal with complex technical problems. Another prominent issue is employment churn, which limits commitments to 3 years or less. The "publish or perish" race, with a retraction rate of articles doubling every 2 years, is also adding an unnecessary pressure on young researchers, depriving the community from a strongly needed generational renewal. As a result, the spreading of code reuse and good practices is quite slower than the production of sharable and reusable software modules.

**Comparison with the climate research community**

One ESL contributor is now experiencing first-hand how software activities are organised in the climate research community, through a position in the Access-NRI infrastructure (https://www.access-nri.org.au/). There, software development is inherently collaborative, since all models require more than one code and have highly complex interactions. Most of the research involves both academic and non-academic institutions, which has had a great impact on the professionalisation of all software activities. Hiring Research Software Engineers (RSE) is part of the core development strategy. Access-NRI has been active since 2022 and is the result of many years of lobbying. It is currently employing 25 RSE and will expand to 35 RSE by 2025. Its activities are evaluated every 5 years to renew its funding. Such an organisation with a long-term view lets RSE serve the whole community all the time, instead of being limited to one research group / one software project as it is the case within the electronic structure community, leading to a much higher impact of the software development outcomes on society. Even if it is quite challenging, the paradigm shift it represents deserves at least to be considered and discussed.

**Possible actions to increase momentum**

One possible way to improve communication and ensure constant progress within the community is to set up an exchange platform for good practices. The following questions are open: How to define a list of experts? Would it be a regular call, e.g. monthly, or an on-demand call when a critical mass of interest is reached? Can this help us save time when addressing software-related issues?
How can we discuss more openly?
One way is to promote the ESL discussion space on Zulip (https://esl-cecam.zulipchat.com/join/uvatdjuxwzytg5sgwv3ojxsq/).
There, discussions can be organised in a way that will make them easy to find even after a few months of inactivity. To make it easier for people to join, the invitation link now appears prominently on the first page of the ESL website (https://esl.cecam.org/).
Another way to improve communication and visibility could be to structure our community around topics and guide new developers through the different kinds of software available: reference implementations vs. fully optimised software, and/or research/experimental software vs. production-grade software. How can the idea of an "electronic-structure ecosystem" be promoted and made more understandable?
An important aspect affecting momentum is to find ways to alleviate the current contributors to the ESL, in particular by identifying what should not be worried about. It is also essential to remember that researchers are generally not software experts and do need training regarding software engineering aspects.
There is a general consensus that the outcomes of ESL efforts should be promoted significantly more than they currently are. More outreach could be achieved by a more prominent involvement of ESL contributors in online communities like Stack Exchange. A well-defined protocol for announcements would help defining an "ESL style".
All this being said, several new developments and connections showcased at the workshop are very encouraging and generated praise - for example, the US DOE funded infrastructure around NWChemEx (Richard), the report on Julia software for DFT development (Herbst), or the experiences of the Psi4 project (Burns), to name just a few. Clearly, our software ecosystem is moving. Connecting the different, rapidly evolving developments in our community continues to be a major function of the ESL workshops and of the ESL.

## 3. What was the take-home message for the participants?

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The ESL initiative is, in fact, centered around a key community need in the experience of the organizers, i.e., a venue to communicate and (where possible) create bridges between the diverse software projects and developments surrounding electronic structure theory.
Since the inception of the ESL, it has sustained a substantial number of consistent participants from the DFT community. However, these same participants are all agreeing that the community needs to do more to bring together developments,

training, and knowledge sharing. This requires close collaboration with entities with expertise, such as HPC centers.
Since GPUs has become mainstream, and we are likely to see more specialized architectures in the future. It is becoming increasingly more difficult for non-research software engineers to tackle the difficulties on achieving performant and accurate software on said architectures. The community needs a continuous communication channel with field experts, such as HPC centers, compiler vendors and hardware designers.
Together with hardware and specialization training, it is equally needed that the next generation electronic structure researchers are learning how to do software developments. Efforts that promote and recognize important, well executed and sustainable software developments, which ultimately enable better science, should be a continuous priority of our community.
Finally, the community needs funding agencies to regard research not only as incremental steps of knowledge and/or new areas, but equally so on sustaining the very platforms where research is made. In the electronic structure community this is directly related to research software where new research is done via extending software, or interfacing it with new paradigms, e.g. machine learning.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Throughout the lifetime of the ESL, a key observation has been that funding of scientific software developments is historically difficult, since it is often viewed as distinct from the scientific outcomes enabled by that software. This problem has been recognized by funding agencies in Europe and in the U.S., with specific calls and initiatives targeting software development. In Europe, large centers (MaX, NOMAD) now exist; the U.K. has had a continuous program focused on software development (e.g., ARCHER2 and its Exascale Initiative), the U.S. Department of Energy has large initiatives and ESL-related activities have also been funded through the US National Science Foundation. All of these funding mechanisms remain intensely competitive, however, creating new divisions through a perceived need to protect funding resources (e.g., competing teams may not be in a position to adjust goals and streamline efforts). A key role played by the ESL is that it bridges these different groups, national initiatives and distinct projects, creating open communication channels towards future proposals and funded projects. As one concrete outcome of the current workshop, Volker Blum will work towards a new grant centered around ELSI and solvers, aiming for US NSF support as in the past. This will involve several key ESL contributors. During the meeting, writing a proposal for a COST network has also been discussed. An action group will be set to take this forward.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The Electronic Structure Library and related collaborative efforts are building a world-wide community and network within the electronic structure theory community. By bringing together developers, researchers, and practitioners from around the world, the initiative fosters a sense of community and shared purpose, facilitating collaboration, knowledge exchange, and professional networking opportunities. This can enhance the visibility and reputation of individuals and institutions involved in the initiative, leading to increased opportunities for collaboration and recognition within the scientific community. Societal benefits are emerging in 4 different areas:

- Accelerating scientific progress: By fostering collaboration and sharing among developers from various academic, industrial, and research institutions, the ESL can foster advancements in areas such as materials science, chemistry, and condensed matter physics, which can ultimately benefit society through the development of new technologies and innovations.
- Democratising the access to cutting-edge software: By sharing and reusing cutting-edge computational tools and libraries developed by experts in the field, as well as good programming practices, the ESL aims at make the access to advanced electronic structure methods easier, enabling researchers from diverse backgrounds, including those in academia, industry, and smaller research institutions, to utilize state-of-the-art computational techniques for their research projects.
- Broadening education and training opportunities: By facilitating knowledge exchange and collaboration among developers with different backgrounds and levels of expertise, the ESL can help cultivate a new generation of computational scientists skilled in advanced electronic structure methods. This can contribute to the growth of the scientific workforce and empower individuals to pursue careers in STEM fields.
- Increasing the impact of publicly-funded research: By defending the modular paradigm and avoiding repetitive efforts and errors, the ESL intends to help researchers and scientific software developers make a better use of their time and resources, which in the long run will improve the impact and returns of the related investments.

## 6. Participant list

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# JNCASR - CECAM conference MD@60

**Location: Bangalore, India**
**Webpage : https://www.cecam.org/workshop-details/JNCASR-cecam-conference-md-at-60-1263**
**Dates: Feb 25, 2024 - Feb 29, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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MD@60 was an International Conference organized to commemorate the sixtieth anniversary of the seminal work of Aneesur Rahman on the MD simulation of liquid argon. Machine learning methods and their application to materials and biosciences were one of the recurring themes of several talks and posters presented in the meeting. Another recurrent topic was enhanced sampling in MD simulations towards accurate and efficient free energy calculations. High-throughput screening and computational drug discovery were other topics of interest. Several applications of MD simulations towards the modeling of electrolytes, electrolyte-electrode interface, polymers, yielding, nanomaterials, enzyme catalysis were presented.
The conference gathered leaders in the field and practitioners at different stages of their careers, providing precious networking opportunities. In particular, the conference immensely benefited the 230 students and post-doctoral fellows who participated by way of interactions with peers.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The conference provided a unique opportunity to consider the state of the field 60 years after the seminal work of Rahman. The interdisciplinary nature of the talks (in terms of topics and methods) was an opportunity for experts to share knowledge across subdomains in molecular dynamics. This was also an important learning opportunity to train the students and early career researchers who attended, gain a broad overview of the field, and understand promising directions.

The special lecture delivered by Prof. Michael Klein, available on YouTube now, provided a much-needed context to simulations and a perspective on the evolution of the field into the current state-of-the-art. This was quite educational for the student and early-career participants.

### 3. What was the take-home message for the participants?

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Participants were able to learn state-of-the-art methods and applications of MD simulations and the evolution of the technique through the special lecture. The 203 poster presenters received valuable feedback. The growing role of machine learning in MD, from interatomic potentials to analyses, was a key message.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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While no immediate and direct societal benefit was intended from the Conference, students trained in the use of state-of-the-art molecular dynamics and related methodologies are increasingly in demand in industries developing new drugs and novel materials. Given the large number of students that attended the Conference, there will likely be a significant societal impact in the future.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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Yes, indeed. A special collection titled “Molecular Dynamics, Methods and Applications 60 Years after Rahman” has appeared in the Journal of Chemical Physics. As of May 2025, 100 publications feature in this collection.
The conference series, “RARE”, which focuses on Rare Event Sampling, has been held in India since 2014 and had its recent meeting in March 2025, after a gap of four years. The ideas for this edition were crystallized by the organizers during the MD@60 conference (personal communication).

### 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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The conference had 300 participants, of whom 50 were senior researchers, 38 were early-career scientists, and 200 were Ph. D. students, drawn from 14 countries. 35% of the 43 lectures were delivered by women. 15 participants were from Industry, and the rest were from academia. Many student participants were drawn from State and private Universities in India who do not possess the financial

means to attend a major International conference in their discipline, had it taken place abroad.

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# Bringing together rare event sampling, excited state dynamics and machine learning

**Location: CECAM-AT**
**Webpage : https://www.cecam.org/workshop-details/bringing-together-rare-event-sampling-excited-state-dynamics-and-machine-learning-1297**
**Dates: Feb 26, 2024 - Feb 29, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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The increase in computational power has come hand in hand with numerous advances to decipher chemical phenomena. A large part of this progress is due to the development of more efficient simulation techniques, including machine learning (ML). ML is increasingly applied as e.g. machine learned force fields [1], for classification of matter [2], the prediction of reactions [3] and generative sampling [4].
While these advances have greatly extended the accessible length and time scales of simulations, chemical processes characterized by rare events are still difficult to model, even if inexpensive ML force fields are used. Approaches to tackle this issue include umbrella sampling [5], metadynamics [6], transition path sampling [7, 8, 9], and forward flux sampling [10], which increase the likelihood of observing rare but important events either by introducing an appropriate bias or by focusing on reactive trajectories.
Especially when investigating rare event processes involving electronic excited states much remains to be done. A number of methods and techniques exist to describe the dynamics of reactions initiated by light, including mixed quantum-classical surface hopping approaches [11], MASH [12], kCSDM [13], AIMS [14], MCTDH [15]. All these methods rely on quantum chemical calculations, and therefore can only be used to simulate short time scales.
The development of new computational methods benefits from rigorous mathematical insights. These are not only vital for understanding the validity and limitation of the methods but also to push improvements. See for instance, publications about the rigorous analysis of surface-hopping algorithms [16, 17] and the investigation of the mathematical foundations of machine learning for materials [18, 19].Recently, some efforts have been made to apply machine learning to rare events sampling [20,21] and excited state dynamics [22, 23, 24], and rare events sampling has been applied to reactions occurring on excited states [25, 26].

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## 2. What were the primary outcomes of this workshop, including limitations and open questions?

Science lives from pushing boundaries bit by bit and building one idea on top of the next. In this spirit many novel and improved methods were discussed at the workshop.
Perhaps unsurprisingly, ML force fields are being applied more and more routinely and oftentimes together with other novel methods. However, still many innovations are made to increase the efficiency and accuracy of ML potentials and several of these were reviewed in the workshop. Additionally, advantages and disadvantages of various different structures of neural networks were presented. In particular, the importance of physics built inside models was discussed.
Many approaches were discussed towards uncovering rare reactions and ideal CVs. Path-based approaches such as transition path sampling and forward flux sampling are being applied to increasingly complex models. Notably, composite schemes were explored, combining trajectory-based sampling approaches with machine learning models to obtain the committor. A particular focus was put on data-efficient sampling and on-the-fly approaches. Further, it is envisioned to eventually generate whole transition trajectories with machine learning. Finding appropriate strategies for the understanding of high-dimensional configuration space is highly relevant, but still an unsolved problem. Approaches towards this goal and the importance of understanding were debated. While most sampling methods are only applicable in equilibrium systems, new approaches were presented for non-equilibrium cases. Sampling beyond the ground state for photoreactions is still an open issue and multiple attempts in pursuit of this goal were discussed.
The efficient and accurate computational investigation of nonadiabatic dynamics itself remains a demanding task. Various dynamics methods --- established as well as only recently developed --- were talked about and thus compared. Although electronic structure computation for excited states was not the focus of this workshop, it clearly is a limiting factor in many cases and improvements thereof would be fairly beneficial for the accuracy as well as time cost of the dynamics simulation. For such simulations the choice of initial conditions can have a huge effect. Therefore, issues connected to the proper choices of these were mentioned. Another open problem is the diabatization of the potential energy landscape.
Mathematical viewpoints on the topics mentioned above were also discussed. Notably, this communication between researchers from mathematical and those with rather application oriented backgrounds is very helpful in steering future research.
One of the central goals of the workshop was to bring together the different communities working on non-adiabatic dynamics, rare events sampling and machine learning. Many interactions between these communities took place in the panel discussions at the end of each session but particularly during informal gatherings.

### 3. What was the take-home message for the participants?

One central goal of the workshop was to bring together researchers from different communities. While some of the participants were sceptical about the chances of success of this aim, we received much positive feedback during the workshop. So we hope that the take-home message for the participants is that it is useful to make an effort to look beyond the boundaries of one's one immediate discipline.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The methods proposed in the workshop lay the groundwork to accelerate the simulation of (photo)reactions. They aim towards extending the currently possible time scales for atomistic simulations on more than one potential energy surface. On the one hand, these approaches lead to cheaper computations, vastly reducing the amount of required HPC resources for some task compared to current strategies, contributing to the battle against climate change. On the other hand, this enables the simulation of processes with societal relevance such as artificial photosynthesis and many more. Furthermore, these simulations assist the design of OLEDs, organic photovoltaics, light activated drugs and much more. We therefore believe, that the methods and problems discussed in the workshop will help in understanding fundamental processes that aid the creation of molecules, structures or materials, which will benefit society broadly. Note, that many of the discussed approaches are still under development. Therefore, the societal benefit will follow long-term and cannot yet be grasped to its full extent.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

One interesting contribution to the workshop was the presentation of MASH, a new method for adiabatic dynamics. A collaboration based on this method between the group of Jeremy Richardson (ETH) and the organizers of the workshop was initiated after the workshop. No other tangible outcomes are known at the moment of submission of this report.

### 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

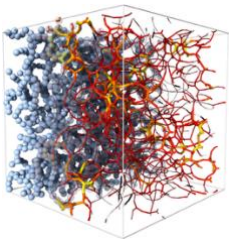
In organizing the workshop effort was made to ensure a good gender balance among the participants. Several slots for presentations were given to early career researchers based on submitted abstracts.

## 7. Participant list

### Organisers

**Dellago, Christoph**
University of Vienna, Austria
**González, Leticia**
University of Vienna, Austria
**Stefanelli, Ulisse**
University of Vienna, Austria

**Aerts, Antoine** - Université Libre de Bruxelles, Belgium



# Network dynamics: synthesis, structure and mechanical properties

**Location: CECAM-FR-RA**
**Webpage : https://www.cecam.org/workshop-details/network-dynamics-synthesis-structure-and-mechanical-properties-1307**
**Dates: Feb 26, 2024 - Mar 1, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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This CECAM workshop brought together 61 researchers from across Europe and the United States to discuss the structure, dynamics, and mechanical behavior of networks. These networks include gels, polymers, and biological systems, with examples ranging from synthetic materials to cytoskeletal assemblies. The workshop was held at the Les Houches School of Physics in the French Alps, a location well known for stimulating scientific exchanges in a quiet and beautiful setting.
The main aim of the workshop was to strengthen connections between different scientific communities working on soft and biological networks. We focused on understanding how the way a network is built (its synthesis and structure) affects its dynamic and mechanical properties. The workshop aimed to bring together theoretical, computational, and experimental researchers and to encourage collaborations between them. It also provided an opportunity for junior researchers to present their work and engage with leading scientists in the field.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop helped to launch several new research ideas and connections. According to the post-event survey, 18 out of 28 respondents (around 64%) reported that they had initiated new collaborations during the week. While some of these are still at an early stage, this shows that the workshop successfully created opportunities for long-term scientific exchange. Several participants expressed interest in organizing follow-up meetings or preparing joint publications. There was also discussion about future funding proposals that could bring together researchers from different groups.
We welcomed 61 participants from a wide range of institutions and backgrounds. The group included established researchers, postdoctoral scientists, and PhD

students. This mix of experience levels helped to create a stimulating and open environment for discussion. Participants came from different fields, including physics, materials science, chemistry, and biology, and many expressed appreciation for the chance to learn about new methods and perspectives.

### 3. What was the take-home message for the participants?

Several highlights emerged during the workshop. These included new experimental techniques for observing fracture and deformation in real time, models linking network microstructure to macroscopic mechanical response, and insights into how biological networks can be used to inspire new material designs. Many speakers also showed how simulations and theory can complement experiments. Some participants shared work using machine learning to analyze and predict network behavior, showing the growing impact of data-driven approaches in soft matter science.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The scientific program combined invited talks, contributed talks, flash presentations, and posters. Twenty invited speakers gave presentations covering a broad range of topics, including network aging, deformation and rupture, rheology of soft matter, and active biological materials. In addition to the main talks, we organized contributed talks for which we favoured young researcher contributions. Further we allowed for flash presentation sessions so that poster presenters could briefly introduce their work. Poster sessions were held in an informal and friendly atmosphere, encouraging long discussions. Discussions also continued over meals and during breaks, which helped to build new connections between participants.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop achieved its goals of connecting researchers, stimulating new ideas, and supporting young scientists in the field. The feedback and collaboration outcomes show that the community is active and ready to grow stronger links between experimental, theoretical, and computational approaches. We thank CECAM and the Les Houches School of Physics for their support in making this event a success.
The Les Houches School of Physics was an excellent setting for the workshop. All participants were housed on site, and meals were taken together in the shared dining hall. The lecture hall and poster rooms were well equipped and located in

the main building. The isolated setting encouraged participants to focus on science and enjoy informal exchanges during walks, meals, and evening gatherings. The organising team received great support from the Les Houches staff and from the CECAM office throughout the planning and the event itself.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

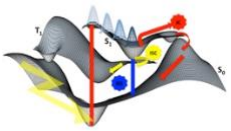
Out of the 61 participants, 29 completed the feedback survey, giving a response rate of around 48%. Overall, the feedback was very positive. Most participants rated the scientific quality of the workshop highly: about 76% rated it as “perfect” and 21% as “good”. Only one respondent gave a lower rating. The venue, facilities, and logistics were also appreciated, especially the poster space, the meals, and the calm and collaborative atmosphere of the site. Several participants commented on the friendly environment and the high level of interaction between junior and senior scientists.

## 7. Participant list

### Organisers

**Barrat, Jean-Louis**
Université Grenoble Alpes, France
**Del Gado, Emanuela**
Georgetown University, United States
**Martens, Kirsten**
Univ. Grenoble Alpes & CNRS, France

**Aime, Stefano** - ESPCI, France



# Quantum and mixed quantum classical dynamics in photochemistry

**Location: CECAM-ES**
**Webpage : https://www.cecam.org/workshop-details/quantum-and-mixed-quantum-classical-dynamics-in-photochemistry-1339**
**Dates: Mar 4, 2024 - Mar 8, 2024**

## 1. What were the major topics presented in the School?

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The school presented an overview of the state-of-the-art in computational photochemistry. This ranges from basic photophysics and photochemistry concepts like absorption/emission processes to non-radiative decays and photochemical transformations, the underpinning electronic structure describing the electron correlation problem and its varying role across multiple potential energy landscapes, and how these estimates are then used both statically and dynamically to model photo-reactions and infer mechanisms to rationalise both steady-state and time-resolved experimental observables.
Particularly, an introduction to photochemistry and spectroscopy set the stage, making connections between the observables measured experimentally and the computable magnitudes that are often used in the literature to elucidate/support them. This was followed by a review of accurate electronic structure methods used in the field, namely multiconfigurational CASSCF approaches and their perturbation theory (CASPT2) extensions, extracting their strengths and weaknesses, and attempting to instruct on their correct use to model a given photochemical problem. These methods, along with TD-DFT, were used to compute different magnitudes (particularly ground and excited state minima, Hessians and transition dipole moments). We note that TD-DFT is not especially covered in the course, but the expected students generally know it. Still, we will try to include it into the content of the course to make it fully self-contained. The computed properties are then used with analytic harmonic models under the Born-Oppenheimer approximation to produce realistic spectra matching the experimental observable and its vibrational lineshape. Subsequent lectures further introduced advanced dynamical treatments, including non-adiabatic couplings that trigger population transfer among excited electronic states. In this sense, both mixed quantum-classical treatments, focusing mostly on surface hoping, and fully quantum dynamical methods were covered. These methods were then shown to pave the way to monitor photochemical phenomena in real time.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The school provides an overview of a highly active area of research, from the basis to state-of-the-art methodologies, highlighting their limitations and associated open scientific questions. Among these, we describe in detail advanced electronic structure methods for excited-states, as CASPT2, and also apply more standard TD-DFT approaches which are applicable to larger and more realistic systems of interest. We also elaborate on various nuclear quantum effects, exploring appropriate strategies to apply cost-effective mixed quantum-classical approaches depending on the specific problem. Several of these challenges are addressed explicitly in the hands-on sessions, equipping students with the tools needed to confront such open questions and apply them to their own research. Moreover, even if TD-DFT is expected to be already known by the students, we plan to incorporate such contents in future editions of the school.
On the practical side, the main limitations were associated to the computing resources available for the workshops, which meant some simulations took a long time to complete and could not be integrated within the activities as well as originally intended. For future editions, we expect to work more closely with the local IT team at CECAM-ES, to better align our needs with the available resources on site. Additionally, another issue that arose in the tutorials is the diversity of systems used to check the different methodologies (i.e. the different molecular systems which were used for each tutorial), which makes extracting general assessments more complicated. In future editions, we will try to adopt a common molecular system across all tutorials.
Another shortcoming intrinsic to the course lies in balancing its duration with the breadth of content: this school brings together a wide range of sub-disciplines to be covered on only one week, exposing participants to a significant amount of new content. There is no easy way around this. In order to address this issue, we are actively working in strengthening the coordination between lectures towards a unified view across them: this includes avoiding unnecessary repetition, use consistent nomenclature and foster connections between them. Moreover, focusing the hands-on sessions around a common molecular system should help students assimilate the content, as it will more clearly illustrate the applicability/limitations of the different strategies covered in the lectures by applying them on top of a shared setting.

## 3. What was the take-home message for the participants?

The main take-home message was to carefully select the model that best fits your problem at hand. The course showcases different methodologies available in open-source software and suggests ways in which they can be applied to solve given photochemical problems, thus showing how to extend well-defined cases to different scenarios applicable to the student's own research.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- The course made all lecture notes (i.e. slides) available to all attending students for future reference.
- The workshops provide the students with valuable example input files as well as tools and strategies to process the outputs, which provide them with the minimum knowledge to start using the software applied in the tutorials to their own research

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The school was attended by 8/32 women, amounting to 25% and far from the 50% we'd hope. Such an issue will be considered in future calls to reduce the gap. Attendees were MSc, which aligns with the introductory scope of the school, but we will try to extend the scope in future editions to also attract PhD students, at least in their initial stages. To lower costs and the associated carbon footprint, most speakers were based in Spain. The school attracted a significant number of Spanish-based participants, but some of them were originally from Latin-American or Asian countries.

## 6. Participant list

### Organisers

**Cerezo, Javier**
Universidad Autónoma de Madrid, Spain
**Segarra-Martí, Javier**
Universidad de Valencia, Spain

**Aleson Gurruchaga, Ander** - UPV, Spain
**Barrios Prieto, Alejandro** - UAM, Spain
**Barroso, Alejandro** - Autonomous University of Madrid, Spain
**Bayo, Miguel** - Universidad Autónoma de Madrid, Spain
**Bello, Roger** - Universidad Autónoma de Madrid, Spain
**Binu Abraham, Alen** - Autonomous University of Madrid, Spain
**Camara Garmendia, Idoia** - Upv/Ehu, Spain
**Catalán Fenollosa, David** - Universidad De Valencia, Spain
**Chacón, Pablo** - University Of Santiago De Compostela, Spain
**Chimarro, Andrea** - Universitat De Valencia, Spain

**Curchod, Basile** - University Of Bristol, United Kingdom
**De La Fuente, Álvaro** - Universidad De Valladolid, Spain
**Diaz-Gutierrez, Miguel Angel** - Universidad Autónoma De Madrid, Mexico
**Fajardo Herrera, Jose** - Universidad De Valencia, Spain
**Gallego De Roa, Alvaro** - Uam (Universidad Autónoma De Madrid), Spain
**Gómez, Sandra** - Universidad Autonoma De Madrid, Spain
**González Pacheco, Alejandro** - Universidad Autónoma De Madrid, Spain
**González Sanz, Aurora** - Universidad Autónoma De Madrid, Spain
**Llorena, Diego** - Universidad Autónoma De Madrid, Spain
**Marković, Danilo** - Autonomous University Of Madrid, Spain
**Martínez Zaragoza, Pedro** - Universitat De Barcelona, Spain
**Mata Rabadan, Fernando** - Uam, Spain
**Miranda Saenz, Edgard Alejandro** - Universidad Autonoma De Madrid, Spain
**Nayeem, S. M. Abdul** - University of Valencia, Spain
**Ndrio De Carvalho, David** - Universitat de Barcelona, Portugal
**Okon, Roza** - University of Barcelona, Poland
**Patiño, Francisco Javier** - Universidad Autónoma de Madrid, Spain
**Qadeer, Abdul** - University of Valencia, Pakistan
**Rodríguez-Arias, Carlos** - University of Oviedo, Spain
**Sobrino Fernández, Cristina** - Universidad Autónoma de Madrid, Spain
**Solares-Knorr, Peter** - Universidad de Valencia, Spain
**Vidal, Lucía** - Universidad de Oviedo, Spain
**Vides Garcia, Nuria** - Universidad de Oviedo, Spain
**Villca Centellas, Danna** - Universidad Autónoma de Madrid, Spain
**Yelamos, Daniel** - Universidad Autónoma de Madrid, Spain

# Theoretical spectroscopy lectures

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage: https://www.cecam.org/workshop-details/theoretical-spectroscopy-lectures-1195**
**Dates: Mar 11, 2024 - Mar 15, 2024**

## 1. What were the major topics presented in the School?

The aim of the school was to give a comprehensive introduction to the theoretical and practical aspects of the electronic excitations that are probed by experimental techniques such as optical absorption, EELS and photoemission (direct or inverse). From a theoretical perspective, excitations and excited state properties are out of the reach of density-functional theory (DFT), which is a ground-state theory. Over the past three decades, alternative ab-initio theories and frameworks capable of describing electronic excitations and spectroscopy, have gained popularity including time-dependent density-functional theory (TDDFT) and many-body perturbation theory (MBPT) or Green's function theory (GW approximation and Bethe-Salpeter equation BSE). In fact, computational solutions and codes have been developed to implement these theories and to provide tools to calculate excited state properties. The present school focused on these points, covering theoretical, practical, and also numerical aspects of TDDFT and MBPT, non-linear response and real-time spectroscopies. Additionally, the school provided valuable insights from an experimental perspective on spectroscopies and magnetic excitations, rarely covered in similar events. Finally, a large part of the school was devoted to getting familiar with the codes that implement such theories (ABINIT, 2Light, Lumen, DP, and EXC).

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The main problems were encountered during the hands-on sessions because of the newly introduced limitation related to the fact that terminals are not any longer made available at CECAM. And participants have to rely on their own personal laptops, coming with the most varied configurations and operating systems, which made difficult to run the hands-on. Even in the cases where the hands-on were run on the local CECAM cluster, some problems were registered even in the use of the

personal laptops as simple terminals. This was especially true for people coming from developing countries. In future, this problem should be cared in advance with respect to the school, by providing the minimum requisites for personal laptops to be used in the hands-on sessions. Or the CECAM could provide a certain amount of laptops to the participants whose laptop is not compatible with the minimum standards.
We didn't see particular limitations regarding the lectures, the hybrid onsite/online system is more and more performant. May be more attention could be devoted to make explanations made by hand at the blackboard more available to online participants.

### 3. What was the take-home message for the participants?

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Our main take-home message for the participants was to make absolutely clear what theoretical spectroscopy can reliably provide, in order to 1) reproduce, 2) explain and 3) predict properties, as in experimental spectroscopy; and of course what cannot, or not yet, so that it is an active field of research.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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For all the lectures we made available:
1) The lecture notes on the CECAM web site;
2) The recording of the lectures on different platforms.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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The overall participation to the event has seen a 40%/60% of F/M gender share, and a 35%/65% of non-EU/EU geographical provenance share, though the latter share reduces if we restrict just only to the onsite participation. In order to promote inclusivity with respect to the latter, we decided to finance supplementary hotel nights across the week-ends for people coming from outside Europe, in order for them to achieve cheaper flight tickets; and, also thank to the CECAM, we financed the travel to two non-EU nationals, particularly a young researcher/PhD woman from the University of Addis Ababa, Ethiopia.

## 6. Participant list

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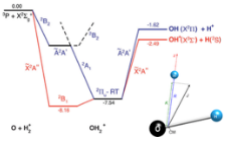
### Organisers

**Olevano, Valerio**
CNRS, France
**Rignanese, Gian-Marco**
Université Catholique de Louvain, Belgium
**Sottile, Francesco**
Ecole Polytechnique, France

**A.Karim, Nabila** - Fuel Cell Institute, Malaysia
**Acharya, Shakti** - Ravenshaw University, India
**Alem, Mamaru** - University of Pretoria, South Africa
**Allen, Tucker** - University of California, Los Angeles, United States
**Andriambelaza, Noeliarinala Felana** - Ecole Polytechnique, France
**Arega, Aseres** - Addis Ababa University, Ethiopia
**Attaccalite, Claudio** - CNRS, France
**Bhagat, Brajesh Rajesh** - The Maharaja Sayajirao University of Baroda, India
**Boukachabia, Samira** - Badji Mokhtar University -Annaba-Algeria, Algeria
**Bulancea Lindvall, Oscar** - Linköping University, Sweden
**Cantarella, Arianna** - University of Parma, Italy
**Corona, Domenico** - University of Rome Tor Vergata, Italy
**De Mestral, Virginie** - ETHZ, Switzerland
**De Vaulx, Jean-Baptiste** - Institut Néel and Université Grenoble Alpes, France
**Dzujah, Diyan Unmu** - Technische Universität Dresden, Germany
**Edwards, Jordan** - Imperial College London, United Kingdom
**Friedrich, Christoph** - Forschungszentrum Jülich, Germany
**Gelabert, Julián** - Universidad Nacional de Rosario, Argentina
**Giantomassi, Matteo** - UCLouvain, Belgium
**Heidari Pebdani, Zeinab** - Helmholtz-Zentrum Hereon, Germany
**Huotari, Simo** - University of Helsinki, Finland
**Huotari, Simo** - University of Helsinki, Finland
**Husain, Munavvar** - University of Warsaw, Poland
**Janovec, Jozef** - University of the Basque Country, Materials Physics Centre, Spain
**Kumar, Vipin** - Technische Universität Darmstadt, Germany
**Lévêque-Simon, Kévin** - Laboratoire des Solides Irradiés, France
**Levy, Andrea** - EPFL, Switzerland
**Mafusire, Cosmas** - University of Pretoria, South Africa
**Mansouri, Masoud** - University of Autonoma de Madrid, Spain
**Mehta, Bijal** - Sardar Vallabhbhai National Institute of Technology, India
**Mishra, Nalin Vilochan** - Indian Institute of Science Education and Research, India
**Muroni, Alessia** - University of Rome "Tor Vergata", Italy
**Rahman, Khalil Ur** - Government Degree College Shewa, Pakistan
**Riemelmoser, Stefan** - EPFL, Switzerland

**Saroka, Vasil** - University of Rome Tor Vergata, Italy
**Solet, Vinod Kumar** - Indian Institute of Technology Mandi, India
**Urquiza, Laura** - Università degli Studi di Milano, Italy
**Veniard, Valerie** - CNRS, France
**Winka, Anders** - ETH Zurich, Switzerland
**Zaari, Halima** - LaMCScI, Morocco



# School on kinetics and dynamics of chemical reactions

**Location: CECAM-ES**
**Webpage : https://www.cecam.org/workshop-details/school-on-kinetics-and-dynamics-of-chemical-reactions-1343**
**Dates: Mar 18, 2024 - Mar 22, 2024**

## 1. What were the major topics presented in the School?

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The school on Kinetics and Dynamics of Chemical Reactions covered the principal aspects of the kinetics and dynamics of chemical reactions from a theoretical point of view but with many hands-on-sessions for practicing the different methodologies exposed during the school. Thus, the main topics presented in the school were kinetics and dynamics of chemical reactions.
The school provided a historical landscape from the beginnings of kinetics and dynamics of chemical reactions up to now focusing on different methodologies, from classical to quantum methods, introducing also methods like ring-polymer molecular dynamics and the use of artificial intelligence in these topics. Besides, the kinetics of heterogeneous catalysis and in macromolecules systems were also considered in the school by introducing kinetic Monte Carlo and QM/MM methods, respectively.
For all the proposed lectures the school offered as many hands on sessions as theoretical lectures so that the attendees could apply the bases obtained during the school to their own research.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

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The only limitation we encountered during the school's organization was the number of available slots in the ZCAM's computer lab used during the hands-on session. The current occupancy of the computer lab is on 30 people. However, for the next edition, we will try to increase the number of attendees since most participants brought their own laptop, so the number of attendees can be higher than the number of computers available in the classroom.
Regarding the material shared during the school we think that was correctly update for this edition avoiding open questions during theoretical or hands-on sessions. This is often an evidence of the efforts given by all the professors involved in the school for preparing the material and hands-on sessions and for

ensuring that all aspects were covered without leaving notable gaps or unanswered queries.
It is clear that several years organizing the School makes it a better school year after year. In our opinion, the contents have been updated in this edition and the participants have been more interested by the school, according to the number of proposals received (more than 40).

### 3. What was the take-home message for the participants?

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The participants greatly enjoyed the school, evidenced by the final session where they applauded for a couple of minutes, thanking for all they learned. The take-home message is: computational simulations are a great tool for understanding chemical reactions, from triatomic reactions until enzyme-based chemical processes, passing through heterogeneous catalysis reactions.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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All the material used during the school has been uploaded into the CECAM's school website (https://www.cecam.org/workshop-details/school-on-kinetics-and-dynamics-of-chemical-reactions-1343) and make available for all, not only for the attendees. This is done in this way since some people that contacted us for participating was unable to attend due to size limitations of the ZCAM's computing room. For the next edition, we will encourage participants to assist with the own laptop and thus, increase the number of potential attendees to the school. This year finally were 31 attendees, but we will propose arrive until 40 since many people was not accepted for the above-mentioned size limitation.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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This is a point in which all the organizers put their best. In our case, we focused on knowing how to communicate orally and in writing using inclusive and non-discriminatory language about the work done. Moreover, we encourage the attendees in working in inclusive and non-discriminatory environment. It is also really interesting that during the lectures, professors stressed the female contributions to the topics in which the school focused.

## 6. Participant list

### Organisers

**Gamallo, Pablo**
Universitat de Barcelona & Institut de Química Teòrica i Computacional, Spain
**Martinez-Nunez, Emilio**
University of Santiago de Compostela, Spain
**Prats, Hector**
University College London, United Kingdom

**Aleson Gurruchaga, Ander** - Upv, Spain
**Barrios Prieto, Alejandro** - Uam, Spain
**Barroso, Alejandro** - Autonomous University Of Madrid, Spain
**Camara Garmendia, Idoia** - Upv/Ehu, Spain
**Chacón, Pablo** - University Of Santiago De Compostela, Spain
**Cuadrado Benavent, Beatriz** - Universidad Autónoma De Madrid, Spain
**Di Liddo, Luke** - University Of Toronto, Canada
**Gallego De Roa, Alvaro** - Uam (Universidad Autónoma De Madrid), Spain
**Gimenez, Xavier** - Universitat De Barcelona, Spain
**González Pacheco, Alejandro** - Universidad Autónoma De Madrid, Spain
**González Sanz, Aurora** - Universidad Autónoma De Madrid, Spain
**Huarte, Fermin** - Universitat De Barcelona, Spain
**Llorena, Diego** - Universidad Autónoma De Madrid, Spain
**Marković, Danilo** - Autonomous University Of Madrid, Spain
**Martínez, Rodrigo** - Universidad De La Rioja, Spain
**Martínez Zaragoza, Pedro** - Universitat De Barcelona, Spain
**Miranda Saenz, Edgard Alejandro** - Universidad Autonoma De Madrid, Spain
**Montagud Andreu, Rubén** - University Of Valencia, Spain
**Ndrio De Carvalho, David** - Universitat De Barcelona, Portugal
**Okon, Roza** - University Of Barcelona, Poland
**Orta Parra, Luis Fernando** - Universitat De Valencia, Spain
**Patiño, Francisco Javier** - Universidad Autónoma De Madrid, Spain
**Revilla-López, Guillem** - Repsol, Spain
**Rodríguez-Arias, Carlos** - University Of Oviedo, Spain
**Sanabria Montalbán, Javier** - Universitat De Valencia, Spain
**Serrano López De La Vieja, Álvaro** - Universitat Jaume I, Spain
**Sobrino Fernández, Cristina** - Universidad Autónoma De Madrid, Spain
**Solares-Knorr, Peter** - Universidad De Valencia, Spain
**Vargas Chaverri, Ximena** - Universidad De Valladolid, Spain
**Vicente Cabello, Vicenta Victoria** - Universidad Nacional Mayor De San Marcos, Peru
**Vides Garcia, Nuria** - Universidad De Oviedo, Spain
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# Theoretical and experimental advances in atmospheric photochemistry

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/theoretical-and-experimental-advances-in-atmospheric-photochemistry-1205**
**Dates: Mar 26, 2024 - Mar 28, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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At first glance, the Earth's atmosphere appears to be mainly composed of simple, inert gases like $O_2$, $N_2$, and $CO_2$. However, the reality is somewhat different, and our atmosphere behaves more like a massive chemical reactor due to the presence of reactive molecules like $CH_4$, halocarbons, $O_3$, $N_2O$, NO, or volatile organic compounds (VOCs). The degradation of biogenic and anthropogenic VOCs takes place via a complex network of chemical processes and is intimately connected to the concentration of OH, ozone, and secondary organic aerosol (SOA) precursors in the troposphere. As a result, VOCs are strong contributors to both global warming and air pollution, and a great deal of effort has been devoted to understanding and predicting their atmospheric concentrations using detailed chemical models. As environmental policy decisions are driven by such atmospheric models, it is essential they accurately reflect the different chemical reactions in the atmosphere.
Historically, these chemical mechanisms have mostly neglected reactions involving the interaction of VOC intermediates with sunlight, and the resulting photochemical reactions. Hence, a complete family of chemical reactions is missing in current atmospheric models, and the influence of these reactions on the composition of our atmosphere is largely unknown, partly as photochemical experiments on (transient) VOCs are highly complex to realize.
How can theoretical and computational chemistry help? Simulating the photochemistry of a molecule requires the inclusion of nonadiabatic effects, i.e., the coupling between electronic states and nuclear motion, which is not straightforward as it challenges several approximations commonly used in theoretical chemistry. For example, nonadiabatic effects lead to a breakdown of the Born-Oppenheimer approximation, classical approximations for the nuclear degrees of freedom may be inadequate, and out-of-equilibrium processes can challenge established reaction rate theories.
While numerous methods have been devised to tackle these issues – e.g., MCTDH, trajectory surface hopping (TSH), ab initio multiple spawning (AIMS) –their application to study the photochemistry of atmospheric molecules faces numerous challenges. Examples are: the complexity in simulating observables of interest for spectroscopists and atmospheric modellers; the challenging electronic structure

of multichromophoric VOCs; the types of excited-state dynamics created by sunlight excitation; the long-time excited-state dynamics associated with VOCs; the importance of intersystem crossings or collisional processes; and the effect of an aqueous environment, such as in atmospheric aerosols and clouds.
Over the last decades, atmospheric chemistry has stimulated the development of new theoretical methods to investigate complex *ground-state* chemical reactions and their mechanisms. Such a connection between theory and experiment *does not currently exist in atmospheric photochemistry* involving electronically excited states, despite the importance for current atmospheric models and a strong push from the experimental side to obtain reliable data for modelling the composition of the atmosphere. With this CECAM workshop, we sought to create a bridge between the worlds of computational photochemistry and atmospheric chemistry to bolster a synergistic discussion between these two groups aiming to (i) connect theory with experiment, (ii) define key targets for theory, and (iii) identify current theoretical challenges and their possible solutions.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The CECAM workshop on Theoretical and Experimental Advances in Atmospheric Photochemistry brought together established and early career researchers from around the world to present and discuss the state-of-the-art in theoretical, computational, and experimental study of photochemical processes of central importance in the chemistry of Earth's atmosphere. Current understanding of atmospheric chemistry has been built on three pillars of complementary research: (i) field observations of the chemical composition of the atmosphere in different global locations (using instruments on ground, satellite, ship, aircraft, and balloon platforms); (ii) laboratory studies of molecular spectroscopy, photochemistry, reaction rates and products; (iii) computer modelling of the sources, sinks, transport, and reactions of atmospheric constituents. In his opening presentation, Professor Joseph Francisco proposed that theoretical chemistry now offers a fourth pillar by providing accurate spectroscopic, photochemical and kinetic data for chemical processes that are challenging to study in laboratory experiments. The subsequent presentations in the CECAM workshop illustrated the value of this proposition, and showed how rigorous intercomparison between theoretical predictions and experimental laboratory measurements is guiding the field of computational atmospheric photochemistry to maturity.
Photochemical reactions can be broadly broken down into the following steps: (i) absorption of a photon of ultraviolet (UV) or visible light of sufficient energy to promote a molecule (the chromophore) to an electronically excited state; (ii) dynamical changes to the molecular structure, driven by ultrafast changes in electronic orbital occupancies, such as bond-breaking (photodissociation), isomerization, intersystem crossing (with a change in electron spin), or conversion of electronic energy into excess vibrational energy; (iii) chemical reactions of the newly formed species, in competition with relaxation and thermalization, for

example by collisions with $N_2$ or $O_2$ in air. While the atmosphere is typically thought of as a gaseous environment, there is growing recognition of the role of small particles dispersed in air (atmospheric aerosols), which provide solid or liquid surfaces and bulk environments where modified chemistry can occur. The theoretical and experimental advances discussed during the CECAM workshop addressed all these aspects of atmospheric photochemistry, as is described below.

Progress in the efficient calculation of molecular absorption spectra in the UV and visible regions is illustrated by remarkable agreement with experimental measurements for a variety of organic compounds present in the atmosphere. This agreement applies to both the wavelengths at which molecules absorb, and their wavelength-dependent absorption cross sections which are a measure of how strongly the molecules absorb light. This progress derives from improvements to electronic structure theory methods for calculation of ground and excited-state energies, and techniques to sample ground-state structures representative of the vibrational motions of the molecule (the nuclear ensemble approach, NEA). NEA methods presented include Wigner sampling, path-integral molecular dynamics, and use of quantum thermostats, which can be combined with transition dipole moment calculations to incorporate non-Condon contributions to the computed spectrum. These methods are being built into openly available computational tools such as ATMOSPEC for wider use. Challenges remain in the accurate computation of the long-wavelength parts of absorption spectra, where overlap with the solar flux in the lower atmosphere (the troposphere) is typically greatest, and the simulation of absorption bands with resolved vibronic structure. Accurate calculation of excited-state properties of reactive species such as Criegee intermediates possessing unusual electronic structures also places considerable demand on computational quantum chemistry methods.

Following the absorption of light, calculation of the nuclear dynamics in an excited-state molecule can simulate changes in electronic state and spin, and the competition between bond breaking, isomerization, and relaxation to the ground electronic state. Such calculations require excited-state potential energy surfaces to be mapped using quantum chemistry, and seams of conical intersection or singlet-triplet crossing between electronic states to be located. Efficient methods for performing such computations were presented and were benchmarked against high-level but computationally expensive methods such as XMS-CASPT2. Computed excited-state potential energies can then be coupled with approaches to simulate the nuclear dynamics using either classical mechanics (e.g., TSH) or quantum mechanics incorporating different degrees of approximation (e.g., MCTDH, vMCG, AIMS). Emerging quantum computing architectures may offer a new paradigm for these dynamical calculations. From such calculations, predictions arise for competing photochemical outcomes and their quantum yields, which can be tested against, or supplement, available experimental data. Pressure and temperature dependent rates of chemical reactions can then be quantitively computed using master equation methods built on transition-state theories. Important examples discussed at the workshop include the photochemical oxidation pathways of hydrofluoro-olefins (HFOs), which are planned replacements for hydrofluorocarbons (HFCs) now recognized as significant

greenhouse gases. One unintended consequence of HFO use is production of HFC-23 (a long-lived and potent greenhouse gas) and trifluoroacetic acid (TFA), which is a persistent environmental pollutant.
The above steps provide a roadmap for first-principles calculation of key atmospheric chemistry processes, and can be incorporated into a computational reactor (e.g. the Nanoreactor of Martinez and coworkers) to predict the complex chemistry. The calculations also provide a toolbox for interpretation of laboratory measurements. New computational methods are constantly being added to this toolbox, such as prediction of X-ray absorption and photoelectron spectroscopy, to match advances in experimental capability.
The workshop programme and discussion also recognized the importance of molecular complexes and heterogeneous chemistry in the atmosphere, whether involving weakly bound dimers with water molecules, molecular nanoclusters, or micron-scale aqueous droplets found in clouds or sea-spray aerosols. Condensed phase chemistry brings new challenges to theory through the (necessarily approximate) treatment of the effects of the surroundings on molecular photochemistry. Examples were presented of computational simulations that required inclusion of explicit hydrogen or halogen bonding interactions for reliable outcomes. Experimental methods must also evolve to study photochemistry in these heterogeneous environments, with advances in spectroscopic and mass-spectrometric investigation of chemistry in clusters and single aerosol droplets now producing quantitative laboratory results.
These scientific outcomes from the workshop will be captured in a perspective article currently being written by the workshop organizers and intended for publication in the Journal of Physical Chemistry (published by the American Chemical Society).
As part of the CECAM workshop, we held two round-table discussions. One was led by senior scientists, and the other by early career researchers. These discussions identified important next steps that we need to take to ensure that the wider atmospheric chemistry community incorporates, and benefits from the scientific advances provided by modern theoretical and computational chemistry. For example, tools developed by the community represented at the CECAM workshop can be disseminated to atmospheric modellers, who can reciprocate by providing expert guidance on the most topical questions in atmospheric chemistry research. One suggested way forward is to hold another CECAM workshop on atmospheric photochemistry (perhaps in 2026) to which representatives of the atmospheric modelling community are invited.

## 3. What was the take-home message for the participants?

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Infrastructure needs for experts in theoretical and computational photochemistry include use of HPC resources, access to existing electronic structure codes, and development of bespoke codes for simulation of spectra and dynamics. The community mostly uses institutional HPC resources, workstations, and in-house clusters of CPUs and GPUs instead of national supercomputers. Electronic

structure packages such as Gaussian, Molpro, Turbomole, and Orca are vital for calculation of ground and excited state potential energy surfaces, and to locate conical intersections. It is common for research groups to use more than one of these codes, depending on the required capability for a desired calculation. Popular computational methods include DFT and TDDFT, or wavefunction methods such as EOM coupled-cluster, ADC(2) and XMS-CASPT2 calculations. Benchmarking of more computationally efficient methods against higher-level, computationally expensive standards is essential.

Most codes developed to compute absorption spectra with NEA sampling of ground-state geometries are developed by individual research groups, but ATMOSPEC (from the Curchod group) is intended for wider release and has a user-friendly interface.

Dynamics calculations might use publicly available codes such as SHARC and Newton-X (for TSH calculations), Quantics for MCTDH and vMCG simulations, or in-house codes for TSH, AIMS, AIMC or other methods. Incorporation of environmental effects may require molecular dynamics simulation packages and QM/MM strategies, possibly also accounting for polarization effects at the solvent level. A new UK project funded by EPSRC and led by Professor Graham Worth (UCL) seeks to develop the COSMOS code which will offer a platform of molecular (nonadiabatic) quantum dynamics simulations and the calculation of time- and energy-resolved quantities. This development of new code in non-commercial settings such as universities greatly benefits from access to research software engineers.

Laboratory based experimental research in atmospheric photochemistry requires dedicated and custom-built equipment such as lasers, mass spectrometers, vacuum systems for gas handling, and instrumentation for aerosol generation and characterization. Capabilities exist in national laboratories and at synchrotrons and free electron lasers (FELs) in some countries to undertake this research using in-situ instruments; an example is the multiplexed photoionization mass spectrometer (MPIMS) instrument operated by Dr David Osborn (Sandia National Laboratory) located at the Advanced Light Source (ALS) at Lawrence Berkeley National Laboratory. X-ray FELs are offering new opportunities to study photochemical dynamics with ultrafast time resolution.

A key outcome of the workshop was the recognition of a need for greater networking and collaboration with specialist atmospheric chemistry modellers. These experts will provide invaluable guidance on topical questions and current challenges in atmospheric chemistry that the theoretical chemistry community can effectively address. Examples might be air quality (which impacts on health) in urban areas and indoor environments. Some of the workshop participants already have such links (e.g. those from the University of Bristol, University of Colorado, University of New South Wales, University of Valencia, University of Salamanca), but these can certainly be broadened and strengthened. Dissemination of new tools such as ATMOSPEC developed by the theoretical chemistry community offers new opportunities to atmospheric modellers. Mechanisms for such dissemination include a follow-up CECAM workshop (tentatively planned for 2026), a community-owned website signposting resources developed for first-principles calculation of absorption spectra, photochemical pathways and reaction

rates, and presentations at major environmental science conferences such as the annual EGU and AGU meetings.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Most of the research presented at the CECAM workshop has been funded through national funders such as UKRI or NSF but several projects have been supported by European funding such as ERC grants. For example, the research groups of the two organizers from the University of Bristol are funded through major grants from UKRI (two EPSRC programme grants, one NERC highlight topic grant) and ERC (one ERC Starting Grant).
Mobility of early career researchers is an essential part of this research, for example for PhD study in other countries, exchange visits, and to take up postdoctoral researcher positions with associated two-way transfer of expertise. Examples of recent exchange visits for postgraduate student participants in the workshop are Yorick Lassmann (University of Bristol), who visited the Martínez group at Stanford University, and Jiří Janoš (University of Chemistry and Technology, Czech Republic) and Vera Brieskorn (Vienna) who are currently visiting the Curchod group at the University of Bristol. The benefits of this early-career research mobility suggest that establishing a Marie Skłodowska Curie Doctoral Network would greatly benefit European-based research in the field of the workshop. This possibility was not discussed in the meeting but could be a follow-on action.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Research in atmospheric chemistry has many societal impacts and benefits. For example, it has identified the impacts of human activity on climate and on stratospheric ozone depletion. In the latter case, rapid intergovernmental action led to restrictions then subsequent bans on the use of chlorofluorocarbons (CFCs). Atmospheric chemistry research, including laboratory studies, field measurements, and computational modelling, has also identified halocarbons as potent greenhouse gases. This research led to international agreements to phase out the use of hydrofluorocarbons (HFCs) in applications such as refrigeration, for which HFOs are proposed as next-generation replacements. Current research, some of which featured in the CECAM workshop, is now identifying potential long-term risks of the widespread use of HFOs.
Poor air quality, in particular in urban areas, is recognized to cause numerous health problems worldwide. The photochemical production of ozone and the growth of organic aerosol particles (which can be inhaled into the lungs) are potent causes of poor air quality, and are processes that can be better understood with input from experts such as those participating in the CECAM workshop.

Atmospheric cycling of toxic metals such as mercury, which can chemically and photochemically switch between Hg(0) and Hg(II) oxidation states, is a major environmental hazard for which remediation will benefit from computational photochemistry studies in combination with atmospheric chemistry modelling. Metals are also being unintentionally introduced into the upper atmosphere through ablation of material from discarded rocket stages, and re-entry of rockets or satellites into the atmosphere where they may "burn up". The consequences of additional metal loading in this sensitive region of the atmosphere are not well understood, but the sudden appearance of high-altitude sporadic metal layers formed from material ablated from meteorites is known to affect global communications.

These examples illustrate the wide significance of the topics covered by this CECAM workshop. Further progress in delivering societal benefits may now require a more coordinated research approach and enhanced collaboration with atmospheric chemistry modellers and observational scientists, for example through European-funded networks.

During the workshop, the question was raised whether we – as scientists contributing to atmospheric chemistry research – currently trust our calculations, simulations and models sufficiently to propose the termination of some industrial processes for the wider benefit of humanity and the planetary ecosystem. A historical example is the current global ban on manufacture and use of CFCs because of the compelling evidence that their use depletes stratospheric ozone and causes the annual Antarctic ozone hole in the southern hemisphere springtime. Concerns are growing about environmental consequences of fluorinated and perfluorinated organic compounds, some of which are referred to as "forever chemicals", the accumulation of long-lived and potent greenhouse gases such as $SF_6$, and the impacts of HFO use as next-generation refrigerants. The existing evidence for potential harm is not yet sufficient to advocate for a ban in the production and use of HFOs, but scientists such as the CECAM workshop participants have an important role to play in challenging industry and governments about the real environmental impacts of these supposedly benign new chemicals.

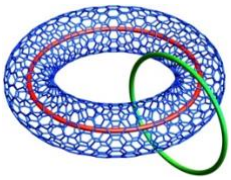
## 6. Participant list

### Organisers

**Curchod, Basile**
University of Bristol, United Kingdom
**Orr-Ewing, Andrew**
University of Bristol, United Kingdom

**Brieskorn, Vera** - University of Bristol, United Kingdom
**Carmona-García, Javier** - University of Bristol, United Kingdom
**Cigrang, Leon** - University College London, United Kingdom
**Dettlaff, Krispin** - Lab. für Physikalische Chemie, Switzerland
**Eklund, Elliot** - University of Sydney, Australia

**Francisco, Joseph S.** - University of Pennsylvania, United States
**Gerber, Robert Benny** - Hebrew University of Jerusalem, Israel
**Hansen, Christopher** - UNSW Sydney, Australia
**Hernández Rodríguez, Javier** - University of Salamanca, Spain
**Hollas, Daniel** - University of Bristol, United Kingdom
**Janoš, Jiří** - University of Chemistry and Technology Prague, Czech Republic
**Kable, Scott** - University of New South Wales, Australia
**Kassal, Ivan** - University of Sydney, Australia
**Lahana, Dean** - Stanford University, United States
**Lan, Zhenggang** - South China Normal University, China
**Lassmann, Yorick** - University of Bristol, United Kingdom
**Liberati, Diego** - National Research Council of Italy, Italy
**Liu, Ji** - Tyndall National Institute, Ireland
**Martín Santa Daría, Alberto** - University of Salamanca, Spain
**Martinez, Todd** - Stanford University, United States
**Muchova, Eva** - University of Chemistry and Technology, Czech Republic
**Prlj, Antonio** - Rudjer Boskovic Institute, Croatia
**Roca-Sanjuán, Daniel** - Universitat de València, Spain
**Signorell, Ruth** - ETH Zurich, Switzerland
**Slavíček, Petr** - University of Chemistry and Technlogy, Prague, Czech Republic
**Suchan, Jiri** - Stony Brook University, United States
**Taylor, Jack** - Durham University, United Kingdom
**Tsizin, Svetlana** - ETH, Switzerland
**Vaida, Veronica** - University of Colorado, United States
**Worth, Graham** - University College London, United Kingdom



# Topological order: anyons and fractons

**Location: CECAM-FR-MOSER, CECAM-FR-RA**
**Webpage : https://www.cecam.org/workshop-details/topological-order-anyons-and-fractons-1302**
**Dates: Apr 1, 2024 - Apr 12, 2024**

## 1. What were the major topics presented in the School?

This school, held at the École de Physique des Houches (French Alps), was devoted to topological order. This notion, introduced by X.-G. Wen in the early 90s, provides a natural framework for understanding quantum phases of matter that cannot be described by standard Landau theory. In two-dimensional systems, it is deeply linked to the concept of anyons proposed by J. M. Leinaas and J. Myrheim in 1977 to describe emergent excitations with non-trivial braiding statistics. Such statistics were observed experimentally in 2020 in two famous papers (published in Science 368, 173 (2020) and in Nature Physics 16, 931 (2020)), which attracted much attention in the condensed matter community. In the late 90s, A. Kitaev realized that topologically-ordered systems could be useful for quantum memories and quantum computing giving rise to the idea of topologically-protected qubits. From a theoretical point of view, understanding topological order in two dimensions requires a set of mathematical tools based on category theory (more precisely, an anyon theory is described by a unitary modular tensor category). In three dimensions, the notion of topological order can be extended to more sophisticated (membrane-like) excitations, giving rise to what is known as fractonic order.
This School brought together several communities interested in topological order (mathematicians, theoreticians, experimentalists, computer scientists,..).

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The lectures covered a wide range of topics. In particular, students were very interested in understanding the underlying mathematics useful in the field, as well as the many correspondences with other existing fields. For example, the notions of dualities, correspondence between edges and masses, or correspondence with statistical mechanics problems were widely discussed and opened up fertile

perspectives for future research. The description of topological phases in terms of tensor networks was also at the heart of many discussions, not least due to the presence of leading experts in this field. We also organized open question sessions where anyone could ask any question on any topic, and many students actively participated.
While the topological phases of matter are now fairly well understood in two dimensions (as well as in one dimension, where, in the absence of intrinsic topological order, one rather study symmetry-protected topological (SPT) phases), the situation is different in three dimensions, where there is clearly room for further research as emphasized by several lecturers.

### 3. What was the take-home message for the participants?

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In addition to the speakers, most of the participants were doctoral students or post-doctoral researchers. They all appreciated the wide variety of fields, from mathematics to experiments. They realized that, depending on their interests, there were still many topics to study in relation to topological order. For example, the search for Majorana fermions, the relationship between topological order and entanglement... They also realized that there was a large and active global community.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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- We recorded all the blackboard lectures (except for one or two due to computer problems!).
- The slides are also available on the school website
(see https://topoanyons.sciencesconf.org/resource/page/id/6).

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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We tried to strike a good balance between the participants. The proportion of women and men reflects the proportion of candidates. We also tried to apply the same rule to speakers. In terms of geographical origin, we have also tried to accept people from many different countries and to limit, for example, the number of participants accepted when they come from the same group. Finally, we have ensured that there are not too many students obliged to take long-distance flights.

## 6. Organiser list

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**Fuchs, Jean-Noël**
Sorbonne Université and CNRS, France
**Schuch, Norbert**
University of Vienna, Austria
**Verstraete, Frank**
University of Gent, Belgium
**Vidal, Julien**
Sorbonne Université and CNRS, France

# Transport properties in soft matter systems

**Location: CECAM-AT**
**Webpage : https://www.cecam.org/workshop-details/transport-properties-in-soft-matter-systems-1296**
**Dates: Apr 2, 2024 - Apr 5, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The complex dynamics of soft matter systems have been a focus of study for decades. The importance of dynamic and transport processes is reflected in the many layers of complexity at different scales and areas, spanning from transport inside cells, anomalous diffusion in glasses, cell migration, and information flow in society. Continuous progress in the field of transport properties has been achieved by studying experimental model systems that allow us to break the intrinsic complexity and tackle crucial fundamental physics and engineering challenges. The use of numerical models to study systems at different levels of description continuously allows us to gather new information and support theoretical and analytical approaches often based on a coarse-grained picture.
This workshop aimed at covering the state of the art in various systems and approaches focused on the design, engineering, modelling and study of active and passive Brownian dynamics. Specifically, we focused on connecting the theoretical and mathematical framework to the current experimental development, leading to insightful discussions, and tackling open challenges in the field.
The talks from the invited speakers represented the core activity of the workshop which was carried out in the time range 9:00 -- 17:00, taking place at the Boltzmann Lecture Hall on the Erwin Schrödinguer Institute (ESI) in Vienna. In addition, we organised extra activities to foster networking, interactions and discussions among the participants: Poster Session (Wednesday, 3rd), Round Table (Thursday, 4th), Welcome drinks (Tuesday 2nd), and Social Dinner (Thursday, 4th).

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

Interdisciplinarity
From a more scientific point of view, this workshop brought together communities that are usually focused on different approaches. Indeed, there were participants

from a strongly mathematical background and others more focused on very applied (often experimental) systems. Fostering discussions and interactions between the two communities surely represents one of the main outcomes of the workshop.
Future challenges
During the invited talks, the poster session and the open discussion, data analysis emerged as a key topic across different disciplines (in both mathematical and experimental approaches). In line with this, one of the talks presented "the AnDI challenge", scientific challenges for testing and developing data analysis techniques for various models of diffusion in complex environments. This led to interesting discussions on whether scientific challenges can be beneficial to the scientific community and what can be learnt from them. Such discussions represent another great achievement of the workshop, as they go beyond the specific research topics and help in shaping the general direction and interests of our scientific community.

## 3. What was the take-home message for the participants?

In addition to the 2 points discussed above (Interdisciplinarity and Future challenges), the following points of discussion addressed during the round table represent the main take-home messages for the participants: - mathematical origin and physical relevance of Fractional Brownian motion; - microgravity; - active or driven systems? - issues related to Open Access and publication; - AI in research; - AnDi challenge and challenges as a new tool for the scientific community.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The study of passive & active diffusion is a very general approach that is at the heart of many applications in different fields (transport in crowded environment, near-surfaces, biological scenarios and engineering perspectives at the microscale). In this context, the highly interdisciplinary approach advertised in this Workshop can be very relevant for environment and bio-inspired world and represents a way to converge different perspectives.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The extra activities organised within the workshop were effective in fostering interaction among the participants. In particular, we witnessed good networking among the group of young researchers (around 10 between pre-doctoral students and early post-docs) who did not know each other beforehand.

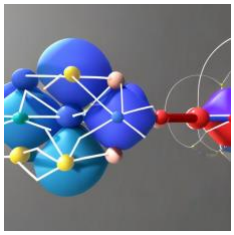
No additional tangible outcomes at the moment.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

During the whole organisation we committed to address and promote inclusivity with respect to gender, geographical provenance, career stage, etc... We continuously checked and made sure that our list of invited speakers and participants would show considerable representation from all the underrepresented groups. During the welcome and introduction speech we explicitly written down a code of conduct to create an environment of respect & inclusivity. Our efforts in this direction were well perceived by the participants who provided very nice feedback on the topic. All the participants acknowledged and appreciated the diverse speaker list, where we not only considered established scientists, but also early career principal investigators and experienced postdocs. This showcases the importance of keeping and open participation not only based on career stage, but also on the quality of the research performed by the scientists.

## 7. Organiser list

**Alvarez, Laura**
University of Bordeaux, France
**Chepizhko, Oleksandr**
University of Vienna, Austria
**Sposini, Vittoria**
University of Vienna, Austria



# Frontiers of Coarse-Grained models: from new developments to modeling dynamics, assemblies, and macromolecular machines

**Location: CECAM-FR-RA**
**Webpage : https://www.cecam.org/workshop-details/frontiers-of-coarse-grained-models-from-new-developments-to-modeling-dynamics-assemblies-and-macromolecular-machines-1311**
**Dates: Apr 3, 2024 - Apr 5, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop provided a comprehensive overview of advancements in coarse-grained (CG) modeling, emphasizing the diverse methodologies and applications propelling the field forward. Among the key themes was the exploration of CG models for intrinsically disordered proteins (IDPs) and multi-domain proteins, as highlighted by Kresten Lindorff-Larsen and Alessandro Barducci. This focus underscores the increasing attention to modeling complex, flexible biomolecular systems that challenge traditional simulation approaches.
Renowned figures in the field, such as Siewert-Jan Marrink, elaborated on the potential of Martini models for simulating entire cells, offering a visionary perspective on CG modeling's scalability. The role of emerging AI-driven methodologies in enhancing transferability and adaptability of CG models was another major topic, with contributions from young researchers like Aldo Pasos-Trejo and established experts such as Michael Feig discussing machine-learned force fields for protein simulation. These approaches demonstrate how data-driven techniques are refining parameterization and improving predictive accuracy.
A particular emphasis was placed on macromolecular interactions and dynamics. Talks such as Herre Jelger Risselada's on lipid membrane recognition and Marco Cecchini's work on cannabinoid binding in glycine receptors demonstrated the applicability of CG models in elucidating specific biomolecular mechanisms. Similarly, Zoe Cournia and Valentina Tozzini explored self-assembly processes in biomolecular and hybrid systems, bridging the gap between biological and materials science applications.
The systematic development of force fields and methods also garnered significant attention. Gregory Voth and Alexander Lyubartsev discussed the theoretical underpinnings and practical applications of bottom-up approaches, such as force-matching techniques, while Adam Sieradzan introduced the UNICORN unified CG model. These efforts represent a concerted move towards rigor and unification in the CG field.

Industrial applications of CG models, showcased by companies like BIOVIA and SAMSON, further highlighted the practical relevance of these tools. The inclusion of cutting-edge topics such as thermo-responsive polypeptides and antimicrobial peptide design added fresh perspectives and underscored the field's growth.
In summary, the workshop's diverse program, featuring contributions from leading researchers and early-career scientists alike, highlighted the interplay between theoretical advances, methodological innovations, and real-world applications. By fostering cross-disciplinary dialogue and identifying future challenges, the event significantly contributed to advancing the state of the art in CG simulations.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop was highly successful, attracting record participation (100 attendees) and substantial sponsorship funding, with a total extra budget of 10,585.19 CHF provided by Zymvol Biomodeling (481.18 CHF), OneAngstrom (481.18 CHF), and METiS Pharmaceuticals (9622.83 CHF). This additional funding enhanced organizational capacity and allowed broader participation.
In addition to academia, companies such as Dassault Systèmes, Sanofi, and AstraZeneca played active roles in discussions, highlighting the growing industrial interest in CG models for real-world applications. However, the condensed 3-day format limited opportunities for extended discussions and in-depth exchanges. Key outcomes included fostering collaborations between CG model developers and AI researchers, with a focus on integrating top-down and bottom-up approaches. Participants emphasized the need to improve CG model transferability across complex biological and industrial systems, addressing factors like chemistry, temperature, and pressure variability.
Open questions remain on balancing chemical fidelity with computational efficiency and how AI can address existing limitations. Future workshops would benefit from longer schedules and more structured discussion sessions to maximize collaborative potential.

## 3. What was the take-home message for the participants?

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Many CG approaches are converging, adopting insights from one another's methodologies. Systematic bottom-up approaches are now tackling systems with broader compositional complexity, while top-down strategies are integrating theoretical insights from bottom-up methods. The rise of AI-based approaches is driving advancements across CG families, from parameterization strategies to innovative potentials, propelling the field toward new horizons.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop demonstrated increasing collaboration between academia and industry, indicating that CG models are maturing for real-world applications. Companies such as METiS Pharmaceuticals, Zymvol Biomodeling, OneAngstrom, AstraZeneca, Dassault Systèmes, and Sanofi underscored the applicability of CG models in drug development, protein delivery design, and materials science.
The potential societal benefits include better understanding of diseases, developing therapeutic interventions, and creating sustainable materials. CG modeling is advancing toward bridging the gap between academic research and industrial needs, showcasing its transformative potential in healthcare, biotechnology, and beyond.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

While collaborators inside of CG families were clearly reinforced, new collaborations were fostered between participants, speakers and organizers, with already some tangible outcomes:
- A book proposed by Adam Liwo about CG approaches, with contributions from participants of the workshop.
- An ICTP school application initiated by Sergio Pantano and other participants of the workshop.
- Integration of CG approaches, as MARTINI CG lipid models into UNICORN/UNRES frameworks.
- AI-based CG strategies from Cecilia Clementi synergized with bottom-up approaches.
- Potential collaboration between polymer physics and biology/chemistry researchers (e.g. Tatiana Morozova and Paulo C. T. Souza).
- The presence of companies such as Sanofi and AstraZeneca also opened doors for potential industry-academia partnerships focused on CG applications.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop achieved notable diversity in geographical representation, career stages, and gender. Approximately 30% of participants were women, reflecting improved gender diversity compared to typical events in the field, though further improvements are still needed. Participants ranged from early-career researchers to senior scientists, including one researcher with a disability. Companies such as Dassault Systèmes, Zymvol Biomodeling, AstraZeneca, and Sanofi participated alongside academic institutions, enriching the event with diverse perspectives.

Speakers and attendees represented various continents, including Europe, Asia, the Americas, and Africa, fostering a truly inclusive environment.

## 7. Participant list

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### Organisers

**Clementi, Cecilia**
Freie Universität Berlin, Germany
**Liwo, Jozef Adam**
University of Gdansk, Poland
**Loverde, Sharon**
CUNY, United States
**Pantano, Sergio**
Institut Pasteur de Montevideo, Uruguay
**Telles De Souza, Paulo Cesar**
ENS de Lyon / CNRS, France

**Akkermans, Reinier** - Dassault Systèmes, United Kingdom
**Andreasen, Mikkel** - Aarhus University, Denmark
**Atmaca, Sumeyye** - University of Gdansk, Poland
**Bacic Toplek, Fran** - Universita' degli Studi di Milano, Italy
**Baltz, Lucia** - Johannes Gutenberg University Mainz, Germany
**Barducci, Alessandro** - Centre de Biologie Structurale, France
**Bezerra Da Cruz, Carlos Henrique** - University College London, United Kingdom
**Bhattacharjee, Nicholus** - Zymvol Biomodeling SL, Spain
**Bini, Margherita** - Scuola Normale Superiore and Istituto Nanoscienze, CNR, Italy
**Bonollo, Giorgio** - University of Pavia, Italy
**Borges Araujo, Luis** - Ecole Normale Superieure de Lyon, France
**Bozoflu, Mert** - University of Groningen, Netherlands
**Brancolini, Giorgia** - Institute of Nanoscience - CNR NANO, Italy
**Brandner, Astrid** - University of Oxford, United Kingdom
**Brannigan, Grace** - Rutgers, United States
**Cascella, Michele** - University of Oslo, Norway
**Cecchini, Marco** - University of Strasbourg, France
**Ceres, Nicoletta** - LBMC UMR 5239, France
**Corne, Léo** - ENS Lyon, France
**Cournia, Zoe** - Biomedical Research Foundation, Greece
**Danielsson, Annemarie** - University of Gdansk, Poland
**De Giovanetti, Marinella** - Sorbonne Université, France
**Dobchev, Dimitar** - SANOFI, France
**Ennis, Jahmal** - Rutgers University, United States
**Everaers, Ralf** - École Normale Supérieure de Lyon, France
**Feig, Michael** - Michigan State University, United States
**Frezza, Elisa** - Université Paris Cité, CiTCoM CNRS, France

**Ghosh Moulick, Abhik** - City University Of New York, United States
**Golon, Łukasz** - University of Gdańsk, Poland
**Gosavi, Shachi** - National Centre for Biological Sciences-TIFR, India
**Goupil, Anne** - Dassault Systèmes, France
**Gront, Dominik** - University of Warsaw, Poland
**Grudinin, Sergei** - CNRS / Inria, France
**Grunewald, Fabian** - Heidelberg Institute for Theoretical Studies, Germany
**Guzman, Horacio V** - CSIC, ICMAB, Spain
**Hazrati, Mehrnoosh** - Ústav Fyzikální Chemie J. Heyrovského, Czech Republic
**Hidayat, Alam Ahmad** - Jagiellonian University, Poland
***, Janusz** - IIMCB Cell Biology, Poland
**Jiang, Yingmin** - Université Paris-Saclay, France
**Karami, Yasaman** - Inria, Université de Lorraine, France
**Kjølbye, Lisbeth Ravnkilde** - AstraZeneca, Sweden
**Klein, Florencia** - Institut de Biologie Physico-Chimique, France
**König, Melanie** - University of Groningen, Netherlands
**Kumar, Ashutosh** - University of Fribourg, Switzerland
**Kusay, Ali** - Linköping University, Sweden
**Leśniewski, Mateusz** - University of Gdańsk, Poland
**Lindorff-Larsen, Kresten** - University of Copenhagen, Denmark
**Loison, Claire** - Université Claude Bernard Lyon 1, CNRS, France
**Lyubartsev, Alexander** - Stockholm University, Sweden
**Malcharek, Madlen** - University of Konstanz, Germany
**Marques, Carlos** - Centre National de La Recherche Scientifique, France
**Marrink, Siewert-Jan** - University of Groningen, Netherlands
**Martin, Juliette** - CNRS UMR5239, France
**Mínguez-Toral, Marina** – CIB Margarita Salas, Spain
**Morozova, Tatiana** - CNRS/ENS Lyon, France
**Musseli Cezar, Henrique** - University of Oslo, Norway
**Muttathukattil Narayanan, Aswathy** - Lund Univeristy, Sweden
**Nascimento Dos Santos, Ricardo** - Sanofi, France
**Ngueldjou Tahabo, Cyrille** - University of Johannes Gutenberg, Mainz, Germany
**Nguyen, Truong Co** - Gdansk University, Poland
**Nieto, Vincent** - Aarhus University, Denmark
**Pągielska, Marta** - University of Gdansk, Poland
**Palmisano, Vito Federico** - Autonomous University of Madrid, Spain
**Pasos-Trejo, Aldo** - Freie Universität Berlin, Germany
**Pasquali, Samuela** - Université Paris Cité, France
**Pedersen, Kasper Busk** - Aarhus University, Denmark
**Pellarin, Riccardo** - CNRS, France
**Pereira, GIlberto** - ENS Lyon, France
**Pitman, Connor** - Rutgers University -- Camden, United States
**Poblete, Simón** - Universidad San Sebastián, Fundación Ciencia y Vida, Chile
**Poma Bernaola, Adolfo** – IPPT PAN, Poland
**Prabhu, Janak** - University of Fribourg, Switzerland
**Redon, Stephane** - OneAngstrom, France

**Risselada, Herre Jelger** - University of Goettingen, Germany
**Rossetti, Giulia** - Forschungszentrum Jülich, Germany
**Scaramozzino, Domenico** - Karolinska Institutet, Sweden
**Schahl, Adrien** - KTH Royal Institute of Technology, Sweden
**Schopmans, Henrik** - Karlsruhe Institute of Technology, Germany
**Schuhmann, Fabian** - University of Copenhagen, Denmark
**Sen, Samiran** - Institut Pasteur/CNRS Paris, France
**Shinoda, Wataru** - Okayama University, Japan
**Sieradzan, Adam** - Fahrenheit Union of Universities In Gdańsk, Poland
**Sikora, Mateusz** - Jagiellonian University, Poland
**Stroh, Kai** - ENS Lyon / CNRS, France
**Szukalo, Ryan** - Princeton University, United States
**Tao, Jianjun** - LAMBE-Univeristé D'Evry, France
**Thallmair, Sebastian** - Frankfurt Institute for Advanced Studies, Germany
**Tozzini, Valentina** - Istituto Nanoscienze, CNR, Italy
**Valerio, Mariana** - ENS de Lyon, France
**Vasin, Semen** - INSA Lyon, France
**Voth, Gregory** - University of Chicago, United States
**Zhang, Qin** - École Normale Supérieure de Lyon, France

# Kardar–Parisi–Zhang equation: new trends in theories and experiments

**Location: CECAM-FR-RA**
**Webpage : https://www.cecam.org/workshop-details/kardar-parisi-zhang-equation-new-trends-in-theories-and-experiments-1312**
**Dates: Apr 14, 2024 - Apr 26, 2024**

## 1. What were the major topics presented in the School?

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Topics :
Scalings of the KPZ universality class: from power-laws to distributions and non-perturbative renormalization group Mathematical tools: random matrix theory, Tracy-Widom and Airy distributions
Statistical mechanics: driven lattice models, from exact analytical solutions to large-scale numerical approaches
Quantum problems: open systems, spin chains, equilibrium and driven-dissipative Bose-Einstein condensates
Experimental realizations (turbulence, front propagation, cold atoms): experimental techniques and modelling realistic phenomena
Numerical methodologies: quantum simulators, simulations of stochastic dynamical equations
Topics cover a wide range of methodologies (experimental and theoretical, both on the analytical and the numerical levels)

Five lectures and practical works will be given by :
**- Elisabeth Agoritsas (DQMP, Université de Genève, Switzerland)**
Interfaces in disordered systems, directed polymer
**- Ivan Corwin (Columbia University, USA)**
Mathematical aspects of the KPZ universality class
**- Sebastian Diehl (Universität zu Köln, Germany)**
Keldysh formalism, open quantum systems, exciton-polaritons, quantum simulators
**- Tomaž Prosen (Univerza v Ljubljani, Slovenia)**
Non-equilibrium lattice (quantum) systems, emergence of KPZ in spin chains, numerical methods for discrete models
**- Kazumasa A. Takeuchi (Tōkyō University, Japan)**
Introduction to the KPZ equation (scaling, numerical approaches) and experimental aspects

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

**Scalings**

Understanding the KPZ universality class involves studying the scaling properties and statistical distributions of growing interfaces. While power-laws have been established for some quantities, a comprehensive characterization of all relevant scaling functions and their crossover behaviors is still incomplete. Non-perturbative renormalization group (NPRG) methods offer potential insights, but developing these methods to fully capture the non-trivial fixed points and scaling functions of the KPZ equation is an ongoing challenge. The connection between the NPRG approach and other methods, like exact solutions and other numerical approaches, needs further exploration.

**Mathematical Tools**

Random matrix theory has been pivotal in understanding the KPZ universality class, particularly in 1+1 dimensions. Extending these mathematical tools to higher dimensions remains a challenge. The exact role of Airy processes and other intricate mathematical structures in higher dimensions, or in different boundary conditions, is not fully understood, although numerical insights point to the existence of universality classes in 2+1 and 3+1 dimensions. Bridging the gap between exact results and numerical results is an ongoing problem, that requires the development of new algorithms to ascertain universality.

**Quantum Problems**

In quantum systems, the KPZ equation finds analogs in spin chains and Bose-Einstein condensates (BECs). Understanding how KPZ-like dynamics manifest in open quantum systems and driven-dissipative BECs is an open problem, particularly concerning the interplay between quantum coherence and classical stochasticity. Developing a robust theoretical framework for these quantum systems, and connecting it to the KPZ universality class, remains a significant challenge.

**Experiments**

Experimental techniques to realize and measure KPZ dynamics in systems like turbulence or front propagation have advanced, but challenges persist. Modelling realistic phenomena requires precise control, alongside numerical models that can accurately capture experimental conditions. Developing new setups that can clearly demonstrate KPZ scaling in higher dimensions or under varying boundary conditions is an ongoing line of research.

**Numerical Methods**

Quantum simulators offer a promising approach for studying KPZ dynamics in controlled environments. However, accurately simulating stochastic dynamical equations and capturing the full range of KPZ scaling behaviors require advanced algorithms. Improving the efficiency and accuracy of these simulations, and validating them against both theoretical predictions and experimental data, is an open problem. Extending these numerical methodologies to explore new regimes (especially those recently unveiled with dynamical exponent z=1) in the KPZ class remains open.

### 3. What was the take-home message for the participants?

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The fields inspired by the seminal paper of Kardar Parisi and Zhang does not cease to grow in diversity, with positive cross-fertilization between fields.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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• PDF of slides used by lecturers, available on the website :
https://kpz-houches.sciencesconf.org/resource/page/id/1
https://kpz-houches.sciencesconf.org/resource/page/id/2
• Recording of Lectures (for lecturers and speakers who accepted), prepared by École de Physique des Houches (soon available).
• Book of abstract available on the main page of the School website
https://kpz-houches.sciencesconf.org/

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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- During the phase of preparation of the school, for lectures and talks, we invited scientists with in mind the promotion under-represented genders, and at a wide spectrum of career stage.
- The publicity of the event was made as wide as possible (worldwide) so as to increase the diversity of geographical provenance of participants.
- As participant subscribed, we provided funding and/or accommodation for students of lesser represented countries or countries with difficult access for travel funding.

### 6. Organiser list

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**Canet, Léonie**
Université Grenoble Alpes, France
**Lecomte, Vivien**
LIPhy, Université Grenoble Alpes, France
**Minguzzi, Anna**
CNRS, France

# Atoms, molecules and clusters in motion

**Location: CECAM-FR-MOSER**
**Webpage : https://www.cecam.org/workshop-details/atoms-molecules-and-clusters-in-motion-1300**
**Dates: Apr 15, 2024 - Apr 18, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

We organized the 5th edition of the international conference on "Atoms, Molecules and Clusters in Motion - AMOC 2024" from the 15th April to the 18st April 2024 at the University Gustave Eiffel. The first version of this series of conferences took place at Paris Region and was initiated by the CECAM-FR-MOSER node of CECAM. Due to the success of this version, several editions of AMOC were organized over Europe in a triennial periodicity. Over the years, AMOC became among the most selective conferences on Physical Chemistry and Molecular Physics. Indeed, this conference tackles the up-to-date experimental and theoretical subjects and deals with problematics to be solved in the following areas:
- Electronic structure theory, in particular for electronic excited states
- Exploring multidimensional potential energy surfaces
- Quantum and semiclassical treatments of nuclear motions
- Approaches beyond the well-established Born-Oppenheimer approximation
- Molecular dynamics techniques and simulations for statistical treatment of the nuclear motion problem
- Establishment of new strategies and approaches for the analysis and the interpretation of recent experimental studies and astrophysical observations, such as high resolution (multi-dimensional) ro-vibrational spectroscopy of molecular species in excited states, of weakly bound clusters, of molecules absorbed on nano-objects or surfaces, and molecules in the interstellar medium.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

This event is an international conference and not a workshop. The oral presentations and the posters were showing the state-of-the-art experimental and theoretical methodologies to treat the above-mentioned topics. The limitations and the open questions concern the consideration of several electronic states and not only a unique one, their couplings and interactions. These cannot be treated straightforwardly and are not implemented in commercial softwares. Participants

expressed the need of close collaborations to tackle such challenges and in particular for the construction of networks at the national, European and international levels. Indeed, several excellent initiatives are developed in labs and in the groups over the world, but we need to develop synergies between these groups to avoid redundancy since it turns out that we are facing similar problems (at different levels) to be overcome.
The attendees proposed to organize the next edition of AMOC to continue discussing such challenges. Therefore, it was decided that the next edition of AMOC. It will be organized in 2027 in Warsaw (Poland). Several attendees expressed their interest to attend and participate to the next edition.

### 3. What was the take-home message for the participants?

Various topics were treated during this conference (and not a workshop). So, several take-home messages were provided. We can gather them in “need of accurate spectroscopic experimental and theoretical methodologies” for better characterization of the Physical and Chemical Processes at the microscopic level and their implications at the macroscopic level.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The applications of the topics treated during this conference are closely connected with environmental (pollution), astrophysics, origin of life and drug design. The understanding of such processes at the microscopic level, tackled in detail during this conference, are crucial for the design and the promotion of eco-friendly products with reduction of pollutants emissions, ...
Besides, three poster prices were given to 3 PhD students as proposed by a committee led by Prof. R. Guntram (U. Stuttgart, Germany). These prices are intended to promote Physical and Chemical Sciences near young scientists and students.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The program included 34 slots for oral presentations of 30 minutes each including 5 minutes of discussions and 6 slots for hot topics (15 minutes). Also, poster sessions were organized during all breaks (coffees and lunches) and also on Tuesday evening, where a cold dinner and soft drinks were proposed to the attendees. We also organized a AMOC 2024 Conference Dinner on Tuesday 16$^{th}$ of April evening.

During the opening of this conference a Tribute to Dr. Philippe Millié who passed away in June 2023 was given by Prof. G. Chambaud (President of the Société Chimique de France).

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Gender balance was ensured by proposing half of the talk slots to men and the second half to women. For such international event, the Local Organizing Committee is composed by 3 women and 4 men.
This conference gathered more than 100 participants from 27 countries from Europe, Africa, Asia and North America.
We had one third of the attendees were seniors, one third are confirmed researchers and one third are early carrier researchers (post docs and PhD students).

## 7. Organiser list

**Brenner, Valérie**
CEA, France
**Hochlaf, Majdi**
Université Gustave Eiffel, France
**Lauvergnat, David**
Université Paris Saclay / CNRS, France
**Morisset, Sabine**
Paris-Saclay University, France
**Palaudoux, Jérôme**
Sorbonne University, France


# Ab initio quantum electrodynamics for quantum materials engineering

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/ab-initio-quantum-electrodynamics-for-quantum-materials-engineering-1294**
**Dates: Apr 15, 2024 - Apr 19, 2024**

## 1. What were the major topics presented in the School?

Quantum electrodynamics (QED) is the detailed theory of how charged particles interact via the creation and annihilation of photons, the gauge bosons of the electromagnetic force. While QED is usually the domain of high-energy and particle physicists, its basic ideas have permeated also the domain of low-energy physics such as condensed-matter physics, electronic-structure theory, chemistry and quantum information science. In condensed-matter physics and electronic-structure theory, for instance, usually only the interaction arising from the longitudinal part of the photon field, the ubiquitous Coulomb interaction, is kept. In contrast, in quantum optics the transverse photons are the focus whereas the Coulomb-interacting matter is reduced to a few effective levels. The vast majority of QED effects are then only considered as perturbations on top of the corresponding reduced models, in agreement with the common formulation of QED as a scattering theory. However, in the 1990s and 2000s mathematicians and mathematical physicists have made great progress in formulating low-energy QED as a non-perturbative quantum theory of light and matter. The resulting QED theory allows for a full self-consistent solution of coupled light-matter systems from first principles, i.e., only fundamental physical parameters are needed. Since the corresponding Schrödinger-like equation of light and matter is very different from the common quantum-mechanical many-body Schrödinger equation, novel ab initio methods have been developed to deal with low-energy QED and the emerging hybrid light-matter states.
Hand in hand with these theoretical developments, experimental results in polaritonic chemistry and polaritonic materials science, where the coupling to optical cavities can influence and control the properties of molecules and solids, have demonstrated that non-perturbative QED effects can also manifest in low-energy physics. This is even true at thermal equilibrium. These experiments together with the emerging ab initio QED methods challenge our artificial distinction between "light" and "matter" and lead to a holistic perspective of low-energy physics.
This CECAM school gave an exhaustive introduction to this novel and exciting field of research at the interface of (quantum) optics, quantum information, (quantum) statistical physics, (quantum) chemistry and condensed-matter physics. It seamlessly combined lectures on mathematical physics (on low-energy QED and foundations of ab initio QED), quantum chemistry and condensed-matter physics

(on the development, implementation and application of ab-initio QED methods) and quantum optics (on macroscopic QED and quantum-optical methods). This school provided a holistic perspective of light and matter and highlighted novel effects and synergies that arise between so far distinct fields of research. Indeed, the school addressed quantum materials in the broadest possible sense

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

This school was unique in the sense that it covered the very basics of light-matter interactions (fundamentals of QED), the novel effects that arise due to non-perturbative interactions in cavities (polaritonic chemistry and materials science), as well as the theoretical and numerical tools to solve the resulting multi-scale problems (ab-initio QED methods). The lectures were supplemented by group exercises and practice classes, where the participants learned to use the available theoretical and numerical tools (e.g. quantum-electrodynamical density-functional theory or macroscopic QED).
From the personal and online feedback, the following points of were identified:
- The mathematical and fundamental aspects of QED were challenging due to the background of most of the participants (quantum chemistry and solid-state physics)
- The time allocated to group exercises and practice classes was too short
- The limitations of the different ab-initio QED methods were not stressed enough
- It remained unclear under which conditions new effects from light-matter hybridizations are expected

## 3. What was the take-home message for the participants?

The participants praised the holistic approach going from basic QED to applications in materials science in one consistent framework. Also, the detailed explanation of quantum-electrodynamical density-functional theory and macroscopic QED was very well received. Given the novelty of the fields of polaritonic chemistry and materials science, the participants appreciated the many open question and that a comprehensive theoretical framework is a good way to answer these questions.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- Second edition in NYC
- Lecture notes will be compiled into a book for after second edition

- Gitlab repository with all the python notebooks
- Binder with pre-compiled simulation software (Octopus) for the exercise classes
- Recordings via CECAM

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

In the selection of the participants, we were trying to balance the gender and geographical composition. Specifically, we had arranged financial support for underrepresented regions (in this case Africa), but the respective applicant could not attend due to personal reasons. At the same time, we actively mixed different career stages (from beginning PhD students to senior researchers) and scientific backgrounds (chemistry, condensed matter and optics) to allow the participants to support each other's understanding. In the group exercises and practice classes we encouraged that the participants worked together and engaged in networking.

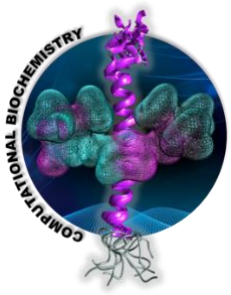
## 6. Participant list

### Organisers

**Latini, Simone**
Technical University of Denmark, Denmark
**Rubio, Angel**
MPI for the Structure and Dynamics of Matter, Germany
**Ruggenthaler, Michael**
MPI for the Structure and Dynamics of Matter, Germany

**Albar, Esra Ilke** - MPI for the Structure and Dynamics of Matter, Germany
**Alessandro, Riccardo** - University of Perugia, Italy
**Angelico, Sara** - NTNU, Norway
**Appel, Heiko** - MPI for the Structure and Dynamics of Matter, Germany
**Bakkestuen, Vebjørn Hallberg** - Oslo Metropolitan University, Norway
**Bonafé, Franco** - MPI for the Structure and Dynamics of Matter, Germany
**Bustamante, Carlos** - MPI for the Structure and Dynamics of Matter, Germany
**Castagnola, Matteo** - Norwegian University of Science and Technology, Norway
**Ciccotti, Giovanni** - University "La Sapienza" and IAC-Rome CNR, Italy
**De La Fuente Diez, Jaime** - École Normale Supérieure de Paris, France
**De La Pena Ruiz, Sebastian** - MPSD, Germany
**De Mestral, Virginie** - ETHZ, Switzerland
**Devescovi, Chiara** - ETH Zurich, Switzerland
**Dos Anjos Cunha, Leonardo** - CCQ, United States
**Even Tzur, Matan** - Technion, Israel
**Fan, Chongxiao** - MPI for Structure and Dynamics of Matter, Germany

**Fiechter, Marit** - ETH Zürich, Switzerland
**Hoffmann, Norah** - New York University, United States
**Horak, Jacob** - MPSD, Germany
**Islam, Md Mursalin** - MPI for the Physics of Complex Systems, Germany
**Kamper Svendsen, Mark** - MPSD, Germany
**Lexander, Marcus** - Norwegian University of Science and Technology, Norway
**Lindel, Frieder** - Universidad Autónoma de Madrid, Spain
**Lu, I-Te** - Max Planck Institute for the Structure and Dynamics of Matter, Germany
**Oue, Daigo** - Instituto Superior Técnico, Portugal
**Penz, Markus** - MPI for the Structure and Dynamics of Matter, Germany
**Ronca, Enrico** - University of Perugia, Italy
**Rossi, Federico** - Norwegian University of Science and Technology, Norway
**Sidler, Dominik** - Paul Scherrer Institut, Switzerland
**Sutter, Sarina** - Vrije Universiteit, Netherlands
**Toth, Oliver** - EPFL/CECAM-HQ, Switzerland
**Vetsch, Nicolas** - ETH Zurich, Switzerland
**Weight, Braden** - University of Rochester, United States




# Computational biochemistry. Efficient tools to fight diseases

**Location: CECAM-ES**
**Webpage : https://www.cecam.org/workshop-details/computational-biochemistry-efficient-tools-to-fight-diseases-1337**
**Dates: Apr 15, 2024 - Apr 19, 2024**

## 1. What were the major topics presented in the School?

The didactic blocks consisted in the following topics:
1st Block:
Lesson 1. Introduction. Biomolecules and their properties. Structural databases of biomolecules. Structure-energy relationship: Biomolecules modeling (Adolfo Bastida)
Lesson 2. Potential energy surfaces in biomolecules. Molecular mechanics force fields. Conformational exploration.
Lesson 3. Solvents. Periodic Boundary Conditions. Molecular Simulations. (Adolfo Bastida)
2nd Block:
Lesson 4. Enhanced sampling techniques and free energy methods 1: Umbrella Sampling, & Metadynamics simulations, Replica Exchange & Accelerated Molecular Dynamics simulations. (Rodrigo Casasnovas).
Lesson 5. Estimation of kinetic data from molecular simulations: Kinetics from metadynamics. Markov State Models. Transition Path Sampling. (Rodrigo Casasnovas)
3rd Block:
Lesson 6. Models to study biochemical reactivity and applications: Continuum solvation models. Cluster models. QM/MM models. Subtractive and additive schemes. Electrostatic and polarizable embedding. (Vicent Moliner & Iñaki Tuñón)
Lesson 7. Reaction free energy profiles in biochemical systems. Application of Transition State Theory to Biochemical reactivity (Vicent Moliner & Iñaki Tuñón)
4th Block:
Lesson 8. The binding processes. Calculation of binding free energies. Alchemical Transformations. Approximate Methods (MMPBSA & MMGBSA). (Vicent Moliner & Iñaki Tuñón)
Lesson 9. Protein-ligand interaction. Quantitative structure-activity relationships (QSAR). Docking techniques. (Vicent Moliner & Iñaki Tuñón)

Practice 1 and 2. Molecular Dynamics simulations of polypeptides in water solution under physiological conditions. Application to fragments of SARS-CoV 3CL protease (Adolfo Bastida & Rodrigo Casasnovas).
Practice 3. Free energy calculations 1. Tutorial on Umbrella Sampling simulations: setup and analysis. Application to the study of inhibitors of SARS-CoV-2 (Adolfo Bastida & Rodrigo Casasnovas)
Practice 4: Free energy calculations 2. Tutorial on metadynamics simulations: setup and analysis. Application to the study of inhibitors of SARS-CoV-2 (Rodrigo Casasnovas)
Practice 5: Protein Ligan Interaction. Reactivity. QSAR. Docking (Iñaki Tuñón & Vicent Moliner)
Practice 6: Free Energy Profile for Ion Pair Formation in the 3CL (or Main) Protease of SARS-CoV-2(Iñaki Tuñón & Vicent Moliner)

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

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**- Limitations in Molecular Modeling Techniques**:
◦ While molecular mechanics force fields are widely used, they still have limitations in accurately representing complex biomolecular systems, such as protein-ligand interactions or conformational changes.
◦ Molecular dynamics simulations often require substantial computational resources, limiting the size and timescale of systems that can be effectively studied.
◦ Enhanced sampling techniques like metadynamics may introduce biases or artifacts depending on the choice of collective variables and simulation parameters.
**- Challenges in Free Energy Calculations**:
◦ Despite the advancements in techniques like umbrella sampling and metadynamics, accurately estimating free energy landscapes and kinetics remains a challenge, particularly for rare events and complex reactions.
◦ Convergence issues can arise in free energy calculations, requiring careful analysis and potentially multiple simulations to obtain reliable results.
**- Validity of Computational Models**:
◦ The accuracy of computational models, particularly in representing biochemical reactivity, ligands-protein docking and binding affinities, depends on the choice of force fields, solvent models, and other approximations.
◦ QM/MM methods offer improved accuracy by incorporating quantum mechanics, but there are still challenges in defining accurate partitioning schemes and balancing computational cost with accuracy.
**- Interpretation of Simulation Results**:
◦ Interpreting simulation results and translating them into meaningful biological insights can be challenging, particularly in complex systems where multiple factors influence the behavior of biomolecules.

◦ Understanding the limitations of computational models and the assumptions underlying simulation protocols is crucial for proper interpretation of results.

**- Relevance and Applicability**:

◦ While computational techniques have shown great promise in drug discovery and enzyme design, their practical applicability and success rates in real-world scenarios may vary.

◦ Open questions remain regarding the transferability of computational models trained on specific systems to novel targets and the generalizability of structure-activity relationships derived from computational studies.

### 3. What was the take-home message for the participants?

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- Computational tools provide a quantitative approach to drug design
- Biochemical processes are complex and their study require adequate simulations
- Free energy changes are the key magnitudes to be computed. Free energies determine the spontaneity and the kinetics of a process
- QSAR methods and exploration of ligand-protein docking, which can be achieved by means of open access programs, provide valuable information for future design of enzyme inhibitors.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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- We have generated lecture notes that are available for the students through the web page of the CECAM course
- We have also generated a set of practical exercises were the students can put their knowledge into practice. These exercises are based on free software so it is very easy for the students to continue their learning.
- With the help of ZCAM technicians we generated a virtual machine where the students were able to carry out the proposed exercises. the access to these virtual machines was granted two weeks after the course so the students could continue practicing.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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We have facilitated the participation of students coming from different countries. We promoted participation from various regions by advertising the course widely. In this edition we have had students coming from Europe, Asia, Africa and both north and south America. We encouraged the students asking by email to

participate in the course, facilitating all the information to help them in the process of enrolling and travelling.
We are aware that there is still a large gap in gender balance in Computational Sciences, which is also reflected in the students enrolled in this course. We ensured gender balance in participant selection through unbiased application processes and actively encouraged diverse representation
The course structure catered to individuals at different career stages, offering content suitable for both early career predoctoral researchers and postdocs that wanted to increase their skills in Computational Biochemistry.

## 6. Participant list

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### Organisers

**Moliner, Vicent**
Universitat Jaume I, Spain
**Tuñón, Iñaki**
Universidad de Valencia, Spain

**Adigun, Temidayo** - University of Ilorin; Omics Code Institute, Nigeria
**Bajia, Donald** - Poznań University of Medical Sciences, Poland
**Barroso, Alejandro** - Autonomous University of Madrid, Spain
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**Binu Abraham, Alen** - Autonomous University of Madrid, Spain
**Casasnovas Perera, Rodrigo** - University of the Balearic Islands, Spain
**Catalán Fenollosa, David** - Universidad de Valencia, Spain
**Chacón, Pablo** - University of Santiago de Compostela, Spain
**Chimarro, Andrea** - Universitat de Valencia, Spain
**Cuadrado Benavent, Beatriz** - Universidad Autónoma de Madrid, Spain
**De La Fuente, Álvaro** - Universidad de Valladolid, Spain
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**Kumar, Prashant** - University College London, United Kingdom
**Lewin, Harry** - University College London, United Kingdom
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**Montagud Andreu, Rubén** - University of Valencia, Spain
**Nayeem, S. M. Abdul** - University of Valencia, Spain
**Orta Parra, Luis Fernando** - Universitat de Valencia, Spain
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**Qadeer, Abdul** - University of Valencia, Pakistan
**Rodríguez-Arias, Carlos** - University of Oviedo, Spain
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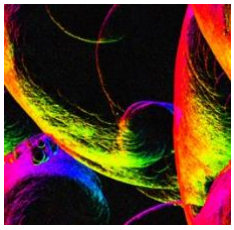
**Vicente Cabello, Vicenta Victoria** - UNMSM, Peru
**Villca Centellas, Danna** - Universidad Autónoma de Madrid, Spain



# Active matter: interfaces and boundaries

**Location: CECAM-CN**
**Webpage : https://www.cecam.org/workshop-details/active-matter-interfaces-and-boundaries-1273**
**Dates: Apr 22, 2024 - Apr 25, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The objective of the workshop was to bring together leading researchers working on the topic and create an atmosphere for brainstorming and exchanging ideas about the role of boundaries and interfaces in active matter. This was going to be achieved through lectures and in-depth discussions. The major topics were mechanical properties and anomalies of active fluids, flocking under confinement, correlation and fluctuation induced forces, onset of liquid - liquid phase separation in confined active fluids, and also organization and collective behaviour of active robotic systems and living matter such as swimming or twitching bacterial motility, or cellular motility. Most of these topics are at the forefront of the state-of-the-art research in active matter and in several cases the discussions resulted in improved understanding of the phenomena and fundamental physics behind them. We also invited a mixture of experimental and theoretical researchers, which further improved the quality of the discussions and the exchange of ideas.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The outcomes follow the objectives: we did bring together leading researchers working on the topic and created an atmosphere for brainstorming and exchanging ideas about the role of boundaries and interfaces in active matter. This was well achieved through excellent lectures and in-depth discussions throughout the workshop on topics such as mechanical properties and anomalies of active fluids, flocking under confinement, correlation and fluctuation induced forces, onset of liquid - liquid phase separation in confined active fluids, and also organization and collective behaviour of active robotic systems and living matter such as swimming or twitching bacterial motility, or cellular motility. We connected the communities in China and Europe and opened new possibilities for collaborations for the future. Moreover, through a healthy mixture of researchers of various ages, and

experimental and theoretical researchers, we managed to improve the quality of the discussions and the exchange of ideas.

### 3. What was the take-home message for the participants?

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The take home message for the participants might be that interfaces and boundaries are of essential importance in active systems and the physics is heavily influenced by these factors. The emerging correlations are complex and difficult to study, but also very rich and interesting, so this might and should be in the focus of the research efforts in the following years.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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Studying living active systems certainly has potential societal benefits. For instance, understanding cellular motility on the substrates might lead to better understanding of cancer and subsequently to better diagnostics and treatment. Likewise, bacterial surface motility is crucial to understand the dynamics of biofilm formation and progress here can offer strategies to prevent the unwanted biofilms in medical applications.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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No specific publications were planned directly from the workshop, however, there are several new collaborations that have started during the event. In particular, the workshop was extremely successful in bringing together European and Chinese active matter communities, and particularly such collaborations (there are many) are the real outcome of the event.

### 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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We tried to achieve as much as possible the gender balance. Despite some rejections, we believe we did reasonably on that front (about 25 percent, a field-typical percentage of female speakers). There was a real good mixture of Chinese and European speakers and participants, and also a mixture of early and not-so-early career stage participants (speakers were ranging from postdocs, to young starting faculty to established professors).

## 7. Organiser list

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**Chaté, Hugues**
CEA Saclay & Beijing CSRC, France
**Dobnikar, Jure**
Institute of Physics, Chinese Academy of Sciences, China
**Pagonabarraga, Ignacio**
University of Barcelona, Spain

# Machine-actionable data interoperability for the chemical sciences (MADICES 2)

**Location: CECAM-DE-MMS**
**Webpage : https://www.cecam.org/workshop-details/machine-actionable-data-interoperability-for-the-chemical-sciences-madices-2-1321**
**Dates: Apr 22, 2024 - Apr 25, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The first working group focused on the challenge of RDM platform interoperability, specifically in a manner agnostic to each other's particular internal mechanics or APIs. It is understood that widespread interoperability is beneficial and generally desired, but that implementing pair-wise interoperability between APIs is a daunting task on the order of $N^2$ (N platforms seeking to interoperate with N other platforms). Hence, a platform-agnostic solution must be devised to facilitate widespread interoperability. To enable such a solution, the group conceived a new transfer protocol rooted in semantically annotated transactional units written in JSON-LD, using the RO-Crate specification for packaging research (meta)data. The group split into two subgroups focusing on drafting open specifications for (i) requests, and (ii) responses. In addition, a demonstrator was developed to showcase the new protocol using mock-up web apps mimicking the openBIS electronic lab notebook (ELN) and the AiiDA workflow management system (WFMS). The demonstrator has since been greatly extended and has proven an indispensable learning tool. A video tutorial is available demonstrating the new protocol using the mock-up apps. The general discussion is ongoing and will continue as we push to finalize the specifications and test our concepts against additional RDM platforms.
The second working group focused on semantic annotations and ontologies. Discussion revolved around which formats to use for RDF serialization, with JSON-LD identified as the most suitable among available options due to its already widespread use and existing JSON-based APIs. Further discussion followed on how much metadata needs to be provided to describe data, how to deal with missing values, and how and where to incorporate units for measurements. There were also discussions on how to write a JSON schema and the need to have GUI-based tools for this for less technically-inclined users. Finally, a contribution from the voc4cat project, which focuses on ontologizing data in catalysis, led to work on the semantic annotation of some of the real-world datasets used at the workshop. A record of the discussions within this working group is available on GitHub.
The third working group was focused on handling data from devices in proprietary formats. Discussions focused on approaches in handling such data, the technical aspects of ingestion of the raw proprietary files into an ELN, their parsing into FAIR

or at least open data, and modern approaches to “streaming” data from continuous experiments.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop provided a major step towards communal understanding of how to best semantically annotate datasets and how to leverage semantically meaningful data to facilitate platform-agnostic interoperability. The collective efforts culminated in a set of tools for semantic dataset annotation (as well as a Python package for semantically handling units), and web apps (and a video) demonstrating the new data transfer protocol, the specifications of which have also been drafted and are currently being expanded. Furthermore, potential partners for collaboration and integration of data extraction tools from binary file types and proprietary data formats have been identified. A batch of such extractors has been successfully integrated into the project during the workshop, with plans for future work with other workshop attendees.

Several open questions remain. With respect to platform-agnostic interoperability of semantically annotated datasets, it is not yet clear the exact level of annotation required to support the protocol. Furthermore, there is the question of how to handle cases where interoperating platforms exchange datasets that have been semantically annotated against disparate ontology knowledge graphs. There is also the issue of whether to handle data format conversion on exchange. These are all being considered and discussed actively on the MADICES repositories. For example, two solutions were offered at the workshop for handling disparate knowledge graphs: (i) community-driven bridge ontologies (and perhaps LLMs at a later stage), and (ii) developing a central format to which each platform implements a converter or adapter. These are both being explored. Note that, at the moment, the new protocol is being tested heavily by the openBIS and AiiDA teams. However, already at the workshop, several RDM platform representatives had expressed interest, including the Chemotion, Herbie, and datalab ELNs, as well as NMRShiftDB. We will continue to involve additional RDM initiatives in the discussion.

In terms of handling data from proprietary files, further work in this area requires an agreement on the level of annotation, discussed above. It is clear that semantic annotations should be incorporated as early as possible in the data pipelines, ideally at acquisition / raw data ingestion time. Therefore, building pressure on instrument vendors to provide open, well annotated data is crucial, and will require a community effort.

### 3. What was the take-home message for the participants?

Providing semantic meaning to research data is invaluable to open science and to facilitating seamless exchange of open and FAIR research data. It can be made simpler through community efforts to develop dedicated tools to streamline semantic annotation, and incentivized by showing the broader value to the community of individual efforts. Such tools should be incorporated as close to the instrumentation producing the data as possible.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

There is a general push for open research in science, with clear benefits to accelerating scientific discovery. However, the crisis of reproducibility is well-known within the science community and often arises from attempts at open research in the absence of clear guidelines. A survey of participants at the first MADICES workshop identified the lack of standards, protocols, examples, and best practices as the primary barrier to the adoption of open research. The collaborative efforts of the MADICES series aim to drive the community towards resolving these challenges. The outcomes of MADICES continue to contribute to and pave the way towards platform-agnostic solutions to exchange open data in a standard way following structured guidelines to ensure research reproducibility, thus securing the benefit of accelerated science.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Several new collaborations have flourished in (and since) the workshop (see the various repositories added to the MADICES GitHub organization and linked above). Additionally, the knowledge exchange on the practicalities of semantic annotation of experimental data will allow attendees to continue with implementation of the work started at MADICES. Representatives from BAM, Chemotion, Herbie, NMRShiftDB, FAIRmat, openBIS, and AiiDA are all presently contributing to the specifications, demonstrators, and implementation of the platform-agnostic data transfer protocol. The web apps developed in and after the workshop are being considered as a future educational playground. Furthermore, in addition to two of the present co-organizers, we identified two participants who wish to co-organize a follow-up MADICES workshop (late 2025), the proposal of which is currently being drafted.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Participants were invited from the networks of the organizers, recommendations from coordinators of research data initiatives, and by surveying relevant activities on GitHub and social media. In particular, due to the hands-on nature of the workshop, junior researchers (PhD students and postdocs) were prioritized in our invitations. In total, 65 people were contacted, out of which 10 were female; from the 35 participants (including organizers), 5 were female. The organizers arranged accommodations for 6 applicants who could not attend otherwise, 5 of whom attended the entire workshop. To find common topics of interest, collaboration partners, and plan the workshop sessions, we organized virtual pre-workshop planning sessions open to all invitees, which were crucial in fostering the right open community and spirit for the eventual workshop. After the workshop, we held a virtual wrap-up meeting to collect feedback, coordinate ongoing work, and discuss the next MADICES event.

## 7. Participant list

### Organisers

**Bainglass, Edan**
Paul Scherer Institut, Switzerland
**Barillari, Caterina**
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**Evans, Matthew**
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**Jablonka, Kevin**
Helmholtz Institute for Polymers In Energy Applications, Germany
**Kraus, Peter**
Technische Universität Berlin, Germany

**Adamopoulou, Despoina** - Empa, Switzerland
**Battaglia, Corsin** - Empa, Switzerland
**Bekemeier, Simon** - Bundesanstalt für Materialforschung Und -prüfung (BAM), Germany
**Brinckmann, Steffen** - Forschungszentrum Juelich, Germany
**Brockhauser, Sandor** - Humboldt University, Germany
**Da Costa Lopes, Fabio Andre** - EMPA, Switzerland
**Dal Molin, Emiliano** - Technishe Universitaet Berlin, Germany
**Danaila, Mihai** - ETH Zurich, Switzerland
**Elbert, David** - Johns Hopkins University, United States
**Held, Martin** - Hereon, Germany
**Hunold, Johannes** - TIB, Germany

**Jung, Nicole** - Karlsruhe Institute of Technology, Germany
**Kirchner, Fabian** - Helmholtz-Zentrum Hereon, Germany
**Kuhn, Stefan** - Tartu University, Estonia
**Laskowski, Adam** - ETHZ, Switzerland
**Linke, David** - Leibniz-Institut für Katalyse E.V., Germany
**Moustakas, Nikolaos** - Leibniz Institute for Catalysis (LIKAT), Germany
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**Pizzi, Giovanni** - Paul Scherrer Institute PSI, Switzerland
**Scheidgen, Markus** - Humboldt-Universität zu Berlin, Germany
**Schumann, Julia** - Humboldt Universität zu Berlin, Germany
**Starman, Martin** - Karlsruher Institut für Technologie (KIT), Germany
**Stier, Simon** - Fraunhofer ISC, Germany
**Yakutovich, Aliaksandr** - Empa, Switzerland

# Towards quantitative cell biology through AI-driven software engineering for molecular simulations

**Location: CECAM-IT-SISSA-SNS**
**Webpage : https://www.cecam.org/workshop-details/towards-quantitative-cell-biology-through-ai-driven-software-engineering-for-molecular-simulations-1319**
**Dates: May 6, 2024 - May 8, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Owing to the emergence of the exascale era in high-performance computing, which is becoming available through advanced facilities such as Frontier from the United States and Jupiter in Europe, and to the development of powerful AI-driven platforms, an unprecedented plethora of biological phenomena are becoming accessible to atomistic description by molecular modeling and simulation techniques. While existing biomolecular simulation codes (often in C++ or Fortran) are optimized for advanced architectures, they can be limited in their broad applicability and adaptability to tackle complex biological challenges. A revolution is underway, driven by big data and AI, to enhance these codes and expand the scope of biomolecular simulations. In this context, several topics were discussed during our workshop in relation to the challenging implementation and application of sophisticated and effective methodologies aiming at treating computationally large-scale biomolecular systems. Among others, various talks discussed in some detail aspects concerning the following research areas:
- Atomistic Simulation Modeling
- Enhanced Sampling Techniques
- Code Optimization and Limitations
- Implementation Challenge in Big Data and AI

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The scientific discussions during our CECAM workshop clearly presented a number of existing limitations that still plague the effective large-scale application of AI-driven software modeling tools for treating biomolecular systems of great scientific and therapeutic interest. Among other limitations, in various talks there were mentioned issues related with code porting to new HPC technologies and the combination and integration of different simulation algorithms. Concerning the

latter point, applied computational methodologies were discussed in depth during the workshop and ranged from quantum mechanics, enhanced molecular dynamics sampling techniques, and coarse-grained molecular dynamics to machine learning approaches. Besides, critical review of the computational techniques employed for these challenging tasks was undertaken throughout the Q&A and discussion sessions, while perspective ones were presented by borrowing ideas from other fields. In the context of current limitations in the field, it was also discussed the limitations of National and International research funding directed towards basic research and computational development programs, in place of highly specific and application-targeted funding programs.

## 3. What was the take-home message for the participants?

The workshop plainly showed already intriguing applications and new possibilities for the forthcoming years. In particular, the fast development of big data and machine learning tools for biomolecular structural predictions opened up new opportunities in the field for unprecedented applications that, however, will also require new needs for our computational community. Among the relevant take-home messages that emerged during the workshop, it is worth mentioning the increasing need for the shareability and accessibility of data throughout the community and the reuse of data to ensure efficient collaboration and transfer of knowledge throughout the scientific communities.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The meeting nurtured some active discussions between researchers from different countries, including the US, inviting future collaborations between the participants. During the exchange and networking (guaranteed through the organized lunches, coffee breaks, and the social event), several opportunities to apply for EU funding were also considered, among which some calls within the coming Exascale HPC calls and the EU ERC programs. We believe that follow-up workshops, seminars, and scientific collaborations, as well as grant applications and student exchanges, are going to be facilitated through the newly established and enforced cooperation network originating from the meeting. Overall, the workshop can have far-reaching societal benefits, advancing both scientific knowledge and practical applications that can improve human health and quality of life.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop presented and stimulated collaboration in various areas of great economic and societal benefit related to the molecular description of biological and pharmacological relevant systems. Opportunities for funding this very important research fields were also discussed since the biological targets discussed during the workshop were of great scientific and biomedical interest. The organization of the workshop allowed to facilitate collaborations and cross-talking among scientists from different fields and institutions, which will ultimately lead to more efficient and effective research, accelerating scientific discoveries and advancements in the field. In the future, we should aim to host and organize more interdisciplinary workshops that join life-sciences with other communities such as computer science and engineering sciences. Additional needs of the community identified during the meeting show the shared view about the necessity to receive more direct support from High Performance Computing centers at National and EU level, especially for helping researchers in computational development activities towards more effective methods and models.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The selection process of the invited speakers to the workshop was carried out keeping in due consideration gender, geographical provenance of the speakers, and their carrier stage. No specific rules were followed in the case of the participants, since the workshop was fully open to any participants (some of which were remotely connected).

## 7. Participant list

### Organisers

**Beck, Thomas L.**
Oak Ridge National Laboratory, United States
**Brancato, Giuseppe**
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**Carloni, Paolo**
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**De Vivo, Marco**
Istituto Italiano di Tecnologia, Italy

**Asthagiri, Dilipkumar** - Oak Ridge National Laboratory, United States
**Baaden, Marc** - Institut de Biologie Physico-Chimique (IBPC), France

**Benedetti, Luca** - Scuola Normale Superiore, Italy
**Bondar, Ana-Nicoleta** - University of Bucharest, Romania
**Boukabcha, Maamar** - Hassiba BEN BOUALI University of Chlef, Algeria
**Chipot, Chris** - CNRS, France
**Ciofalo, Cosimo** - University of Florence, Italy
**Clementi, Cecilia** - Freie Universität Berlin, Germany
**Collepardo, Rosana** - University of Cambridge, United Kingdom
**Dal Peraro, Matteo** - EPFL, Switzerland
**Ezat, Ahmed** - Faculty of Science, Cairo University, Egypt
**Fahlke, Christoph** - Forschungszentrum Jülich, Germany
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**Glaser, Jens** - Oak Ridge National Laboratory, United States
**Gray, Alan** - NVIDIA, United Kingdom
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**Hummer, Gerhard** - Max-Planck-Institut für Biophysik, Germany
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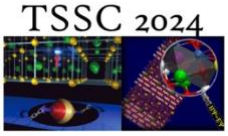
**Joo, Balint** - Oak Ridge National Laboratory, United States
**Kumar, Chettan** - Georg-Speyer-Haus, Germany
**Kurnikova, Maria** - Carnegie Mellon University, United States
**Laughton, Charles** - University of Nottingham, United Kingdom
**Liberati, Diego** - National Research Council of Italy, Italy
**Lin, Jung-Hsin** - Academia Sinica, Taiwan
**Magistrato, Alessandra** - CNR-IOM@SISSA, Italy
**Mandelli, Davide** - FZJ, Germany
**Mariani, Valerio** - Stanford University, United States
**Meloni, Simone** - University of Ferrara, Italy
**Merz, Kenneth** - Michigan State University, United States
**Messer, Bronson** - Oak Ridge National Laboratory, United States
**Mitusinska, Karolina** - CNR-IOM at SISSA, Italy
**Nechushtai, Rachel** - Hebrew University of Jerusalem, Israel, Israel
**Nimigean, Crina** - Weill Medical College, United States
**Nussinov, Ruth** – NCI Frederick, United States
**Parrinello, Michele** - Istituto Italiano di Tecnologia, Italy
**Perez, Danny** - Los Alamos National Laboratory, United States
**Piquemal, Jean-Philip** - Sorbonne Université, France
**Pizzorusso, Tommaso** - Scuola Normale Superiore, Italy
**Ramos, Maria João** - University of Porto, Portugal
**Rempe, Susan** - Sandia National Laboratories, United States
**Roethlisberger, Ursula** - EPFL, Switzerland
**Rosato, Antonio** - University of Florence, Italy
**Rossetti, Giulia** - Forschungszentrum Jülich, Germany
**Sagresti, Luca** - Freie Universität, Germany
**Salvadori, Giacomo** - Forschungszentrum Jülich, Germany
**Sharma, Himanshu** - Seth G. L. Bihani Sd Pg College, India

**Sinha, Dhirtaj** - UT Southwestern Medical Center, United States
**Spivak, Mariano** - CNRS, France
**Stevens, Mark** - Sandia National Lab, United States
**Suarez, Estela** - Forschungszentrum Juelich GmbH, Germany
**Tourassi, Georgia (Gina)** - Oak Ridge National Laboratory, United States
**Turan, Haydar Taylan** - Scuola Normale Superiore, Italy
**Wang, Yuhan** - UCL, United Kingdom
**Wang, Feiyi** - Oak Ridge National Laboratory, United States
**Wimley, William** - Tulane School of Medicine, United States
**Wolf, Steffen** - University of Freiburg, Germany
**Xie, Song** - Forschungszentrum Jülich, Germany
**Zuo, Ke** - University of Cagliari, Italy




# Theoretical solid-state chemistry: theory, modelling, and simulation

**Location: CECAM-ES**
**Webpage : https://www.cecam.org/workshop-details/theoretical-solid-state-chemistry-theory-modelling-and-simulation-1336**
**Dates: May 6, 2024 - May 10, 2024**

## 1. What were the major topics presented in the School?

- Electronic Structure. Cluster and periodic models. Kohn-Sham equations and DFT methods.
- Thermodynamic Properties. Static models. Equation of state of solids. Phase transitions.
- Macroscopic Maxwell equations. Hamiltonians for light-matter interaction. Time-dependent evolution of a periodic system under electric fields. Absorption and reflectivity.
- Multiscale methods. Scaling in the construction of the Hamiltonian. Linear scaling techniques. Metals, insulators, and the Fermi energy. QM/MM and force-fields. Excitons and polarons.
- Structure of solids' surfaces: relaxation, rumpling, and reconstruction of surfaces. Surface energies. Surface defects. Reactivity at surfaces.
- Phonons and dispersion curves. Free energy. Quasi-harmonic approximation. Thermal properties. Anharmonicity and thermal transport.
- Topologies of scalar fields in crystals. Electron density, electron localization function and reduced density gradient chemical functions.
- Effective Magnetic Hamiltonian theory. Spin waves for ferromagnets. Antiferromagnetic lattices. Electron transport.
- Magnetic anisotropy, double exchange, and spin wave theory.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

The different specialists of each area paid particular attention to the approximations used in the simulations so that the students can critically understand the advantages and limitations of each approximation. The level of the school is too basic as to enter into open questions in the atomistic modelling of solids. Anyway, know limitations of current state-of-the-art density functional methods in relation to their applications to the study of the solid state are examined. With respect to surfaces, the limitations of models regarding experimental coverages of adsorbates, the modelling of complex dynamic catalytic

systems, and the open problem of predicting surface reconstructions in real catalytic conditions (temperature and reactant pressure) have been presented. The need to go beyond the harmonic or quasi harmonic approximation to properly describe heat transport have also been addressed.
During the practical sessions the students made the presenters questions about their particular projects in many cases related to their master and PhD thesis.

## 3. What was the take-home message for the participants?

The school provides the students with a wide toolkit with which to approach many facets of Solid-State Chemistry with applications in important current topics of the area.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture notes for theoretical sessions and hands-on tutorials for the practical sessions are deposited in the CECAM web page for the school. In addition to these, input files for the practical sessions are also provided to ensure that all exercises can be completed within the tight schedule of the course.

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

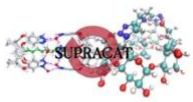
We had students from México (1), Italy (3), Belgium (1), Sweden (1), Norway (1), Brazil (1), and Spain (16). One third of the speakers are female as well as about 30% of the students.
We are open to geographical provenance of the participants, but its geographical location results in a majority of students coming from European countries.

## 6. Participant list

### Organisers

**Díaz, Cristina**
Universidad Complutense de Madrid, Spain
**Garcia Fernandez, Pablo**
Universidad de Cantabria, Spain
**Márquez, Antonio M.**
Universidad de Sevilla, Spain

**Aleson Gurruchaga, Ander** - UPV, Spain
**Camara Garmendia, Idoia** - UPV/EHU, Spain
**Cuadrado Benavent, Beatriz** - Universidad Autónoma de Madrid, Spain
**Custódio Silva Lemos, Samantha** - Universitat Jaume I, Spain
**De Armas Rodriguez, Raúl** - IMDEA Materiales, Spain
**Dhali, Rama** - University of Mons, Belgium
**Diaz-Gutierrez, Miguel Angel** - Universidad Autónoma de Madrid, Mexico
**González Pacheco, Alejandro** - Universidad Autónoma de Madrid, Spain
**González Sanz, Aurora** - Universidad Autónoma de Madrid, Spain
**Jena, Nityasagar** - IFM, Linköping University, Sweden
**Loprete, Fabio** - University of Bologna, Italy
**Marković, Danilo** - Autonomous University of Madrid, Spain
**Mas Garcia, Josep** - ICMUV, Spain
**Mata Rabadan, Fernando** - UAM, Spain
**Miranda Saenz, Edgard Alejandro** - Universidad Autonoma de Madrid, Spain
**Pistillo, Simone** - Università degli Studi di Trieste, Italy
**Putra, Jouvan Chandra Pratama** - University of Agder, Norway
**Ribeiro, Israel** - University of Sao Paulo, Brazil
**Rodriguez Almeida, Lucas Francisco** - University of Bologna, Italy
**Romani, Anna** - University of Bordeaux, France
**Sifuna, James** - The Catholic University University of Eastern Africa, Kenya
**Varela, Miguel** - Fundacion IDONIAL, Spain
**Vidal, Lucía** - Universidad de Oviedo, Spain
**Vides Garcia, Nuria** - Universidad de Oviedo, Spain
**Villa, Jean** - Universitat de Barcelona, Spain
**Villca Centellas, Danna** - Universidad Autónoma de Madrid, Spain
**Villegas, Orlando** - Université de Poitiers, France
**Youbi Kemmogne, Marie Rose** - Université Catholique de Louvain, Belgium




# Modelling supramolecular catalysis: methods and applications

**Location: CECAM-FR-MOSER**
**Webpage : https://www.cecam.org/workshop-details/modelling-supramolecular-catalysis-methods-and-applications-1301**
**Dates: May 12, 2024 - May 14, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop started with D. Tantillo on modeling carbocation rearrangements, and he advocates that most of comp. tools are nowadays mature but needs to be used in combination to reach scientific consensus and that in particular environmental effects are critical for large systems. The 2nd talk was presented by FX Coudert and was about modeling with machine learning supramolecular materials. One of his conclusions was that going back to simpler DFT calculations in a pragmatic approach is interesting when the model obtained allows to be predictive. The last speaker of the first day was W. Li and she presented comp. analysis of reactive supramolecular systems, showing that the catalytic system is very sensitive to local electric field and are functioning like enzymes.
The next day started with G. Ujaque and he presented computational results highlighting the importance of understanding the substrate binding within the supramolecular catalyst and the interplay with solvent displacement. T. Piskorz then introduces some automatic tools for analyzing molecular cages (size of the cavity and automatized force field parametrization involving metals). The next two talks were focusing on catalytic events analysis: one by L. Xu who has been showing that the selectivity of Diels-Alder in cages is indeed controlled by non-covalent interactions and one by F. Masera who emphasizes that reactivity emerges from multiple bindings pose of the substrate inside the supramolecular cage. Another interesting point of this talk was the complete integration of a microkinetic model based on computational data to fit the experimental results. Then G. Piccini concluded the day by showing that despite differences between the various field of catalysis, many concepts are similar (and in particular when modeling it).
We start the last day with F. Himo. During his works on supramolecular catalysis, he found that performing extensive conformational search was more important than extensive DFT benchmarking. Of course, it requires to parametrize FF and to ensure proper convergence of the conformational search, but for large systems, conformations are more important than a systemic error of DFT. the next talk was given by J. Peters who emphasizes that the most complex task was to determine what binds into the cavitand and when during the catalytic cycle, hence showing again that the main problem is not to determine the nature of the elementary steps.

The workshop was concluded by E. Derat, showing that cyclodextrins can act like enzymes by establishing electrostatic control and modifying mechanisms known without the supramolecular environment.
In summary, the field of comp. supramolecular cat. has many computational tools at its disposal. There is no more major technical problems. We have now entered time when more subtle effects can be analysed by these various tools: solvent effects, long-range electrostatic effect, substrate unbinding, etc... It will allow the community to focus on describing and creating new catalytic systems.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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During the workshop, we dedicated a session to discussing what are the acquired points and what are the current limitations in the field of computational supramolecular catalysis. It appears that hybrid QM/MM methodologies are sufficiently developed to tackle most of the problems in this field. There is probably some needs related to adaptative QM/MM (for example exchange of solvent/substrate within the cavity), but these are relatively minor problems.
Similarly, investigating non-covalent interactions is not really a problem, with various topological approaches currently available from the literature. But what remains more problematic is to quantify a specific non-covalent interaction within a large subset of interactions. What would be even more interesting is an automatised tool able to distinguish between the various kinds of non-covalent interactions and able to classify them qualitatively and quantitatively.
During the discussions, one point which was coming back regularly is the need of benchmarking carefully the computational methods used for describing supramolecular catalysis. There is plenty of database related to DFT calculations for various systems, but none of them take into account the reactivity in large systems. It could be interesting to build a database of carefully checked experimental supramolecular reactions (barrier and enthalpy), as well as binding energies for prototypical systems. This DB would serve to check the various complex computational protocol used by the researchers in the field.
Another limitation was coming back in the discussion: sampling and conformational analysis. Supramolecular catalysis is at the border of two domains: classical synthetic chemistry with relatively small objects (±100 atoms) and chemical biology (with size up to several thousands of atoms). We have a few tools at our disposal but none of them were properly evaluated for supramolecular catalysis. Using force fields developed for chemical biology can also be problematic and requires careful checking of the parameters before conducting any conformational analysis. Here, the current situation is a compromise between accuracy and quality of the exploration of the chemical space.

### 3. What was the take-home message for the participants?

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Three points here:
-1- An emerging community based on a few groups doing computational supramolecular catalysis with some specific methodologies
-2- Lots of challenging (and sometimes very complex) questions are opened in this field.
-3- A field with many connections to enzymatic/homogenous/heterogenous catalysis simulations

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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The field of supramolecular catalysis is in between classical catalysis and enzymatic catalysis. Potential benefits for the society is thus relatively similar to the outcome of theses catalysis: obtaining complex products while minimizing the environmental cost. Simulations are currently mainly used to understand the machinery at work but further developments will help to make the field more predictive.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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We are currently starting to write a Perspective article summarizing what has been achieved in the field of computational supramolecular catalysis and discussing what needs to be developed. We envisage to submit this Perspective to Nature Communications since one of the editors has shown interest to the subject. Most of the participants to the workshop will be authors of this perspective article.

### 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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The organizers have send invitations to researchers working in many countries (EU, US, China, Japan, India), irrespective of their genders and nationalities.
Two female researchers were not able to come for teaching reasons (they are head of department in the US and the workshop was corresponding to end of semester with heavy duties).
PhD student/ PDRA/ young researchers were given the same opportunity to talk during the workshop.

## 7. Participant list

### Organisers

**Coudert, François-Xavier**
CNRS, France
**Derat, Etienne**
Sorbonne Université, France
**Himo, Fahmi**
Stockholm University, Sweden

**Braïda, Benoît** - Sorbonne Université, France
**Davila, Brenda** - Sorbonne Universite, France
**Frison, Gilles** - CNRS, France
**Li, Wanlu** - University of California San Diego, United States
**Lombardo, Giacomo** - Universite Paris Cite, France
**Maseras, Feliu** - Institute of Chemical Research of Catalonia (ICIQ), Spain
**Norjmaa, Gantulga** - Stockholm University, Sweden
**Peters, Joannes** - Stockholm University, Sweden
**Piccini, GiovanniMaria** - Università di Modena e Reggio Emilia, Italy
**Piskorz, Tomasz** - University of Oxford, United Kingdom
**Prejanò, Mario** - University of Calabria, Italy
**Tantillo, Dean** - University of California, Davis, United States
**Ujaque, Gregori** - Universitat Autonoma de Barcelona (UAB), Spain
**Wang, Qian** - Shandong University of Technology, China
**Xu, Li-Ping** - Shandong University, China


# Machine Learning modalities for materials science

**Location: Ljubljana, Slovenia**
**Webpage : https://www.cecam.org/workshop-details/machine-learning-modalities-for-materials-science-1282**
**Dates: May 13, 2024 - May 17, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop showcased advancements in machine learning methods applied to materials understanding, characterization, discovery, and design. From machine learning potentials to generative models (variational autoencoders and diffusion models), from large language models for structure-property predictions to convolutional neural networks and transformers for the analysis of spectroscopy and microscopy data.
Panel discussions and question-times enabled to discuss the need for integration of multi-modal data, which involves combining disparate data types like microscopy images, spectroscopy results, simulation outputs, and performance metrics. This integration aims to create comprehensive models that predict material behavior with greater accuracy. Additionally, the concept of multi-objective optimization, especially in the context of generative approaches, was explored, highlighting how ML can help balance trade-offs between different material properties. Transfer learning emerged as another promising approach, where models trained on one set of materials or properties can be adapted to predict others, thereby accelerating discovery. Challenges and opportunities inherent to multi-fidelity approaches, where models leverage data of varying quality and resolution to enhance predictive power and robustness, were also analyzed.
Collaboration and interdisciplinary efforts were a significant theme, with attendees from diverse backgrounds discussing how to best combine their expertise. Workshops and panel discussions provided platforms for sharing experiences, addressing challenges, and identifying future research directions. Keynote speakers from leading institutions and industries offered insights into the current state and future potential of ML in materials science. Additionally, the workshop aimed to equip young researchers with a solid foundation in cutting-edge ML methods, ensuring they are well-prepared to drive future innovations.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The field appeared as rather mature when accounting for “single-modality” approaches, where the word modality refers to a single property evaluated through a single method. Machine learning potentials predict forces and energies almost with chemical accuracy. Observables typical of characterization methods, such as spectra and image, may be assessed in an automated fashion, with the latter analysis providing statistics and insights in agreement with the ones of domain-experts.
Challenges do exist when facing noisy data or non-univocal structure-property mappings. Open questions remain on how to practically foster shared data and approaches across different modalities, laboratories, and materials-domains communities to shed light on these more complex situations.
A significant challenge is also to establish standardized protocols and platforms that enable seamless data sharing and integration across various research settings. Different laboratories and research communities often use diverse methodologies and formats, making data interoperability difficult. Overcoming these barriers requires the development of universally accepted data standards and the creation of centralized repositories where researchers can upload and access datasets.
Fostering collaborations between academic institutions and industry is also crucial. Industrial stakeholders possess vast amounts of proprietary data and practical insights that, if shared under appropriate frameworks, could substantially accelerate research and development in materials science. To facilitate this, it is essential to build trust and establish mutually beneficial partnerships where data privacy and intellectual property rights are respected.
Democratization of methods, approaches, and training of a diverse and inclusive community is also an additional key opportunity to address the current competition for talent and resources. By making advanced machine learning tools and educational resources widely accessible, we can level the playing field and ensure that researchers from varied backgrounds and institutions can contribute to and benefit from advancements in materials science. Encouraging participation from underrepresented groups and providing them with the necessary training and support can unleash a wealth of untapped potential, driving forward new discoveries and solutions. This democratization effort requires sustained investment in educational initiatives, mentorship programs, and inclusive policies that promote equal opportunities for all researchers, regardless of their geographic or institutional affiliations

## 3. What was the take-home message for the participants?

An holistic approach, integrating various data types and leveraging advanced machine learning methods, is essential for advancing materials design and

discovery. A diverse and horizontal community, which fosters collaboration across disciplines, and the adoption of multi-modal, multi-objective, and multi-fidelity approaches could significantly enhance the predictiveness and efficiency of materials research, driving innovation.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop discussed applications of machine learning to accelerate materials in the context of green energy, sustainable chemistry, pharma and agropharma, thus holds significant potential for societal benefits.
Machine learning acceleration of new materials design for renewable energy technologies, includes solar cells, batteries, and fuel cells more efficient and cost-effective, and promises to reduce reliance on fossil fuels and lowering greenhouse gas emissions.
By enabling the discovery of new catalysts and chemical processes, machine learning can minimize waste and reduce the environmental impact of chemical manufacturing, promoting greener industrial practices.
Similarly, machine learning promises to accelerate the identification and optimization of novel compounds, streamlining drug discovery and developing environmentally friendly pesticides and fertilizers, contributing to sustainable agriculture.
Furthermore, the workshop fostered (international) collaboration between experts in various fields, leading to innovative, integrated solutions that address complex societal challenges more effectively. Also, the skills and knowledge shared during the workshop empower researchers and practitioners, enhancing their capacity to apply machine learning in tackling critical problems in materials science and beyond, also at industrial level.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

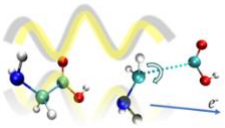
The workshop is part of the activity of a European Network on machine learning for materials (https://www.cost.eu/actions/CA22154/), which was successfully funded after its bottom-up emergence from previous CECAM workshops. Under the framework of this network, and also thanks to the event, it is expected that new collaborations will start on specific topics of interest decided by PIs and students attending the event. A review/perspective on multi-modal approaches for machine learning in materials science could be also expected to be kick-started in the next year(s). The submission of collaborative EU projects (e.g. MSCA ITN) is also under scrutiny.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote inclusivity we implemented several measures. We ensured geographical diversity by hosting the event in Ljubljana, with 135 participants, including several from South-east Europe, oftentimes facing challenges to reach more distant locations, joining the event. Gender and financial inclusivity was also a priority, reflected in our travel support, which was awarded to 25 participants, 9 of whom were female. We also aimed for gender diversity among our invited lecturers, achieving 1/3 female representation despite scheduling conflicts, which precluded the availability of additional female speakers. Finally, we note that the workshop also focused on young researchers, featuring introductory pedagogical lectures and hands-on demonstrations in the first two days to support their development.

## 7. Organiser list

**De Gironcoli, Stefano**
Scuola Internazionale Superiore di Studi Avanzati - International School for Advanced Studies, Italy
**Dzeroski, Saso**
Jozef Stefan Institute, Slovenia
**Rinke, Patrick**
Technical University Munich, Germany
**Rossi, Kevin**
TU Delft, Netherlands
**Stevanoska, Sintija**
Jozef Stefan Institute, Slovenia
**Todorovic, Milica**
University of Turku, Finland



# Ultrafast phenomena in chemistry: laser-matter interactions at the femto- and atto-second time scales

**Location: CECAM-ES**
**Webpage : https://www.cecam.org/workshop-details/ultrafast-phenomena-in-chemistry-laser-matter-interactions-at-the-femto-and-atto-second-time-scales-closed-reached-full-capacity-1342**
**Dates: May 20, 2024 - May 24, 2024**

## 1. What were the major topics presented in the School?

The school presents advanced computational techniques for Femtochemistry and Attochemistry. It was structured in 4 modules:
Module 1: Introduction to laser technologies.
1.1. (A. Palacios, UAM) Introduction to the fundamentals of light and matter interactions (perturbation theory, time-dependent Schrödinger equation – exact simulations for few-particle systems). Overview of quantum chemistry methods for the description bound and continuum states of molecules (i.e., light-induced excitation and ionization).
1.2. (K. Chirvi & Jens Biegert lab from ICFO; and W. Gawelda from IMDEA. Technical aspects for laboratory-based XUV and X-ray lasers, and large-scale accelerator driven light sources (free electron lasers). The most illustrative applications on gas-phase targets, solvents and condensed matter are discussed. A practical session on laser pulse characterization and spectral analysis is given.
Module 2: High-order harmonic generation (HHG) techniques.
2.1. (C. Hernández-García, USAL). Theoretical tools for the description of HHG spectra, including tools to account for macroscopic effects. It then presents novel concepts on structured light (light with angular momenta). The practical sessions are prepared through Jupiter notebooks.
Module 3: Light-induced ultrafast processes in real systems.
3.1. (J. Feist, UAM) Theoretical description of laser pulses in time and frequency domain using open source codes (https://github.com/jfeist/laserfields). Extensive module for the description of light interacting with atoms and molecules, connecting the weak-field regime introduced in Module 1, with non-perturbative approaches to treat high-intensity regimes where non-linear phenomena arise in atoms and molecules (light-induced electronic wave packets, dressed states). The lecturer provided premade Jupiter notebooks, using Python libraries and homemade libraries.
3.2. (F. Zapata, UAM) Numerical solution of the time-dependent Schrödinger equation. A premade Fortran-based code and Python scripts are provided to simulate photoelectron spectra using attosecond interferometric techniques.

Module 4: (A. Castro, UNIZAR-BIFI) Fundamentals on time-dependent density-functional theory (TDDFT). The attendants learnt to use of the OCTOPUS software to describe excitation processes in large molecules (https://octupus-code.org/). The lecturer, Alberto Castro (UNIZAR/BIFI) has been one of the developers of this package, and offered a tutorial and 4 hours of practical sessions.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

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The school is very interactive. The attendants are encouraged to participate at any moment and, thus, asked many questions to deepen in the different lectures. They were particularly interested on the description of the light itself (weak *vs* strong fields; laser parameters definitions). Not limitations detected in the hands-on. These are some of the attendants' comments regarding the interactivity of our course or their main interests:

"*Introductions are done well and I felt comfortable asking questions with everyone being roughly the same knowledge level. I learned lots of new terminology and ideas such that the harder concepts were not obfuscated by the language.*"

"*..., all the professors was very kind and careful in review the learning processes, with nice interactions with the students.*"

"*There were many opportunities for people to network and exchange ideas. Liked the availability of all lecturers during and after the sessions. Also really appreciated that in the beginning of the school we had introductory sessions towards the topic and then went more in-depth. Also the topics were nicely arranged in time - moving from smaller towards bigger systems."*

We also got some comments regarding the hands-on sessions. Their positive view is also the result of our previous accumulated experience in other schools, and the previous edition of the present one, where we analyze our surveys to improve:

"*The hands on portions were a great introduction to modeling these sorts of systems. I really appreciated how easy it was to access the programs via Jupyter notebook.*"

"*It was great to see that some of the lectures were connected, or that at least each professor -- or most of them, more on that later -- knew what the other was doing, so that they didn't explain the same thing over and over again, and they could reference each others materials, making the whole experience seem very well organized."*

There is always room for improvement. In our survey, we explicitly ask them to find the weakest points of the course and provide suggestions to improve the school. Two issues are detected: better whiteboards and more (smaller) breaks:

"*New Whiteboard Pens in a black color, as there was instances when speaker notes were very difficult to read. The sessions themselves are of a good length but to maintain concentration i think it would be a good idea to take 5-10 minute breaks at intervals so that everyone does not get tired...*"

*"I would suggest that more, but small breaks, are made between the lectures, so students can rest and move a little bit...*"

While no specific limitations were identified, the above issues (shorter but more breaks), will be incorporated if a new edition takes place.

### 3. What was the take-home message for the participants?

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A solid formation to describe coherent light interacting with matter. An overview of the state-of-the-art methodology and technological progresses in Attosecond and Femtosecond Science. They learnt the most fundamental tools to be able to tackle new problems in these areas and obtain the necessary material to work in an autonomous manner. In the words of one of the attendants: "*moreover the material provided is very useful for reviewing and deepening the topics in the future.*"

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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- Lecture notes and tutorials are still available at the CECAM-ES platform in the tab "Documents". Lecture notes from all professors are made available, in most cases, before the class, so the attendants can review the information.
- Jupiter Notebooks and home-codes are made available to the attendants, so they can keep using them after the classes.
- Attendants employ our libraries for the description of light sources and to reproduce the interaction with simple systems (few-level systems). The software has been developed by the Lecturers and the students have access through notebooks, and libraries available through github (i.e. : https://github.com/jfeist/laserfields).
- Attendants are taught to employ OCTOPUS software, which is installed and available in several centers and computational networks.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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We announce it in international distribution lists and networks. Our school includes female teachers (as role model) and teachers in different career stages (7 to 25 years post-PhD). Attendees came from different countries: Spain, USA, UK, Italy, Czech Republic, Poland, Norway, Germany and Bulgaria. We had 1/3 of Master and 2/3 PhD students. We prioritize female and international attendants, for acceptance and reimbursement. BIFI facilities are fully accessible for everyone.
Gender balance should be improved, although the ratio (6/30) reflects the % of females working on this field (~20% of female scientists in Europe working on AMO Physics). See statistics in https://ww2.aip.org/statistics/women-in-physics-and-

astronomy-2019 or https://www.aps.org/apsnews/2022/10/mixed-progress-women-marginalized.

## 6. Participant list

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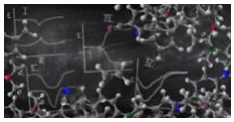
### Organisers

**Palacios, Alicia**
Universidad Autónoma de Madrid, Spain
**Zapata Abellan, Felipe**
Universidad Complutense de Madrid, Spain

**Barrios Prieto, Alejandro** - UAM, Spain
**Binns, Edward** - Imperial College London, United Kingdom
**Binu Abraham, Alen** - Autonomous University of Madrid, Spain
**Biró, László** - University of Debrecen, Hungary
**Broad, Mitchell** - Imperial College London, United Kingdom
**Castro, Alberto** - ARAID Foundation, Spain
**Chirvi, Katharina** - ICFO (Institute of Photonic Sciences), Spain
**Cortivo, Riccardo** - Università degli Studi di Padova, Italy
**Crhán, Martin** - Charles University, Czech Republic
**De La Fuente, Álvaro** - Universidad de Valladolid, Spain
**Diaz-Gutierrez, Miguel Angel** - Universidad Autónoma de Madrid, Mexico
**Dinvay, Evgueni** - UiT, Norway
**Djumayska, Simona** - Sofia University, Bulgaria
**Fajardo Herrera, Jose** - Universidad de Valencia, Spain
**Farhat, Afifa** - MPI for the Structure and Dynamics of Matter, Germany
**Faria, Felipe** - University of Central Florida, United States
**Feist, Johannes** - Universidad Autónoma de Madrid, Spain
**Gallego De Roa, Alvaro** - UAM (Universidad Autónoma de Madrid), Spain
**Gawelda, Wojciech** - Universidad Autónoma de Madrid, Spain
**Gindl, Adam** - Charles University, Czech Republic
**Hernández-García, Carlos** - Universidad de Salamanca, Spain
**Husain, Munavvar** - University of Warsaw, Poland
**Jena, Nityasagar** - IFM, Linköping University, Sweden
**Lafiosca, Piero** - Scuola Normale Superiore, Italy
**Lewis, Nicholas** - University of Central Florida, United States
**Mata Rabadan, Fernando** - UAM, Spain
**Mohammed, Lablali** - M'Sick, University Hassan II of Casablanca,, Morocco
**Rashid, Md Harun Or** - Temple University, United States
**Sepali, Chiara** - Scuola Normale Superiore, Italy
**Snowden, Henry** - University of Warwick, Coventry, United Kingdom
**Sobrino Fernández, Cristina** - Universidad Autónoma de Madrid, Spain
**Trinari, Marco** - Scuola Normale Superiore, Italy
**Vargas Chaverri, Ximena** - Universidad de Valladolid, Spain

**Vicente Cabello, Vicenta Victoria** - UNMSM, Peru
**Villca Centellas, Danna** - Universidad Autónoma de Madrid, Spain
**Yadav, Nitin** - Indian Institute of Science Education and Research Mohali, India
**Yelamos, Daniel** - Universidad Autónoma de Madrid, Spain
**Zhong, Kai** - University of Groningen, Netherlands



# Standardizing nonadiabatic dynamics: towards common benchmarks

**Location: CECAM-FR-MOSER**
**Webpage : https://www.cecam.org/workshop-details/standardizing-nonadiabatic-dynamics-towards-common-benchmarks-1304**
**Dates: May 21, 2024 - May 24, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop was animated by extensive discussion sessions centered around the idea of "benchmarking" different methodologies for nonadiabatic dynamics. Since this workshop was the first meeting of this kind, the representatives of the community worked primarily towards defining this idea. Indeed, various research groups already work(ed) on benchmarking some nonadiabatic methodologies, but these efforts have not been well-organized, systematic or rigorous, as there was no agreement on standards from the community. Therefore, together with the participants of the workshop, we worked towards discussing the key issues and establishing these standards.

The first point that was addressed was about the reference for the benchmark: Can the community identify a method that will be treated as a reference against which to benchmark other methods? Can one simply benchmark methods by comparison? Is it adequate to discuss benchmarks against experiments? Related to this point, the discussion focused on the possibility of comparing methodologies based on the representation of the nuclear dynamics in terms of trajectories or in terms of wavefunctions.

The second aspect discussed was the role of the electronic structure, which in some cases is crucial for the outcome of the dynamics. Mainly, the necessity to fix the electronic structure method (and code) to allow a comparison between different dynamics was underlined. Related to this, we discussed the suitability of benchmarking and of comparing methodologies that are based on different representations of the electronic part of the problem. Specifically, often the trajectory-based or trajectory-guided techniques give access to electronic properties expressed in the adiabatic representation, whereas wavefunction-based methods usually work in the diabatic representation.

Therefore, as a third main point of discussion we agreed that not only electronic properties should be used for the benchmarks, but the analyses need to be organized in various kinds of "system properties". For this, analysis codes/scripts need to be discussed and developed, so as to perform analogous post-processing treatment of the data produced by the various codes and methods.

Finally, the community aims to share the codes and the data that are the focus of this benchmarking work. In particular, we anticipate needing support from CECAM

to create a repository for the data produced on the systems identified during the workshop.
It is worth noting that "prediction challenge" on the photodynamics of cyclobutanone was recently launched by the Journal of Chemical Physics, and the results of the prediction were published at the beginning of 2024. Nonetheless, the work we started in the framework of this workshop is not a challenge, but rather a concerted and organized effort of the nonadiabatic community towards improving our understanding of the power of this kind of simulations.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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One major outcome of the workshop is the fact that some representatives of the community and methods developers themselves agreed to sit together and organize their efforts to discuss how to introduce the ideas of standards and benchmarks in the field of nonadiabatic dynamics.
The main outcome of the discussions that took place during the workshop was the agreement on the molecular systems that will represent the first set for benchmarking nonadiabatic dynamics methodologies. The simulations and the analyses will be performed by different groups using different dynamics codes and different techniques, ideally at least those represented at the workshop. However, our goal is to advertise our efforts to other research groups aiming to include a large variety of simulation schemes.
The identification of the systems chosen for the first set of benchmarks have been selected as they are characterized by diverse underlying physical and chemical phenomena (isomerization, dissociation, intersystem crossing and proton transfer). As discussed above, the data produced by the simulations will be analyzed using analogous post-processing treatments, so as to propose a set of observables or properties that can be directly compared to one another. In addition, in order to ensure that only the actual dynamics methods are benchmarked, we plan to adopt the same sets of initial conditions and the same electronic-structure theories (thus, the same quantum chemistry packages).
Indeed, due to the limited time of the workshop and due to the fact that we decided to limit our focus in this initial phase of the benchmarking, some aspects of nonadiabatic dynamics were not covered. These, however, are not really limitations, but questions that will be addressed in the years to come, and hopefully in the framework of other CECAM workshops. In particular, as said above, we are not covering exhaustively all possible simulation methods. In addition, we only proposed systems and phenomena occurring in the gas phase and we proposed to study only ultrafast processes, thus dynamics on short time scales.

## 3. What was the take-home message for the participants?

The participants understood that if we want to improve our methodologies and understand their limitations, we have to work together as a community. There is a lot of work to do, we have to put together our efforts and discuss frequently. Also, the community of nonadiabatic dynamics was well-represented at the workshop, but other people with different expertise need to be involved. Benchmarks are not meant to be difficult to calculate, and there is a clear distinction between benchmark and challenge.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The field of nonadiabatic molecular dynamics (NAD), although part of fundamental scientific research, has numerous indirect societal benefits. Nonadiabatic phenomena play a decisive role in areas such as organic electronics, optoelectronic devices, photobiology, photocatalysis and photochemical synthesis, atmospheric chemistry, and many others. Advancements in NAD methods will certainly drive future discoveries with potentially more direct societal impact. However, this requires dedication to improving current theoretical frameworks and progressing towards simulating more realistic systems and experimental observables. The creation of molecular benchmarks and standardization within the field will help identify the limitations of existing methods and likely contribute to the development of new approaches. However, these aspects of societal benefits were not the focus of the workshop and were, therefore, not discussed in detail. Indeed, our efforts will have repercussions on the methodologies used for these kinds of studies, and, once the preliminary rounds of benchmarks are concluded, challenges towards application-oriented discoveries could be launched based on the key points that have been discussed for the benchmarks.

One topic actively discussed during the workshop is the significant carbon footprint of our current NAD simulations, which negatively impacts the environment and the sustainability of scientific research. Establishing standardized benchmark systems will help identify the most efficient methods for studying specific problems. If more approximate methods are found to be sufficiently accurate and trustworthy, it may be possible to avoid computationally intensive simulations that require extensive CPU usage. Therefore, the creation of benchmark sets may not only enhance the performance of our methods but also challenge the way we approach studying realistic problems.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

To maintain and stimulate further the connection among the members of the community who attended the workshop, we created a Slack channel and all participants accepted our invitation to join it. One of the purposes of this Slack channel is to initiate a short-term collaboration to write and publish a roadmap. In this roadmap, we plan to discuss the necessity for the community to propose benchmarks and to present our viewpoint on the aspects to be addressed in producing standards for nonadiabatic dynamics. This will allow researchers who did not attend the workshop to contribute to the subsequent effort of creating and publishing a common set of molecular benchmarks, which we hope will be accepted as a standard by the broader community in our field.
In addition, a group of participants of the workshop proposed to organized a new workshop next year to address some of the questions that remained open in our first meeting and applied for a July 2024 CECAM call to organize a workshop titled "Future Directions in Non-Adiabatic Dynamics: Towards Complex Systems and Long Time Scales"

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

As organizers, we put a lot of effort into promoting principles of equity and inclusivity. Regarding gender balance, we involved 5 invited female speakers out of a total of 11. Although we aimed for a higher number, some of our invitees had to decline. Unfortunately, the gender ratio among all participants was less balanced, being around 1/3 female. This is indeed a point needing improvement in the future.
In terms of geographic diversity, budgetary constraints primarily allowed to cover a wide variety of European countries. However, we also invited speakers from South Korea and from the United States, and had a participant from India. Thanks to the additional funding received by CECAM HQ, the participant list included many early career researchers as well as experienced researchers. Specifically, we provided financial support to all early career researchers who expressed a need for additional funding.
We did not receive any applications requiring accommodations for disabilities.

## 7. Participant list

### Organisers

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**Worth, Graham** - University College London, United Kingdom


# Tensor contraction library standardization

**Location: CECAM-FR-GSO Toulouse, Franced**
**Webpage : https://www.cecam.org/workshop-details/tensor-contraction-library-standardization-1315**
**Dates: May 22, 2024 - May 24, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop gathered major players in the field, representing users, developers and vendors. Extensive discussions on standardization and other topics were carried out. On the second day of the workshop three groups of developers had a longer breakout session discussing previous proposals of a standard low-level interface. On the third and final day of the workshop, these three groups sat together working on the unification of their proposals. An immediate outcome was the generalization of the binary tensor contraction to D := α A*B + β C, where C and D may be different tensors. The difference is not as minor as it might seem, and not everybody was in favor of this operation. The alternative would be to offer two functions, C := α A*B + β C and D := α A*B + β C, where in the latter C and D must be distinct. Agreement was furthermore reached on using an einsum format for the specification of the contraction, whereas further discussion is needed to converge on whether specific hardware information, in particular for GPUs, should be added at this level. A working group was set up to work on further unification. Concerning the higher-level interface, there was mostly consensus about the operation itself (i.e., its algebraic definition); the major topic of discussion was about data types (input, output, computational).

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop gathered major players in the field, representing users, developers and vendors. Extensive discussions on standardization and other topics were carried out. On the second day of the workshop three groups of developers had a longer breakout session discussing previous proposals of a standard low-level interface. On the third and final day of the workshop, these three groups sat together working on the unification of their proposals. An immediate outcome was

the generalization of the binary tensor contraction to D := α A*B + β C, where C and D may be different tensors. The difference is not as minor as it might seem, and not everybody was in favor of this operation. The alternative would be to offer two functions, C := α A*B + β C and D := α A*B + β C, where in the latter C and D must be distinct. Agreement was furthermore reached on using an einsum format for the specification of the contraction, whereas further discussion is needed to converge on whether specific hardware information, in particular for GPUs, should be added at this level. A working group was set up to work on further unification. Concerning the higher-level interface, there was mostly consensus about the operation itself (i.e., its algebraic definition); the major topic of discussion was about data types (input, output, computational).

### 3. What was the take-home message for the participants?

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Overview talks by users, developers and vendors allowed all participants to get up to speed on all aspects of the workshop topic. Further insight and awareness was brought by the panel discussions, the breakout sessions and debriefings. Major take-home messages is the need for a clear separation of low- and high-level interfaces as well as a standard low-level interface.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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Tensor contraction is a key element of numerous modern-day computations, such as machine learning as well as high-level simulations of the electronic structure and properties of molecules and materials. Vendors are very much aware of the potential of the first domain and work on software for tensor computations according to the needs of this field. However, there is less awareness of the specific features required for the second domain. We have identified an urgent need to create a standard for tensor libraries, which will pave the way for efficient tensor contraction on modern supercomputers, allowing for instance theoreticians to interact with experimentalists in the characterization and development of new materials, with immediate societal benefits. It will also allow users to focus on what they are experts on.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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An extended report about the workshop will be prepared and posted on arXiv. A working group has been set up to continue working on a unified low-level tensor interface and will set up a repository (e.g. GitLab) for this. There will also be work on a reference implementation of such a low-level interface. We will apply for a

follow-up workshop at the Lorentz Center in 2025. Depending on the progress of the working group, the workshop will either focus again on tensor contraction or possibly expand to other aspects of tensor computations, such as decompositions.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Diversity was from the outset a key for a successful workshop. We were able to gather key players from both users, developers and vendors, from major European countries, but also the US and Canada. Both junior and senior scientists were present. The selection of speakers for the overview talks was based on who, independent of career stage, would provide best incentive for the discussions that were at the core of the workshop. Specific instructions were given about this. A difficult point, however, is gender balance. Females are poorly represented in this domain, and, much to our dismay and despite our best efforts, including trying to find childcare solutions, we ended up with an all male workshop. CECAM may consider possible financial assistance for childcare. In the feedback survey after the workshop we have asked the participants to suggest female participants for future workshop.

## 7. Organiser list

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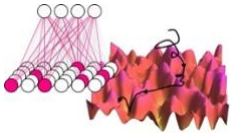

# From Machine-Learning theory to sriven complex systems and back

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/from-machine-learning-theory-to-driven-complex-systems-and-back-1287**
**Dates: May 22, 2024 - May 24, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This workshop focused on links between Machine Learning (ML) and Statistical Physics (SP). For many decades, there has been a strong commitment by researchers in SP to investigate ML problems with a slightly different perspective than computer scientists. This workshop's topics were chosen from this perspective, focusing on connections between driven complex systems, extensively studied by statistical physicists, and modern ML problems. The workshop therefore gathered invited experts respectively in the field of ML (E.Agliari, F.Cagnetta, C.Furtlehner, A.P.Muntoni), in stochastic dynamics and complex systems (M.Ruiz Garcia, A.Manacorda, F.Mignacco, Y.Roudi), or more focused on disordered systems (G.Catania, C.Lucibello, P.Urbani, F.Zamponi).
During the workshop we discussed 3 distinct topics: (i) stochastic dynamics: optimization, sampling and generative models; (ii) symmetry breaking and phase transition in learning dynamics and their statistical physics' description; (iii) ML models as disordered systems.
For (i), many discussions focused on the possibility of using ML methods to improve e.g. sampling and hard optimization problems. In particular, it was emphasized how ML techniques can be used to develop fast samplers to simulate complex systems, and how their performance should be evaluated compared to standard methods. We had a structured discussion on this topic on day 2 led by Martin Weigel.
At the intersection of (i) and (ii), many experts discussed the relevance of the concept of phase transition in generative neural networks, which is associated with symmetry breaking as a modus operandi to describe the hierarchical structure of datasets, and how learning dynamics are influenced or driven by such phenomena. The connection between these physics phenomena underlying ML will allow us to better understand how models are shaped and constrained by the presence of these transitions.
Finally, in the context of (iii), it was shown that recent advances in driven complex systems and disordered systems are relevant to ML. In the application part, we have seen that concepts of temperature and jamming are very useful to understand and study ML models, while the classical replica approach allows understanding fundamental properties such as the critical capacity or the ML

behavior from a static point of view. A structured discussion on this topic was organized on day 1, led by Hajime Yoshino.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

As for the results of this workshop, we believe that bringing together different experts, all working on different aspects of machine learning and statistical physics, shows the diversity of approaches to solving some problems related to ML.
For example, various experts have shown us that the study of ML models that started in the 1980s is still of great importance. They have managed to produce highly non-trivial analyzes of neural network models (modified Hopfield models with exponentially increased capacity, feed-forward networks with hidden layers, restricted Boltzmann machines) that shed light on our understanding of the learning mechanism on the one hand and the phenomenon of memorization on the other. These studies are also related to the phenomenon of symmetry breaking, which is being rediscovered in generative modeling, and on which we had several talks during these three days. In particular, it was shown that these phenomena occur in diffusion models and in the learning of energy-based models. These two approaches are in a way complementary, as symmetry breaking is related to the phase transition, so participants on both sides had the opportunity to exchange their points of view on this topic.
Another topic that was discussed is the fact that learning some models relies heavily on sampling processes, which can be particularly challenging in the presence of a possible second-order phase transition. In this context, the community now faces the theoretical problem of working with real data sets. In the usual approaches, the artificial data sets typically used are too simple. While the recent approach of hidden manifolds, which was also discussed during these three days, is a first step in this direction, we still lack a theoretical framework from which we could connect the statistical properties of the model with the statistical properties of the data.

## 3. What was the take-home message for the participants?

1) Concepts and techniques developed for driven complex/disordered systems have the concrete potential to extend our understanding and improve ML approaches, on both the static theoretical behavior and learning dynamics.
2) While ML for traditional problems such as sampling and optimization provides a set of new customizable tools, very hard paradigmatic problems remain and are not “solved” by ML approaches.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The topics discussed in this workshop are not directly relevant to the aspect of “social benefit". The outcome that we believe is closest to social utility is that it is important not to forget the fundamental aspect of research aimed at understanding the efficiency/capacity and pitfalls of modern techniques (such as ML) in order to make better use of them - better in terms of understanding their mechanisms, their limitations and ultimately improving their training algorithms and their reliability, thus enabling the use of more frugal and less computationally intensive models, a challenge that ML should better address sooner rather than later.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

This workshop will certainly contribute to the development of a new collaboration between some of the participants. We have observed intense scientific discussions during these three days, be it during the day (coffee breaks, lunches, discussion sessions, poster session) or during more mundane events (dinner). This was confirmed by the statistics of the survey among the participants.
As most of the works presented had already been published, we decided not to push for a conference proceedings. However, with the consent of the speakers, ⅔ of the recordings and half of the slides are publicly available on the CECAM website of the workshop.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We prioritized diversity, especially gender balance, with 3/4 women in our team. Despite this, we only received ~8 applications from women. After a thorough review, we accepted those that fit the theme of the workshop. In the end, ~11 of the ~45 participants were female, including the organizers, and 1/4 of the invited speakers were women (one female speaker could not attend and had to be replaced).
With participants from ~12 countries, including Japan and the US, we ensured diversity in terms of career stages, and institutions. We received ~25 applications from Italians, reflecting the strong Italian SP school and skewing the nationality of the final group.
Two concurrent events at ICTP Trieste and Bocconi University, announced after the CECAM dates were confirmed, may have impacted our applicant pool, particularly women who are underrepresented in ML.

## 7. Participant list

### Organisers

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# COST/ZCAM School on new computational methods for attosecond molecular processes

**Location: CECAM-ES (Zaragoza)**
**Webpage : https://www.cecam.org/workshop-details/costzcam-school-on-new-computational-methods-for-attosecond-molecular-processes-1338**
**Dates: May 27, 2024 - May 31, 2024**

## 1. What were the major topics presented in the School?

The school was motivated by the recently born field of Attosecond Chemistry, which aims to study dynamical processes occurring in the attosecond time scale, the natural time scale for electronic motion in atoms and molecules, using attosecond light pulses. The complexity of these experiments requires a theoretical support to provide an interpretation of the experimental results and to design new experimental approaches. For this reason, new theoretical methods and computational tools have been developed during the last decade.
The aim of the school was to provide a comprehensive training on these new computational tools, which describe the electron and nuclear dynamics upon interaction with attosecond pulses or strong IR fields, resulting in highly relevant phenomena such as photoionization or high-order harmonic generation. The lectures included state-of-the-art ab-initio and hybrid time-dependent approaches, as well as more advanced methods that can cope with the electronic continuum of molecules, with emphasis on strong-field and weak-field ionization and on methods that properly account for electron correlation in the ionization continuum
The school format was 5 days, each one focused in a different topic, and starting with the most basic concepts with an increasing complexity level along the week. The specific topics of each day are listed below.
1st day: Overview of strong-field and attosecond physics with a tutorial on analytical models for ionization and high-harmonic generation. Hands-on: calculation of high harmonic spectra and photoelectron spectra resulting from the interaction of strong IR fields with simple systems by solving the TDSE for one electron.
2nd day: Merging quantum chemistry approaches with scattering theory methods for strong field ionization of molecules: electronic structure calculations in the ionization continuum. Hands-on: computational packages for strong-field ionization of molecules with correlated electrons, including MO-ADK, TD-RIS and ECS-MP2.
3rd day: Numerical and theoretical challenges associated to the description of strongly driven electrons in the continuum, with the introduction of ir-ECS and t-

SURFF methods. Hands-on: Calculations of ionization rates from simple and medium size molecules with the t-SURFF software.
4th day: State-of-the-art methodologies to access attosecond molecular processes driven by attosecond pulses, with emphasis in the hybrid Gaussian/B-spline multi-reference CI method XCHEM. Hands-on: Calculations of photoelectron spectra from simple molecules in the region of Feshbach resonances by using the XCHEM computational package.
5th day: Extension of the concepts introduced in the 4th day with emphasis on the UK-Rmol+ methodology (based on R-matrix) for the description of molecular ionization and pump-probe spectroscopy. Hands-on: Calculations of photoelectron spectra in medium-size molecules with the UK-Rmol+ package.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

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- One of the main open questions raised by the participants during the lectures was the scalability of the mentioned computational methods towards larger molecules. Some of the tools (e.g. the XCHEM and the UK-Rmol+ packages) are highly accurate in their description of molecular ionization and thus very computationally expensive. Therefore, some of the participants were interested in knowing until what extent such tools could be used to study their own molecules of interest.

- During the lectures, the speakers also pointed out the main challenges in the development of computational tools to describe the phenomena of interest (namely molecular ionization or high-order harmonic generation), such as the deficiencies of the single active electron picture, the different levels of accuracy in the description of the electron correlation, the boundary conditions, the difficulties in developing analytical models, the selection of the basis sets and discretization methods, the description of nuclear dynamics, the description of resonances, etc. They also pointed out what advantages and disadvantages of the different approaches are, depending on different parameters such as the interaction regime (e.g. perturbative vs non-perturbative).

- The speakers also mentioned some of the open questions regarding the most recent advances in the field, such as the existence of a third path in RABBITT experiments.

- An important constraint of the theoretical study of attosecond chemistry is the necessity of large computational resources. This aspect was experienced by the participants during the hands-on sessions, where they used their laptops to connect to individual virtual machines where the required software was previously installed and where they could directly perform the designed numerical simulations. One of the practical limitations encountered during the hands-on of the first 2 days was the slow performance of the virtual machines when all of them

were used at the same time. This obstacle was circumvented by organizing the participants in pairs, so only half of the virtual machines where used.

### 3. What was the take-home message for the participants?

The school provided an overview of the formalisms, mathematical expressions and a description of the most relevant computational tools used in attosecond chemistry nowadays. Thus, the participants learnt how to distinguish which are the best approaches and computational packages for the description of each specific phenomenon, within a variety of accuracy levels. They also received a practical training on how to access and employ these tools.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- Lecture material: most of the lectures provided the slides of their lecture presentations, which were sent to the participants via email.

- Lecture notes: the participants continuously wrote down notes of the morning lectures. These lectures mostly consisted of slide presentations, but also included mathematical derivations on the physical whiteboards, which incentivized their active participation.

- XCHEM Software: Participants were provided access to the AMOS Gateway platform where the XCHEM software (4$^{th}$ day) is installed and where it is possible to directly run computational simulations in situ. Thus, they can perform calculations on their own after the school. This platform also provides access to other computational chemistry packages, such as OpenMolcas or t-Surff (described on the 3$^{rd}$ day). They retained access to the platform after the school.

- R-matrix software: Participants were provided access to a Canvas, an online platform where they accessed the R-matrix tutorial (5$^{th}$ day). They retained access to the course after the school. The participants were also informed that the UK-Rmol+ software is publicly available in the Zenodo platform.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The school was co-founded by the Next COST Action (CA22148) which covered the expenses of the speakers from different countries and career stages. COST

also reimbursed the expenses of 6 participants, following a gender and geographically balanced selection: 4 female and 2 male from diverse countries.
The school was announced through worldwide-popular email distribution lists to ensure that the information was accessible from any geographical region and diverse researcher profiles. In the announcements, we mentioned that it was aimed to both PhD students or postdoctoral researchers (we had 75 % PhD students, 21 % postdocs, 4% professors) and in the initial program, 30% of the speakers were females (33% of the participants were presumably females).
The school was carried out in a wheelchair-accessible building. The combination of the tangible material, oral lectures and practical training made the content of the school accessible for diverse learning preferences.

## 6. Participant list

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### Organisers

**Martin, Fernando**
Universidad Autonoma de Madrid, Spain
**Rego, Laura**
ICMM - CSIC, Spain
**Svetina, Cristian**
IMDEA Nanociencia, Spain
**Vozzi, Caterina**
Consiglio Nazionale Delle Ricerche, Italy

**Baeck, Kyoung Koo** - National Gangneung-Wonju University, Republic of Korea
**Broad, Mitchell** - Imperial College London, United Kingdom
**Brown, Graham** - Max Born Institute, Germany
**Buczolich, Katharina** - TU Vienna, Austria
**Carlström, Stefanos** - Lund University, Sweden
**Christou, Elena Aethra** - Max Born Institute (MBI), Germany
**Crhán, Martin** - Charles University, Czech Republic
**Dinvay, Evgueni** - UiT, Norway
**Dvorak, Jan** - Lawrence Berkeley National Laboratory, United States
**Eric, Vesna** - Max Planck Institute for Polymer Research, Germany
**Faria, Felipe** - University of Central Florida, United States
**Flores, Philip Caesar** - Max Born Institute, Germany
**González Vázquez, Jesús** - Universidad Autónoma de Madrid, Spain
**Gorfinkiel, Jimena** - Open University, United Kingdom
**Heilemann, Rico** - MBI for NOSPS, Germany
**Jena, Nityasagar** - IFM, Linköping University, Sweden
**Lafiosca, Piero** - Scuola Normale Superiore, Italy
**Lewis, Nicholas** - University of Central Florida, United States
**Maier, Pablo** - Max-Born-Institute, Germany
**Masin, Zdenek** - Charles University, Czech Republic

**Mazza, Francesco** - Scuola Normale Superiore, Italy
**Mirahmadi, Marjan** - Max-Born-Institut (MBI) Berlin, Germany
**Mohammed, Lablali** - University Hassan II of Casablanca,, Morocco
**Morales Moreno, Felipe** - Max Born Institute (Berlin), Germany
**Oakley, Séraphine** - King's College London, United Kingdom
**Patchkovskii, Serguei** - Max-Born Institute, Germany
**Roos, Aycke** - Max-Born-Institut, Germany
**Schrader, Simon** - University of Oslo, Norway
**Scrinzi, Armin** - Technical University of Vienna, Vienna, Austria, Germany
**Sepali, Chiara** - Scuola Normale Superiore, Italy
**Tahouri, Rezvan** - Lund University, Sweden
**Terentjevas, Justas** - Max-Born Institute, Germany
**Tomaselli, Anna** - King's College London, United Kingdom
**Trinari, Marco** - Scuola Normale Superiore, Italy

# YRM 2024 – 20th ETSF young researchers' meeting 2024

**Location: CECAM-FR-GSO (managing node), CECAM-FR-RA.**
**Webpage : https://www.cecam.org/workshop-details/yrm-2024-20th-etsf-young-researchers-meeting-2024-1308**
**Dates: May 27, 2024 - May 31, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The discussed topics pertain to the research lines of the groups of the European Theoretical Spectroscopy Facility (ETSF), falling in the broad field of theoretical spectroscopy. Reflecting the research breadth of ETSF network, and along the lines of previous editions, the scientific topics covered in YRM2024 were diversified and arranged in five different thematic sessions of oral presentations: (1) Advanced electronic structure methods development, (2) Optical properties of materials, (3) Vibrational properties of materials and transport, (4) Strongly correlated systems and magnetism, and (5) Machine learning in materials science. Additionally, there was a specific session with a scientist from industry sharing their experience on the possibilities outside academia and how such career opportunities can be pursued. A poster session was also present selecting representatives abstracts.
On the one hand, novel results on new challenging systems (molecular, solids or hybrids) with increasing precision have been presented, as well as the description of new phenomena (optical, vibrational, magnetism...). On the other hand, new theoretical and computational methodologies or approaches relevant for the problems of interest were presented. All the invited presentations, especially of the invited speakers as experts in the field, were done with an accessible and interdisciplinary approach to ensure to reach the broader audience. Overall, the conference showed an interesting overview of recent developments in the field of theoretical spectroscopy.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The primary and most broad outcome for the attendants, namely researchers at the beginning of their career, was the successful participation in a conference that provided an overview of the research directions in the field, from the point of view of students and researchers that are directly working on them. Stimulated by the

informal setting, all attendants interacted in a friendly and constructive manner, discussing and extending their network among peers.
Overall, the sessions provided a broad overview of the progress in the field of theoretical spectroscopy. In particular, on the one hand, new methodological approaches in the field of materials and molecular sciences have been presented (theoretical models, computational methods, application of artificial intelligence), along with new developments of the state-of-the-art existing ones. On the other hand, spectroscopic properties (optical, vibrational,..) computed on novel systems of interest (solid, molecules, hybrid) have been presented.
As the experimental research on the field progresses, as well as the accuracy of descriptive models increases, once again it was confirmed that the main limitation is still represented by the computational feasibility. Therefore, open questions remain on how to achieve simulations of systems increasingly challenging in terms of dimension and complexity, for more and more accurate interpretation of experimental results.

## 3. What was the take-home message for the participants?

A transversal aspect evident from all sessions was the inherent interdisciplinary nature of the field. Hence different technical approaches and expertises are necessary to achieve good results and, consequently, an important message is that collaboration and ideas exchange among peers is particularly beneficial. The success of this conference modality suggests that it can be productively encouraged from the beginning of the scientific career.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The themes of the workshop were centered on theoretical chemistry and physics, with particular orientation on academic basic research. Many of the discussed topics concerned the discovery of new materials or phenomena that can have benefits for society and are timely. In particular, new materials were presented, along with the development of new models to interpret and engineer properties of interest. Systems with improved optical properties were discussed, with applications to energy conversions (eg. photonics) or to the improvement of solar cells (e.g. organic molecules, perovskites). Additionally new developments in the investigation of phenomena such as conductivity (thermal and electrical) and superconductivity have been presented. Finally, a specific session of this year's edition of the conference was specifically devoted to developments of artificial intelligence applied to materials science.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop organization did not actively plan specific tangible outcomes. However, the lively discussion, encouraged by the informal atmosphere, is going to be beneficial for new collaborations and ideas exchange. When designing the workshop organization, an effort was made in order to ensure the creation of an informal yet productive environment, since it is particularly important, for young people at an early career stage, to create or expand their network in order to increase future career possibilities.
As an additional important outcome, the good success of this conference will probably encourage the organization of the next editions by confirming the interest in this conference format for the people in the field.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity and diversification were promoted through a careful selection of organizers and speakers, with particular attention to the scientific background, gender and geographical provenance. Overall, the attendance numbers of the event show a good result. Scientifically, attendants had different backgrounds (chemistry, physics, material sciences) and worked on different disciplines (computational physics/chemistry, methods development, theoretical modeling). Particular attention was paid to the gender balancing of the invited speakers (50% women) with an overall 35% of participating women. The provenance of attendants institutions was differentiated (12 European countries) with different affiliations (universities, research centers, industry). Within the audience target (non-established scientists), there were mainly PhD students, whose presence we supported by making the participation to the conference free. Also postdocs and master students were present.

## 7. Participant list

### Organisers

**Ammar, Abdallah**
LCPQ, CNRS, France
**Biancorosso, Leonardo**
University of Trieste, Italy
**Canola, Sofia**
Institute of Physics of the Czech Academy of Sciences, Czech Republic
**Saravanabavan, Karthikeyan**
CEA, France

**Castellano, Aloïs** - Université de Liège, Belgium
**Filip, Maria Andreea** - Max Planck Institute for Solid State Research, Germany
**Giarrusso, Sara** - Université Paul Sabatier, Toulouse France, France
**Janke, Svenja** - University of Warwick, United Kingdom
**Levi, Gianluca** - University of Iceland, Iceland
**Mejuto Zaera, Carlos** - SISSA, Italy
**Nys, Jannes** - EPFL, Switzerland
**Urquiza, Laura** - Università degli Studi di Milano, Italy
**Vanzan, Mirko** - University of Milan, Italy

# Les Houches-Telluride workshop on protein dynamics

**Location: CECAM-FR-RA**
**Webpage : https://www.cecam.org/workshop-details/les-houches-telluride-workshop-on-protein-dynamics-1299**
**Dates: Jun 2, 2024 - Jun 7, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The motions of proteins and other biological macromolecules are intricate and important because they are often closely linked to the biological function. However, the detailed investigation of biomolecular dynamics is a formidable challenge, because it requires methods that have a very high resolution in both space (ideally atomic) and time (ideally picoseconds or even faster). Consequently, despite impressive progress during the last years, there is no single individual experimental method that can simultaneously fulfil all these requirements. Instead, the most promising approach is the synergistic combination of experimental methods with computational approaches, in particular, molecular dynamics (MD) simulations. On the computational side, steady progress of both hardware and software, coupled with the development of effective coarse-grained potentials, now enable to tackle large systems, such as multicomponent biomolecular condensates, on long time scales (microseconds and beyond). This bridges the spatial and temporal gap between computations and experiments, enabling the use of simulations as computational microscopes for detailed, molecular-level interpretations of experimental data. The ongoing advancements also bring up new challenges, which need to be overcome for a most fruitful combination of experiments and computations. One challenge concerns simulation of molecular dynamics on slow time scales (micro- to milliseconds), which are often required to observe the relevant conformational changes, or the spatial (re-)organization of the components of large biomolecular objects such as dense biocondensates. Next to enhanced sampling methods and hardware, also innovative machine-learning approaches emerge. Another active area is the development and validation of computationally effective, yet predictively accurate, coarse-grained force fields, which need to be carefully validated against experiment. At the workshop, these aspects were discussed by an interdisciplinary group of scientists, both experientialists and theoreticians. Major topics discussed, as reflected in the session titles, were order and disorder, membrane protein dynamics, light-induced dynamics, protein dynamics from NMR and from single-molecule techniques, allostery, protein dynamics and artificial intelligence, protein hydration water dynamics, as well as dynamics of photoactive proteins and in crystals. Thereby, the integrated workshop sessions encompassed both experimental and computational approaches and covered biomolecular dynamics across a broad

range of time- and length scales. A contribution to advancing the field was also the very close and fruitful interchange between the scientists, across different experience levels, resolving any boundaries and fostering a common language between experimentalists and theoreticians.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

One of the primary outcomes of the workshop was to make participants aware of the current state-of-the-art, challenges, and frontiers in the field of protein dynamics, and to provide a platform for starting new collaborations. (One participant even explicitly mentioned in his feedback email that he started a new collaboration, and another group of principal investigators decided to write a review on the topic, and agreed on the plan with an editor present at the workshop.) During the workshop, biomolecular dynamics specialists exchanged on the latest advances in the field, covering a wide spectrum of disciplines between biology, (bio-)chemistry, (bio-)physics, and biomolecular simulation. This multi-disciplinarity is a hallmark of this workshop, but it also involves the challenge of "speaking the same language". Therefore, all invited speakers were asked to spend the first 15 min of their 45 min lectures on a pedagogical presentation of their research techniques and methods, followed by a presentation of their latest research results. The discussion after each presentation was an important part of the workshop. In addition to the 24 invited speakers and 8 selected contributed talks (by PhD students and postdocs), 30 participants (PhD students, postdocs, researchers) presented a poster and gave a 2-minute flash presentation. All participants very actively contributed to the discussions, both in the 15 min discussion slots directly after the talks, but also during the poster sessions and the entire workshop. A prize sponsored by the Federation of European Biochemical Societies (FEBS) was awarded to the best poster, and the best flash presentation was also awarded a prize. The flash talks by the poster presenters were very well received by the participants, as is also reflected in the very good evaluation in the feedback form (61% very good (N=27), 21% good (N=9)).
Concerning limitations and open questions, the main points of the discussions evolved around three major topics. First, how can the accuracy and predictive capacity of the current energy functions ("force fields") used in the biomolecular simulation field be advanced to further increase the predictive power of the simulations, especially also at the coarse-grained level? Second, how can the time- and length-scales accessible to the simulations be increased, and, at the same time, the spatiotemporal resolution of the experiments be further improved, so that the overlap of experiments and simulations is enhanced? Third, how can machine-learning based methods be best used and integrated into protein dynamics research (in both experiments and in simulations)? We explicitly encouraged discussions, at least 15 min after each talk, and provided time for discussions during evenings and an excursion (half a day).

## 3. What was the take-home message for the participants?

Studying protein dynamics is more relevant than ever, especially since AI solved part of the structure prediction problem. It has also become clear that addressing protein dynamics is best achieved when combining several methods. In this respect, many participants gave positive feedback about the fact that they were exposed to such a wide range of topics, including a pedagogical introduction and the latest state of the field.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

At the science level, it is clear that studying protein dynamics is important for drug design, as explicitly discussed, e.g., in the invited talks of Dorothee Kern (U Brandeis) and Birthe Kragelund (U Copenhagen), and on several posters, e.g., by Galyna Volynets et al. from the NAS of Ukraine, Kyiv.
At the social and science education levels, the multi-disciplinary and multi-cultural nature of the workshop and the open-minded and constructive atmosphere have, in our view, a great potential to benefit society because that fosters the development and education of a new generation of future scientists. This was also one of the major results of the feedback form, selected parts of which are quoted in the following:
- "As a student, I was so stimulated the entire time that the 12-hour days of science felt wonderful."
- "The free time allows for fruitful discussion amongst people."
- "I want to send my most sincere thanks to the organizers for putting together an excellent scientific program and providing a wonderful forum for senior scientists and the next generation of scientists to mingle and exchange ideas and socialize in an amazing setting. It was really great. As I expressed to some of the organizers, it was one of the very best workshops I have attended in three decades."
- "The workshop was great! Friendly atmosphere and diverse experiences were very helpful."
- "This is one of my favorite meetings. The choice of topics and quality of speakers was just great, not to speak of the friendly atmosphere."

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

In addition to considering the participants themselves as a tangible outcome, we heard about several plans for new collaborations, and one invited speaker (Tom Perkins, U Colorado) explicitly mentioned a new collaboration in a feedback email

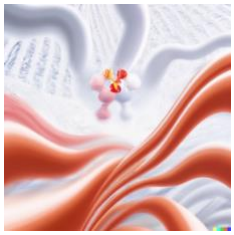
to the Organisers. As mentioned above, a group of PIs decided to write a broadly accessible review article on integrated studies of protein dynamics.
We are positive that these developments will eventually provide interesting and valuable scientific results, which might eventually then also lead to publications and joint proposals.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

In the selection process (invited speakers, other participants), inclusivity concerning gender, geographical location, career stage, etc, was carefully considered. Out of the total of 32 talks, 10 were given by women (31%) and 22 by men (69%). Out of the 30 posters, 13 (43%) were presented by women and 17 by men (57%). Concerning career stage, the participants were a mix of experienced and established researchers (mostly the invited speakers) and ECRs. Out of the total of 62 participants, 24 were invited speakers (at the professor or equivalent level). Among the 38 other participants, there were 19 PhD students, 16 postdocs or experienced researchers (e.g., staff scientists), and 3 professors. Geographical provenance (judged by home institute): Germany (12), USA (12), France (11), Switzerland (8), Austria (5), Denmark (4), United Kingdom (2), Canada (2), Italy (1), Spain (1), Czech Rep. (1), Netherlands (1), Israel (1), and Ukraine (1).

## 7. Organizers list

**Bordignon, Enrica**
Université de Genève, Switzerland
**Schäfer, Lars**
Ruhr University Bochum, Germany
**Schanda, Paul**
IST Austria, Austria
**Schuler, Benjamin**
University of Zurich, Switzerland
**Weik, Martin**
Institut de Biologie Structurale, Grenoble, France, France
**Yano, Junko**
Lawrence Berkeley Laboratories, United States



# Polymer physics in cellular organization and function

**Location: CECAM-ES**
**Webpage : https://www.cecam.org/workshop-details/polymer-physics-in-cellular-organization-and-function-1341**
**Dates: Jun 3, 2024 - Jun 5, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop has addressed open challenges in the use of polymer physics concepts and tools for biologically relevant systems. Specifically, we have focused in two main areas:

**Chromatin Organization:** The availability of experimental data on contact maps, 3D distances, phase separated nuclear condensates and TAD organization of chromatin have given us key insights into the three-dimensional structure of chromatin. These organizing structures, which are heterogeneous across cells and dynamic and short lived in time, have key implications for transcriptional regulation. There are two approaches to exploit polymer physics to understand chromatin. One set examines the nature of intra-chromosomal interactions that can generate experimentally observed contact probabilities and 3D distances.

The second set consists of the effects of loop extrusion, intra-chromatin interactions and their interplay, resulting in the experimentally observed 3D organization.

Current challenges include the development of models and theories that account for the rich structure, heterogeneity of the multiscale organization of chromosomes.

**Biomolecular condensates and liquid/liquid phase separation:**

Biomolecular condensation processes are recognized as a fundamental mechanism that living cells use to organize and control biomolecules in time and space. Biomolecular condensates appear in numerous locations in cells where they carry out many biochemical functions. They modulate enzymatic activity, modulate buffer protein concentration, reduce noise in gene expression, and regulate cell migration.

The mechanical properties of these aggregates, usually composed by intrinsically disordered proteins, are also critical to determine their biological function. Although many biomolecular condensates are fluid, they do not behave as simple liquids.

It has been conjectured that reversible phase separation is indicative of cellular health while irreversible rigidification of biomolecular condensates marks a cell's transition into disease states. The mechanistic understanding of how the molecular architecture of intrinsically disordered proteins controls their structure and mechanical properties remains a challenge.
We have advanced the state of the art by bringing together biologists and polymer scientists into a workshop and discussed the above topics. A leer idea about current polymer physics based models to address the relevant biological questions has emerged
from the discussions.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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chromatin structure and function.
how is chromatin organized.
Biologists presenting organization and structure. Presentations form physics how to model chromosome and relationship with experimental info (HiC, Fish).
Limitations of the models: what they should include.
Models from atomistic to CG: nucleosome level. discuss chromosome structure from atomistic resolution to global organization at the scale of the condensed chromosomes. Interface chromatin.
Also the structure of condensed chromatin in mitosis.
Polymer physics on liquid-liquid phase separation, and how to model them. The role of heterogeneity, polydispersity in polymer aggregates.
Role of electrostatics and dipolar interactions in heteropolymers. pH regulation.
Nonequilibrium transport and response of protein aggregates (role pf PhD gradients) new means to control polymer aggregates. Liquid/solid transitions of polymer aggregates.
Heterogeneity induced by complex solvents (e.g. solvent and co-solvent).
Address the role of topology on the structural and dynamical properties of polymer suspensions. Relevance of topology for bacterial DNA (ring polymers under confinement).
Topic on CG: techniques for CG to ensure they capture relevant biological information (Tamar, Rosana, Ranjith). New approaches to quantitative CG and how to benchmark models.
How mechanical forces affect chromatin structure (Marco, Shiva).
A lot of emphasis on chromosome as the most relevant nuclear polymer structure.
Relevance of non-coding regions of chromatin (they can transcribe as well) Role of nuclear RNA as crowders.
Need to look at polymer properties in presence of crowders: importance of nuclear environment in chromosome structure and function.
There were a number of high quality experimental talks: Possibility use of complementary experimental techniques to covers the broad range of length

scales relevant for chromosome structure in the polymer. Assessing relevant time scales.
Signaling and function of chromosome (expression) relevance of memory and how information is stored.
Shiva: mechanical properties of chromosome and nuclear envelopes. Emerging structures: dynamics.

### 3. What was the take-home message for the participants?

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Challenges to develop chromatin and nucleic acids CG models that capture relevant biological information
Protein condensates as structured liquids: needs to understand structure properly. Their mechanical response (viscoelastic, gels). Phase transitions
Need to develop multiscale models that cover relevant time scales and that can cover ability of experiments to combine techniques that cover from molecular to chromatin scale
Role of physicochemical aspects that affect the structure and dynamics of the physics of heteropolymers and proteins and their impact in biological function

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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The workshop has highlighted the relevance of the structure and mechanical properties of chromatin in the biological processes inside the cell.
This is a fundamental understanding that will open new venues to tackle diseases.
Examples of diseases associated to the malfunction of chromatin, e.g. genetic diseases
such as Hutchinson and progeria.
The ability to manipulate and control protein aggregates can also offer biotechnological venues to identify and control diseases.
The workshop mentioned examples of disease associated to protein aggregation and their transition from a liquid like (where they are functional) to solid or gel like structures.
amyloid diseases
The understanding between the physical behavior of these aggregates and their biological implications remains an open challenge

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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The workshop brought together participants with a diverse background. There was frank and open exchange between biologists, physicists and chemists.

The biologists were very receptive to the potential that polymer physics can bring to understand cellular processes. The advance sin quantitative biology offers a possibility in polymer physics to work closely to the regimes and conditions that are biologically relevant.
Therefore, the workshop was a fruitful playground to establish new connections among disciplines and research groups and their open clear possibilities for new collaborations.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We have taken care of diversity during all the stages of the workshop preparation and deployment.
We have ensured attendance of participants from different parts of Europe, USA, India and China. We have ensured a reasonable number of contributions from women, and have accepted all requests to attend coming from women.
We have also been sensitive to inclusivity in a broader sense. We are glad to see a good number of participants from Aian countries.
Also, we have ensured a good representation of early stage researchers and make them active participants by giving them the possibility to present their work.
We have also allowed remote presentations by two people who were not able to attend in person. One of them mentioned explicitly her restrictions to travel due to their maternity duties, and she expressed her gratitude to be able to attend remotely during this period in which travelling is challenging for her.

## 7. Participant list

### Organisers

**Antoli, Beatriz**
University of Zaragoza, Spain
**Kumar P B, Sunil**
IIT, Madras, India
**Pagonabarraga, Ignacio**
University of Barcelona, Spain

**Ahmadian Dehaghani, Zahra** - Sissa, Trieste, Italy, Italy
**Chan, Brian** - Duke University, United States
**Chatterji, Apratim** - IIISER-Pune, Pune, India-411008, India
**Chauhan, Akshay** - Indian Institute of Science Education and Research-Pune, India
**Chervanyov, Alexander** - University of Münster, Germany
**Collepardo, Rosana** - University of Cambridge, United Kingdom
**Conforto, Filippo** - University of Edinburgh, United Kingdom
**Dahirel, Vincent** - Sorbonne Université, France

**Das, Rakesh** – MPI for the Physics of Complex Systems, Germany
**De Corato, Marco** - Universidad de Zaragoza, Spain
**Di Stefano, Marco** - Université de Montpellier, , France
**Falo, Fernando** - University of Zaragoza, Spain
**Forte, Giada** - University of Edinburgh, United Kingdom
**Franzese, Giancarlo** - Universitat de Barcelona, Spain
**Girard, Martin** - Max-Planck-Institut für Polymerforschung, Germany
**Gomez-Benito, Maria Jose** - University of Zaragoza, Spain
**Guha, Sougata** - INFN Napoli, Italy
**Ipsen, John** - University of Southern Denmark, Denmark
**Joyeux, Marc** - CNRS & Université Grenoble Alpes, France
**Knowles, Tuomas** - University of Cambridge, United Kingdom
**Kremer, Kurt** - Max Planck Institute for Polymer Research, Germany
**Kumar, Amit** - Weizmann Institute of Science, Israel
**Likos, Christos** - University of Vienna, Austria
**Marcato, Davide** - SISSA, Italy
**Marenduzzo, Davide** - University of Edinburgh, United Kingdom
**Micheletti, Cristian** - SISSA, Italy
**Mitra, Mithun Kumar** - Indian Institute of Technology (IIT) Bombay, India
**Mohanta, Dibyajyoti** - Lund University, Sweden
**Muthukumar, Murugappan** - University of Massachusetts, United States
**Notani, Dimple** - National Centre for Biological Sciences, India
**Padinhateeri, Ranjith** - Indian Institute of Technology Bombay, India
**Rajput, Satyendra** - Indian Institute of Technology Delhi, India
**Rivas Barbosa, Rodrigo** - Sapienza University of Rome, Italy
**Rubinstein, Michael** - Duke University, United States
**Sáinz-Agost, Alejandro** - University of Zaragoza, Spain
**Schlick, Tamar** - New York University, United States
**Shen, Xiaohua** - Tsinghua University, China
**Shillcock, Julian** - EPFL, Switzerland
**Shivashankar, G. V.** - ETH Zurich and Paul Scherrer Institute, Switzerland
**Smrek, Jan** - University of Vienna, Austria
**Thirumalai, Dave Thirumalai** - The University of Texas at Austin, United States
**Tubiana, Luca** - University of Trento, Italy
**Valei, Zahra** - The University of Edinburgh, United Kingdom
**Van Der Hoek, Pieter** - SISSA, Italy
**Zidovska, Alexandra** - New York University, United States


# Defects in solids for quantum technologies

**Location: Budapest, Hungary**
**Webpage : https://www.cecam.org/workshop-details/defects-in-solids-for-quantum-technologies-1279**
**Dates: Jun 10, 2024 - Jun 14, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Quantum devices of the next generation are expected to actively create, manipulate and read out quantum states of matter. This may revolutionize information and communication technology, and also has great potential for life-science and medical applications. Considerable effort has been spent to develop a basic unit of quantum information processing (or qubit) from different individual quantum systems, such as single atoms or ions trapped in a crystal lattice, single Josephson superconducting devices, single photons emitted from quantum dots or single photons/spins associated with point defects in semiconductors. However, most of these systems can only operate at cryogenic temperatures or in ultra-high vacuum. Quantum states due to point defect in solids may realize single photon sources and quantum bits that can be harnessed in quantum information processing and nanoscale sensor applications at room temperature.
First principles theoretical simulations have been demonstrated as an essential tool in understanding the underlying physics of these atomic scale systems as well as in identification of potential new quantum bits and single photon emitters in semiconductors. Therefore, tight collaboration of experimental research and atomistic simulations is essential for a rapid progress in the field. We organized the workshop to discuss the recent advances in the development and application of theory in exploring and characterization of novel defect qubits and the progress in experiments.
The workshop program included scientific sessions “Theory for scaling up: searching and characterization”, “Theory: screening and excited states”, “Color center in 2D materials”, “Diamond NV: novel control schemes”, “Silicon carbide qubits”, “Diamond NV center: electrical control”, “Diamond NV center for quantum sensing”, “Theory of excited states in periodic models”, “Color centers in silicon”, “Diamond NV center: quantum simulation and sensing”, “Color centers in diamond”, “Search for qubits in 3D and 2D materials”, “Theory of 2D materials”, “Color centers in hexagonal boron nitride” as well as a “Discussion session” with Profs. Benedict Murdin and Steven Clowes from University of Surrey and Prof. Yuan Ping from University of Wisconsin-Madison. In experiments, they discussed the progress towards single defect engineering in solids with ion beams techniques (also sharing the knowledge from the RAISIN network in the UK to the audience) and the key theoretical questions of theoretical defect spectroscopy. There were two

poster sessions too with significant contributions, dominantly from young researchers. Two poster prizes were awarded by the Prize committee composed of Prof. Hannah Stern and Prof. Adam Gali. They were awarded to Theresa Pfau, a young female scientist from University of Copenhagen, and Pim Vree from University of Delft where both young scientists presented results on ground breaking quantum sensor concepts and demonstrations.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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Before discussion the scientific outcome, let us briefly summarize the statistics of DSQT2024 Flagship workshop. Including the organizers, 154 participants from 28 countries registered for the workshop from 5 continents. The participants showed up in person at the workshop site and attended the scientific talks except for one attendee with on-line participation and one attendee had to cancel the trip in the last minute because of illness. The final scientific program of the workshop lasted for five full days, included 18 invited talks, 41 contributing talks, and a poster session with 87 posters, and a Discussion session about single defect engineering with leading experimentalists and theorist.

DSQT2024 workshop succeeded to bring together world-leading theoreticians and experimentalists active in the field of quantum information processing based on solid state qubits. Our discussions improve interdisciplinary cooperation overcoming traditional boundaries between scientific disciplines. Invited speakers at DSQT2024 workshop represented electronic structure theory community, theory at phenomenological and atomic scale level, materials growth, defect engineering, surface chemistry, quantum optics and spin physics. Recognized leaders in the field, like Volker Blum (Duke University), Kristian Thygesen (Technical University of Denmark), Sivan Refaely-Abramson (Weizmann Institute of Science), Jörg Wrachtrup (Stuttgart University), Fedor Jelezko (Ulm University) and young researchers, like Hannah Stern (University of Manchester), Aparathija Singa (Max Planck Institute - Stuttgart), Anton Pershin (Wigner Research Centre for Physics) highlighted recent progress and discuss challenges and opportunities in their invited talks. Invited talks, contributed talks, posters, and the Discussion session stimulated the exchange of methodological expertise and new developments between scientists working on different aspects of the field, illuminate opportunities for optimizing the materials properties and device design aided by theory. Discussions during the breaks provided opportunity to form new interdisciplinary collaborations on solid state quantum bits for the mutual benefit of theoretical, experimental and applied researchers, especially following talks demonstrating the potential of this field in various interdisciplinary areas.

The attendees well agreed that the tight collaboration of theory and experiment can only advance the field. In the theory front, further development in the excited states calculations together with geometry optimization is a key issue: various attempts (time-dependent density functional theory, many-body perturbation methods and wavefunction techniques) have been presented but further progress

is required to implement methods with periodic boundary conditions tractable for hundreds of atoms in the model.
In summary, based on numerous feedbacks from the participants, we conclude that the DSQT2024 workshop goals are achieved.

## 3. What was the take-home message for the participants?

Many challenges in the field remain to be overcome such as accurate theoretical description of excited-state kinetics for spins and electrons, description of nonequilibrium doping processes such as ion implantation and annealing in experiments. Constant developments of theoretical and experimental spectroscopy are needed to explore novel quantum defects that may exist in 2D and 3D solids. However, strategies and proposals have been made and rapid progress can be foreseen in the future.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Quantum technology requires ultimate control of material to a single defect level in materials and to develop spectroscopy techniques and devices to be able to observe single atom species. The connection of quantum technology to present semiconductor industry is obvious: the bit – the basic unit of information – will have to be stored in atomic- and subatomic-scale systems, such as individual atoms, ions, electrons or photons, whose behavior is governed by the laws of quantum mechanics. Sensors on the atomic scale are also required for monitoring single molecules. The transition from conventional technologies to quantum technologies is therefore unavoidable. To develop a basic unit of quantum information processing based on point defects in semiconductors has huge potential for applications. Beside the well-known nitrogen-vacancy defect in diamond, other defects in various host materials such as silicon carbide, silicon, wide band gap oxides and hexagonal boron nitride and other two-dimensional materials were discussed. Among these materials single optically addressable spins were demonstrated, with long coherence time even at room temperature in some cases, embedded in a high-performance electronic material such as silicon carbide. Scientific and industrial developments in this direction may ultimately lead to the realization of quantum applications operating at elevated temperatures, which may eventually enable the widespread of quantum devices and influence our society in many respects. Furthermore, novel spectroscopy tools have been developed and presented at the conference which opens new avenue in the microwave field detection and control which has an impact in the telecommunication and defense industries.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Discussions amongst the attendees of the conferences highlighted the interest in not only continuing DSQT in its current form but also the idea of holding more specific workshops that focus on different topics within the area of 'defects for quantum technology'. One idea that was discussed is a meeting focused on defects in two-dimensional materials, or a meeting that would include the community of those working on molecular spins for quantum technology. This could include not only the traditional EPR community interested in inorganic high spin complexes, but also the organic molecular community where the photophysics of optically addressable spins resembles that of defects in wide bandgap solids. By combining the two fields (molecular spins and solid-state defects) we would hope to broaden the theoretical and experimental approach to studying these systems. Separately, grant proposals and collaborations were discussed by participants at the meeting forming European/UK consortia.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We found sponsors to finance the “Best poster award” that were given to a youth male scientist and a female scientist to maximize the inclusivity in both career stage and gender. We believe that we could indeed inspire the young generation of scientists by the award. Furthermore, contributed talks from early career stage scientists were given and we had a very positive feedback from these scientists in social media after the conference (e.g., LinkedIn posts). We had 5 female invited speakers to encourage youth female scientists of the audience in their career. Although, the workshop was planned exclusively in person but we offered to one female invited scientist to present her results on-line because of the difficulties to travel with her recently born baby. In the organization and local organization teams we have women and men with diverse cultural background to run the conference in order to secure an inclusive environment for people with any gender or geographical locations of various habits.

## 7. Participant list

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# Open databases integration for materials design

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/open-databases-integration-for-materials-design-1280**
**Dates: Jun 10, 2024 - Jun 14, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The OPTIMADE API provides a unified approach to query multiple materials databases that greatly benefits materials design and broader materials informatics. With the OPTIMADE API, researchers and scientists can use the same query syntax to access data from all participating databases, eliminating the need to learn and adapt to different interfaces for each database, as showcased at optimade.science. The OPTIMADE API streamlines the data retrieval process and facilitates cross-database searches, saving time and effort for materials researchers, and empowering them to access a wider range of materials data.
The OPTIMADE API follows the FAIR principles that are gaining prominence in the materials community, to enhance the discoverability, accessibility, interoperability, and reusability of materials data. FAIR enables researchers to easily find relevant data, access data in a standard manner, integrate data with other datasets, and reuse data for various purposes, fostering collaboration and advancing materials research.
It is crucial to involve and engage important players in the materials community to ensure the success and continued development of the OPTIMADE initiative. Collaboration with key stakeholders, such as developers from organizations like ColabFit and MPDD, is essential to encourage the implementation of the OPTIMADE API across different databases.
The community that is forming around this initiative is leading to advances beyond the direct benefits of the OPTIMADE API. Workshops and gatherings that bring together a diverse group of experts can facilitate these discussions, leveraging the collective expertise and influence of the participants to drive the adoption of standards in the broader materials community. For example, the community has been used as a platform for defining standards and developing an ontology for materials [Workshop on Ontologies for Materials-Databases Interoperability, Sweden. October 2021].
The materials community recognizes the value of the OPTIMADE API in facilitating materials design and promoting the FAIRification of materials data. Sustaining and expanding the OPTIMADE initiative by involving important stakeholders, fostering a common target, and leveraging the community's potential for standardization

efforts will not only enhance data access and interoperability but also drive advancements in materials research, development, and collaboration.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The first day of the workshop allowed participants to finalize and publish the 1.2 version of the OPTIMADE specification. A significant scientific output is the publication of the second paper on OPTIMADE on 24 June 2024. The paper details not only the 1.2 release developed during previous CECAM OPTIMADE workshops, but also updates on participating and new databases that support OPTIMADE, use cases to inspire future use, and upcoming features.
As usual the workshop included numerous discussions in subgroups followed by plenary sessions in which the different subgroups would report about their advances.
Additional properties were included in the OPTIMADE definition. This is a significant step forward as it allows researchers to access material properties to train machine learning models, which can in turn be used to develop and design materials. It was decided to categorize properties in name spaces according to the underlying physics, with groups of cheminfo, stability, electronic, magnetic, thermo, phonon, transport, optical, defect, mechanical, superconductivity, radiological, chemical, and acoustic. Further discussion focused on proposing the first tranche of properties that should be included, namely: density (3D), electron density of states at Fermi level, and work function, and that these should be in name spaces(s) and not the core. It was further agreed that if a database cannot return a property then they should be left null. The group also considered how a series of runs (likely DFT) intended for use to train a machine learning potential should best be curated. Following consultation with the trajectories working group it was agreed that they should all be stored within a trajectory if they have the same composition, and a collection for changing composition.
Continued ongoing work for making molecular dynamical trajectory data available over the OPTIMADE API. A prior prototype implementation had been developed in the past meetings but had limited features and lacked the capability to efficiently serve large amounts of data, or to filter subsets of the data (e.g., slices of a trajectory). In order to enable such features, several extensions to core features of OPTIMADE have been necessary to facilitate the sharing of (possibly) very large but still indexable information. The majority of the time in this subgroup was thus dedicated to defining and specifying a general protocol for a client to request, and for a server to deliver, parts of a large data object. The in-person discussion and access to invited participants with specialist knowledge about trajectory formats greatly facilitated progress in this area.

## 3. What was the take-home message for the participants?

The materials community recognizes the value of the OPTIMADE API in facilitating materials design and promoting the FAIRification of materials data. Sustaining and expanding the OPTIMADE initiative by involving important stakeholders and leveraging the community's potential for standardization efforts will not only enhance data access and interoperability but also drive advancements in materials research, development, and collaboration.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The OPTIMADE API enables users to query multiple databases using the same query syntax, so it grants access to a wealth of materials knowledge. By combining data from various sources, researchers can enhance the training and performance of machine learning models, enabling more accurate predictions and accelerating materials discovery and design processes.

The accelerated pace of materials design holds immense potential in addressing numerous societal challenges. For instance, as we navigate through the ongoing energy transition, there is a pressing need for materials with tailored properties suitable for various applications such as batteries, photovoltaics, thermoelectrics, and catalysts. The ability to efficiently identify these materials can lead to significant advancements in industries like renewable energy, transportation, and electronics.

Moreover, the OPTIMADE API's contribution to materials discovery indirectly supports broader societal progress by enabling researchers to develop materials that offer tangible benefits to individuals and industries alike. For example, high-performance batteries with longer lifetimes can lead to more efficient electric vehicles, reducing our reliance on fossil fuels. Similarly, photovoltaic cells with enhanced efficiency can contribute to a cleaner energy grid by maximizing the conversion of solar power into electricity.

In summary, the OPTIMADE API's ability to query multiple databases using a consistent syntax and merge data from various sources empowers researchers to improve machine learning models for materials design, accelerating the discovery process and addressing societal challenges in areas such as energy storage, conversion, and transportation.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The OPTIMADE workshops have consistently produced tangible outcomes that significantly advance materials science research. Two papers have been published on the design and implementation of the OPTIMADE API, with a third paper

focusing on the optimade-python-tools for deployment. The OPTIMADE API's adoption in various databases has attracted more collaborators, strengthening the community and expanding materials research. The optimade-python-tools have simplified integration and utilization of the API in workflows. These workshops foster collaborations among researchers from diverse backgrounds, including the biosimulations community. They provide opportunities for early career researchers and students to engage with experts. The impact of these workshops goes beyond immediate outcomes, leading to long-term research projects that drive progress in materials science. The OPTIMADE workshops have been pivotal in inspiring new discoveries and driving innovation.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We have to be as inclusive as possible. In terms of career stage, we have made sure to invite both young researchers and more experienced ones, by sponsoring mainly the former. In terms of the geographical provenance of the participants and speakers, we have invited representative from many different countries (14 in total taking into account remote participants as well), including India, Mexico, Morocco, Turkey, and the USA. On the gender balance, one can say that we have completely failed despite various invitation towards women. As far as disabilities are concerned, we did take any specific measures.

## 7. Participant list

### Organisers

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# 8th Les Houches School in computational physics: variational approaches for quantum matter in and out of equilibrium

**Location: Ecole de Physique, Les Houches**
**Webpage : https://www.cecam.org/workshop-details/8th-les-houches-school-in-computational-physics-variational-approaches-for-quantum-matter-in-and-out-of-equilibrium-1314**
**Dates: Jun 10, 2024 - Jun 21, 2024**

## 1. What were the major topics presented in the School?

On the methodological side the school was focusing on tensor network and machine learning approaches to neural quantum states. Introduction to matrix product and tensor networks have been presented, but also more recent representations based on tensor trains and their applications to perform highly dimensional integrals, e.g. in diagrammatic calculations and constrained tensor networks. Ruther the use of tensor networks for dynamics has been discussed. We then had introductional lecture on Monte Carlo methods, neural quantum states, and stochastic gradient optimization, and their use in time dependent Monte Carlo calculations. Physical questions addressed the variational description of strongly correlated systems, frustrated magnets and quantum Hall physics, as well as unitary and non-unitary time-dependence of many-body quantum systems. Semi-classical approaches based on phase space representations have been presented. The use of quantum computers have been presented discussing variational algorithms and a contact to experiments studying quantum matter under the microscope.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Many questions during the lectures were concerning the representability of quantum states: Matrix product and tensor network states are efficient to represent states in one dimensions and with low entanglement. How can they be used to efficiently represent two dimensional systems, and long time evolutions? Tensor cross interpolation algorithms have been presented to learn compact matrix product state representations to perform highly dimensional integrals and partition functions, but how good will they perform on hard problems. Concerning variational Monte Carlo approaches, physical inspired wave functions with few parameters may provide a better understanding of possible phases than

optimization of neural quantum states with million of parameters. The stability of the time-dependent variational Monte Carlo was further discussed and the influence of the stochastic noise intrinsic to the Monte Carlo evaluation. The reduction of the stochastic noise seems to be very important to the stability in time.

### 3. What was the take-home message for the participants?

Matrix product and tensor network approaches are powerful tools to resolve exactly quantum problems in low dimensions if the entanglement does not grow fast enough. Machine learning methods can efficiently represent quantum states in two or three dimensions.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

All lectures have been recorded and are available over the Les Houches webpage. Lecture notes and further material have been distributed via Slack.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Whenever possible, we tried to give priority to female lecturers and students. One female Organiser for three Organisers in total, and four female lecturers out of forteen. Concerning the participants, 17 female/others students out of 59. This ratio of 1/3 probably reflects that theoretical and computational physics has still more male applicants as well as permanent researchers. We attributed grants to an Indian, Argentinian and African student to wave the participation fee. However, at the end, the African student was not able to come due to Visa problems. The other students came from all over Europe, US, and Canada.

### 6. Participant list

Organisers

**Holzmann, Markus**
CNRS, France
**Repellin, Cecile**
LPMMC, CNRS, France
**Roscilde, Tommaso**
Ecole Normale Supérieure de Lyon, France


# International summer School in electronic structure theory: electron correlation in physics and chemistry (ISTPC)

**Location: CECAM-FR-RA, CNRS Center Paul Langevin, France.**
**Webpage : https://www.cecam.org/workshop-details/international-summer-school-in-electronic-structure-theory-electron-correlation-in-physics-and-chemistry-istpc-1309**
**Dates: Jun 16, 2024 - Jun 29, 2024**

## 1. What were the major topics presented in the School?

The main topic of the summer school was correlation in electronic structure theory. Its description has been approached from the perspective of both quantum chemistry and condensed matter physics. Starting from the well-established wave function-based methods in the treatment of weak (Moeller-Plesset, configuration interaction, and coupled-cluster theories) and strong electron correlation (complete active space self-consistent field and multi-reference perturbation theory), density functional theory, which has been extensively discussed during the school, served as a gateway to Green function-based methods (GW, in particular) and their application to molecules and solids. While most lectures focused on the ground-state problem, the description of excited states has also been addressed through various approaches: state-averaging (in quantum chemistry), linear response time-dependent density functional theory, and the Bethe-Salpeter Equation. Emphasis was also put on the more specific treatment of strong electron correlation in extended systems through quantum embedding (dynamical mean-field theory and density matrix embedding theory).

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Various open questions in electronic structure theory have been raised during the evening discussions that were scheduled every day after dinner. Among them, the description of non-conventional superconductivity within static quantum embedding theories such as density matrix embedding theory (DMET) has been mentioned. The formal exactification of the full-size low-level Bogoliubov calculation has been briefly discussed from a density functional theory (DFT)

perspective. The construction of a correlated quantum bath within DMET, with a particular focus on its nature (one- or many-body?), has also been mentioned, as well as the possibility to construct the one-electron reduced density matrix as a functional of the density. In connection with the former topic, quantum information is envisioned as an efficient tool to systematically improve correlated orbital spaces. Like in DMET, defining a proper low-cost reference calculation remains challenging. Finally, the question of extending DFT beyond the ubiquitous Born-Oppenheimer approximation has been raised by the participants.

## 3. What was the take-home message for the participants?

Properties of interest in electronic structure theory are evaluated from functionals of a basic quantity that differs from one theory to another. As that basic quantity gains in simplicity, the functional gains in complexity, thus making the development of approximate functionals challenging. Making compromises in terms of accuracy and computational cost on the basis of these considerations is central in numerical simulations.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Lecture notes and exercises are available on the website of the school: https://lcqs.unistra.fr/istpc-2024/lecture-notes/.

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Particular attention was paid to gender balance when validating pre-registrations. Ultimately, 25% of the participants were women. One female student came from India. She could not afford paying the registration fee (in addition to her flight tickets). In order to make sure she could participate, we did secure extra funding.

## 6. Organizers list

**Fromager, Emmanuel**
University of Strasbourg, France
**Loos, Pierre-Francois**
CNRS, France
**Robert, Vincent**

Institut de Chimie de Strasbourg, France
**Romaniello, Pina**
Université de Toulouse, France
**Toulouse, Julien**
Sorbonne Université, France

# Electrochemical interfaces in energy storage: advances in simulations, methods and models

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/electrochemical-interfaces-in-energy-storage-advances-in-simulations-methods-and-models-1199**
**Dates: Jun 18, 2024 - Jun 21, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on how to incorporate electrochemistry into simulations of relatively large systems, since most simulations of redox processes are still limited to ab initio approaches, and large-scale analytical models are often incompatible with atomistic simulations due to concentration, time, and size limitations. In this context, we discussed how to incorporate nanoscopic mechanisms into existing analytical models and how to assess the validity of existing analytical models for nanoscopic systems, since these continuum models typically lack an atomistic description of, e.g., solvent layering at the electrode/electrolyte interface. In addition, it was mentioned that the commonly used ICC (induced charge computation) method neglects molecular details of the liquid and solids. Therefore, the constant potential method is a valuable tool to study these effects. Improvements and requirements of this method, e.g. under which conditions (confinement, importance of the DOS, etc.) and how it can be applied to heterogeneous electrodes, were intensively discussed in the discussion session after the lectures and at the posters. The variations in the surface tension upon (electrochemical) adsorption of chemical species were intensively discussed and it was concluded that this would probably require a many-body description, which is usually not done in current simulations.
The experimentally observed underscreening of the electrolyte was also discussed from different perspectives, e.g. DFT, molecular dynamics and continuum. It was concluded that from a theoretical point of view, there is no reason why electrostatics alone can capture the underscreening, and the MD simulations are in full agreement with the liquid state theories from the 1990s.
Data-driven / machine learning techniques have emerged as a major tool to advance research on electrochemical interfaces and material science in general. Some examples of how machine learning could help improve the design of batteries and supercapacitors were shown, and ways to improve the machine-learning prediction of quantities based on structure-property relationships of

electrolyte additives were discussed, as well as ways to use data-driven techniques to predict the behavior of electrode materials.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

During the workshop, several ideas were discussed on how to move more towards hybrid simulations, e.g. via QM/MM and MM/coarse-grained approaches. It was also discussed how the density of states (DOS) in the electrodes affects the structure of the electric double layer. The representation of the DOS is currently a limitation of the continuum models (since in principle it does not matter whether the electrode is Pt, Au, Cu or another metal, although the electrode material has a significant effect on the electrochemical performance). More specifically, the solvent at the interface strongly affects the final macroscopic properties, such as capacitance or surface tension, of an electrochemical device, which is often not properly accounted for in continuum models. The possibility of learning the DOS with some of the machine learning schemes, including long-range, was discussed. The use of Long-Range descriptors (LODE) as input for QSPR models to predict the surface stress was also discussed.
Regarding the surface stress, the importance of many-body effects, especially for frustrated chemical bonds, the alteration of the electronic structure at surfaces in contact with electrolytes, especially when an electric potential is applied, were discussed. There are many open questions about this important aspect. Another point that came up was the experimental validation of theoretical models. For example, models for the time to form an electrical double layer based on the Nerst-Planck equation are well established in the literature, but there is little experimental data to confirm these models.

## 3. What was the take-home message for the participants?

Given the breadth of the participants list each participant carried different insights home. Yet, the common denominator between all these participants was their interest in solid/liquid interfaces relevant to electrochemical devices. To our opinion, the breadth of the participants list was the strong point of this workshop. We sensed that the participants appreciated the different perspectives on the solid / liquid interface offered by the different modeling communities.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The potential of electrochemical interfaces to affect society in general is vast as they are a key element in a large variety of application areas ranging from energy

generation, storage and conversion, advanced manufacturing, health and biomedical application, power electronics and many more. The workshop focused on the application of simulation techniques (physical and data-based modelling) to advance research in materials research either by unraveling fundamental mechanisms at electrochemical interfaces or by optimizing processes to obtain materials with superior properties without the need to rely on traditional try-and-error approaches. The majority of the discussed topics depict fundamental contributions for the design and application of engineering materials and associated technologies, by which society can address the above mentioned critical challenges leading to a more sustainable and healthier future. In particular, understanding the charging of electrodes and particularly the electrode/electrolyte interface is vital for the further development of electrochemical devices. In turn, these devices will play a major role in the implementation of intermittent renewable energy sources into the electricity grid and also to (electro-)chemical synthesis. Developing better models can lead to a deeper understanding of these devices, which, in turn, will help in their rational design and further optimization and thus enable a shift away from fossil fuels. As efficient energy storage systems, batteries and supercapacitors may become key components in this "green energy transition". In many research domains, modelling approaches constitute an essential tool to reduce the environmental footprint of scientific research (e.g. by short-listing promising material systems for synthesis / application rather than solely relying on high-throughput screening techniques). However, for some of the discussed high-fidelity simulations that require high performance computer systems to be run, the footprint of research might slightly increase but we are confident that the gained knowledge will still reduce the net footprint of society in general.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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We held two poster sessions and group discussions after every second talk. To our opinion, the participants used these times for discussion very well. There were many people who stayed very late during the poster sessions, where they made many new connections. And the discussions after the talks never stopped before the 30 minutes we scheduled for them. Through these interactions, all participants extended their networks.
Regarding publications, it is too early to judge, but we organizers have several ongoing projects with the other workshop participants, some of which involve new connections.
Regarding software development, one conclusion from the discussions was that Qeq should be implemented in the ELECTRODE package

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The list of speakers was established in order to have a diversity of gender, geographical provenance and career stage. The final program includes 24 speakers from 10 different countries and 3 continents (with a majority from Europe). Several early career researchers (with a postdoctoral position or who have recently obtained a permanent academic position) gave a talk, representing almost a third of the speakers. The other participants were also very diverse in terms of their career stage, ranging from PhD to emeritus. There were 19 male and 5 female speakers (35 male and 10 female participants), giving a female presence of 21% (22% for the participants), slightly above the estimated representativity of women in the specialised field of research corresponding to this workshop. We left a lot of time in the program for discussions after the talks. These long sessions allowed all participants to ask questions and bring insightful comments to the various topics.

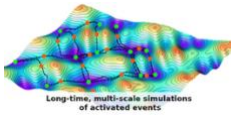
## 7. Participant list

### Organisers

**Feiler, Christian**
Helmholtz-Zentrum Hereon, Germany
**Janssen, Mathijs**
Norwegian University of Life Sciences, Norway
**Meißner, Robert**
Hamburg University of Technology, Germany
**Merlet, Celine**
CIRIMAT - CNRS - Université de Toulouse, France

**Ahrens-Iwers, Ludwig** - Hamburg University of Technology (TUHH), Germany
**Aslyamov, Timur** - University of Luxembourg, Luxembourg
**Bazant, Martin** - MIT, Cambridge, MA, United States
**Bi, Sheng** - Xiamen University, China
**Boda, Dezső** - University of Pannonia, Hungary
**De Freitas Martins, Ernane** - ICN2, Spain
**Deringer, Volker** - Oxford University, United Kingdom
**Duivenvoorden, Tanika** - The University of Queensland, Australia
**Fertig, David** - NMBU, Norway
**Gaudy, Nicolas** - CIRIMAT-Paul Sabatier, France
**Goloviznina, Kateryna** - Sorbonne Université & CNRS, France
**Gor, Gennady** - New Jersey Institute of Technology, United States
**Härtel, Andreas** - University of Freiburg, Germany
**Hartkamp, Remco** - Delft University of Technology, Netherlands

**Holm, Christian** - University of Stuttgart, Germany
**Iannuzzi, Marcella** - University of Zurich, Switzerland
**Joly, Laurent** - Université Lyon 1, France
**Kim, Hyemin** - Helmholtz-Zentrum Hereon, Germany
**Kondrat, Svyatoslav** - Institute of Physical Chemistry, Polish Academy of Sciences, and Stuttgart University, Poland
**Kornyshev, Alexei** - Imperial College London, United Kingdom
**Kowalski, Piotr** - Forschungszentrum Juelich, Germany
**Kramer, Denis** - Helmut-Schmidt-University, Germany
**Lahrar, El Hassane** - CIRIMAT-CNRS, France
**Loche, Philip** - EPFL, Switzerland
**Nair, Swetha** - CNRS, Sorbonne Université, France
**Neugebauer, Joerg** - Max-Planck-Intitut for Sustainable Materials, Germany
**Nickel, Ole** - Hamburg University of Technology, Germany
**Olsson, Emilia** - University of Amsterdam, Netherlands
**Ordejon, Pablo** - Institut Català de Nanociéncia i Nanotecnologia - ICN2, Spain
**Rossmeisl, Jan** - Technical University of Denmark, Denmark
**Schlaich, Alexander** - University of Stuttgart, Germany
**Serva, Alessandra** - Sorbonne Université & CNRS, France
**Shin, Seung-Jae** - Imperial College London, United Kingdom
**Sprik, Michiel** - University of Cambridge, United Kingdom
**Stärk, Philipp** - GS SimTech Stuttgart, Germany
**Stooß, Henrik** - University of Stuttgart, Germany
**Sudhakar, Hari Haran** - Sorbonne Université, France
**Sulpizi, Marialore** - Ruhr University Bochum, Germany
**Tee, Shern** - Griffith University, Australia
**Warnicka, Agnieszka** - CEA, France
**Waysenson, Zacharie** - Sorbonne Universite, France




# Long time multi-scale simulations of activated events: from theory to practice

**Location: CECAM-IT-SISSA-SNS**
**Webpage : https://www.cecam.org/workshop-details/long-time-multi-scale-simulations-of-activated-events-from-theory-to-practice-1317**
**Dates: Jun 24, 2024 - Jun 28, 2024**

## 1. What were the major topics presented in the School?

The long-time evolution of nanoscale and multiscale systems, e.g., heterogeneous catalysis, surfaces, and metallic alloys, typically involves morphological changes of the atomic structure, and chemical reactions. Simulation of many of these processes can be severely limited, since these processes are rare-events with respect to simulated time of an atomistic simulation by tiny time steps (i.e. molecular dynamics). The school covered a range of topics related to the simulation of long-time evolution (i.e. rare-events), starting from the atomic level.
The foundation for such simulations is the transition state theory (TST), and its harmonic variant (hTST), which was introduced, discussed, and covered in great detail at the school.
A major part of TST is the knowledge of the probability for a system to transition from a current state into another, which is given by the knowledge of all possible transition mechanisms, or reaction pathways. The rate for a given pathway can be deduced from the knowledge of the saddle point of the potential energy surface (PES) along that pathway, therefore the computation of saddle points is essential. The topic of saddle point exploration was covered in two essential approaches: (i) the double-ended approach by Nudged-Elastic Band (NEB), and (ii) the open-ended approach by Dimer, and ARTn algorithms.
Equipped with the knowledge of saddle points, TST is directly used in kinetic Monte-Carlo (kMC) simulations. The algorithmic approach of kMC was introduced and discussed, at two main levels of approximation, on-lattice (with the software kmos3), and off-lattice (with software akmc in eOn, and k-ART). The kMC algorithm is based on statistical probabilities, and Markov chains. The foundations of mathematical probability, and ergodicity were laid out, and discussed in the school.
For more complex systems, such as (bio)molecular systems, the number of possible transition paths becomes extremely large, and simple saddle point exploration algorithms do not suffice. The algorithm suited for the task of transition path sampling and computing the rates in such systems, OpenPathSampling (OPS), was introduced and discussed.
Beyond the atomic-scale simulations, coarse-grained approaches can be used to simplify the description of a system, and open the possibility to simulate very large systems such as needed for the computation of transport coefficients in crystals. The algorithm KineCluE was introduced and discussed, which is suited for this task.

Each theoretical talk was accompanied by a hands-on session designed to demonstrate the respective technique using various computational packages, providing practical experience and reinforcing the theoretical concepts discussed.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

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The support of computational packages on various operational systems and platforms is one of the limiting factors in the field, due to the somewhat diverging development teams in academic software. Besides that, the prerequisites to operate the edge-cutting packages may be too demanding for researchers who are just end-users, instead of developers. These background knowledge requirements include the proper configuration, adaptation, and compilation of computational environments across platforms, which is not at all common-knowledge.
Additionally, the package ecosystem within the saddle point searching community presents significant challenges. Currently, multiple packages address similar problems using different methodologies but lack a unified standard for input and output data. This fragmentation impedes interoperability and complicates the integration of results across different tools. Furthermore, the absence of a common programming platform, or interface, spanning from transition state searching to mesoscopic-level simulations (e.g., kMC), exacerbates the issue. A more standardized and cohesive platform like ASE in the atomic simulation community could streamline workflows, enhance reproducibility, and accelerate research progress by enabling easier integration and comparison of results.

## 3. What was the take-home message for the participants?

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All software used during hands-on sessions is freely accessible, and open-source. The demonstrations offered simple but practical examples and insights. Kinetic parameters of a system can be extracted from saddle search algorithms, and used by a microkinetic model. Beyond the atomistic description, more sophisticated methods need to be used for sampling, and for the computation of larger-scale kinetic properties, other proper tools need to be used.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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- github page of the event, https://github.com/CECAM-LTS-MAP with associated repositories for each of the hands-on sessions;
- includes lecture materials like slides;

- all software used in hands-on is freely accessible and open-source

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The invited speakers and tutors came from eleven countries to contribute to the event, ensuring a broad and inclusive perspective across various research fields. The lectures began with the fundamentals of transition state theory, which helped cater to the diverse interests of our participants, including those working on organic molecules, inorganic catalytic surfaces, and more. The participant group was equally varied, encompassing master's and doctoral students, postdoctoral researchers, and professional from the tech industry. This diversity fostered a rich environment for meaningful social networking and interdisciplinary exchange. In addition to the lectures and hands-on sessions, all participants of the school were given a chance to present their work either orally, or by poster. There were 6 contributed talks, and 7 posters, while no contributions were refused.

## 6. Participant list

### Organisers

**Connétable, Damien**
CNRS, France
**Gunde, Miha**
Institute Rudjer Boskovic, Croatia
**Hemeryck, Anne**
LAAS-CNRS, France
**Lai, King Chun**
Fritz Haber Institute of the Max Planck Society, Germany
**Martin-Samos, Layla**
CNR-IOM (Democritos) C/o SISSA, Italy
**Mousseau, Normand**
Université de Montréal, Canada
**Poberznik, Matic**
Jozef Stefan Institute, Slovenia
**Salles, Nicolas**
CNR-IOM Democritos, Italy

**Aldana Delgado, Samuel** - Tyndall National Institute, Ireland
**Béland, Laurent Karim** - Queen's University, Canada
**Bertoni, Ilaria** - University of Milano Bicocca, Italy
**Bolhuis, Peter** - University of Amsterdam, Netherlands
**Cannizzaro, Francesco** - Fritz Haber Institute of the Max Planck Society, Germany
**De Armas Rodriguez, Raúl** - IMDEA Materiales, Spain

**Deimel, Martin** - Fritz Haber Institute of the Max Planck Society, Germany
**Dlouhy, Matjaz** - Jozef Stefan Institute, Slovenia
**Ebrahimi Viand, Roya** - Fritz Haber Institute of Max Plank Society, Germany
**Fankam Fankam, Jean Baptiste** - University of Witwtersrand, South Africa
**Fioccola, Simone** - LAAS-CNRS, France
**Flaibani, Matteo** - Università di Trieste, Italy
**Gašparič, Lea** - Jozef Stefan Institute, Slovenia
**Ghosh, Prasenjit** - Indian Institute for Science Education and Research, Pune, India
**Gönnheimer, Nils** - Universität Bayreuth, Germany
**Goswami, Rohit** - University of Iceland, Iceland
**Gregori, Erik** - Jožef Stefan Institute, Slovenia
**Henkelman, Graeme** - University of Texas at Austin, United States
**Jay, Antoine** - LAAS-CNRS, France
**Jónsson, Hannes** - University of Iceland, Iceland
**Jung, Sung Hoon** - The University of Texas at Austin, United States
**Keshavarz, Fatemeh (Sarah)** - LUT University, Finland
**Lipin, Raju** - University of Limerick, Ireland
**Loprete, Fabio** - University of Bologna, Italy
**Mahamiya, Vikram** - International Centre for Theoretical Physics (ICTP), Italy
**Massa, Dario** - NCBJ, Poland
**Matera, Sebastian** - Freie Universität Berlin, Germany
**Mishra, Nalin Vilochan** - IISER Bhopal, India
**Moison, Hugo** - Géosciences Environnement Toulouse, France
**Rahman, Md. Mljanur** - Polytechnique Montréal, Canada
**Sahu, Rahul** - Indian Institute of Technology Kharagpur, India
**Sallermnn, Moritz** - University of Iceland, Iceland
**Sarkar, Arka Prava** - Iit Kharagpur, India
**Schrautzer, Hendrik** - University of Iceland, Iceland
**Schuler, Thomas** - CEA, France
**Settem Narasimha, Manoj** - Sapienza University of Rome, Italy
**Sidler, Elizaveta** - NTNU, Norway
**Singh, Akksay** - The University of Texas at Austin, United States
**Son, Won-Joon** - Samsung Electronics, Republic of Korea
**Song, Zichen** - Southern University of Science and Technology, China
**Tirunelveli Vallinayagam, Ram Mohan** - BCAM, Spain
**Toffoli, Hande** - Middle East Technical University, Turkey
**Toffoli, Daniele** - Universita' degli Studi di Trieste, Italy
**Upterworth, Anna Luisa** - Martin Luther University Halle-Wittenberg, Germany

# Out-of-equilibrium soft matter: challenges and perspectives

**Location: Isaac Newton Building , University of Lincoln, Lincoln, UK**
**Webpage : [https://www.cecam.org/workshop-details/out-of-equilibrium-soft-matter-challenges-and-perspectives-1344](https://www.cecam.org/workshop-details/out-of-equilibrium-soft-matter-challenges-and-perspectives-1344)**
**Dates: Jun 26, 2024 - Jun 28, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The main topic of the workshop was out-equilibrium soft matter systems, and how they can be understood, described and predicted with modern computer simulation tools. Specific systems, which were addressed were two classes: i) variety of active colloids and self-propelling particles, including active nematic, magnetic colloids, bacteria, ii) polymers, emulsions and block polymer system in non-equilibrium conditions such as electric fields and shear flow. The discussion also included applications to such long standing questions as static vs dynamic friction, nucleation rates.
Relation between dynamic processes and the structure in the soft matter was one of the main questions addressed in the symposium with a particular challenge how one can model such systems on multiscale, from electronic states to mesoscopic structures. A new element, which received considerable discussion is the hybrid of the two systems, such as active polymers, swimmers in viscoelastic medium and active moving particles in block copolymer structures.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop allowed for ample discussion and cross fertilisation of ideas. Its layout was ideal for the purpose. The five sessions other 3 days consisted of a mixture of longer and shorter talks with separate Questions and Answers 30 minute sessions after every two talks. These Q&A sessions were organised so that both speakers can answer questions but also discuss between themselves, that resulted in very lively discussions which continued during extensive coffee breaks (30 minutes as well) and 1.5 hour lunches. Further discussions were supported by over 2 hours long poster session with reception and by a conference dinner. That patten of networking resulted in a very fruitful exchange and new ideas interchange between two main areas. One of the technical questions which was discussed is development of combined field-based and particle based methods for the hybrid systems composed of both nano-particles and polymer matrix. The use

of several computational tools of different degree of coarse-graining was discussed as well, it was demonstrated, that it is a good strategy to address hybrid systems.

### 3. What was the take-home message for the participants?

The primary message of the workshop was that different non-equilibrium systems exhibit many similarities in their physical behaviour and as a result simulation techniques developed for one system can help in development of methods for another. Another take-home message is that creation of hybrid systems can exhibit novel structures and dynamical behaviour. Creation of multiscale simulation methods and platforms remains a challenge and a combined effort is desirable.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Soft matter materials can offer substantial benefits to the society. They can be applied in health as drug delivery vehicles, in chemical engineering as scaffolding for creating nano-catalytic containers, as matrixes for creating nano-structures with tailored properties, which can be used as energy materials for instance. Development of computational tools to predict such structures can make the creation faster and cheaper.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop was very useful for starting new funding proposals, development and enhancement of software and potential joint publications. The participation in the workshop of a Japanese software company JSOL was a manifestation of such usefulness.

### 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Firstly, we attempted to have a diverse selection of invited and contributed participants: in terms of gender, we invited ...
In terms of geographic provenance, we invited and accepted participants from various countries, with UK and Germany being the most represented ones, largely accounting for geographic proximity and population. We provided supporting letlers for participants in need of visa applications to facilitate their participation.

In terms of career stage, we invited and accepted participants from a wide variety of stages. Invited speakers were of various stages (postdoc P. Digregorio, early career PI L. Alvarez), instead of merely well-stablished PIs. We provided ample time for discussions and coffee breaks. We provided Q&A sessions after two or three talks in order to facilitate discussions in a more suitable environment for early career researchers.

## 7. Participant list

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### Organisers

**Diaz, Javier**
University of Barcelona, Spain
**McIlroy, Claire**
University of Lincoln, United Kingdom
**Zvelindovsky, Andrei**
University of Lincoln, United Kingdom

**Alvarez, Laura** - University of Bordeaux, France
**Bhowmik, Bhanu Prasad** - University of Edinburgh, United Kingdom
**Cammann, Jan** - Loughborough University, United Kingdom
**Charan, Harish** - Durham University, United Kingdom
**Cristín, Javier** - Insitute of Complex Systems-CNR, Italy
**Digregorio, Pasquale** - Universitat de Barcelona, Spain
**Elschner, Jonas** - University of Bayreuth, Germany
**Govorun, Elena** - ESPCI Paris - PSL, France
**Kudryavtsev, Yaroslav** - ESPCI Paris - PSL, France
**Löwen, Hartmut** - Heinrich-Heine Universität Düsseldorf, Germany
**Maity, Ruma** - Technischen Universität Wien, Austria
**Mazza, Marco** - Loughborough University, United Kingdom
**Mueller, Marcus** - Georg-August University Göttingen, Germany
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# Out-of-equilibrium phenomena in the presence of curvature and non-reciprocal interactions

**Location: CECAM-HQ-EPFL, Switzerland & online**
**Webpage : https://www.cecam.org/workshop-details/out-of-equilibrium-phenomena-in-the-presence-of-curvature-and-non-reciprocal-interactions-1284**
**Dates: Jul 2, 2024 - Jul 5, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The major topics discussed at the event were nonreciprocal interactions in active systems, the role of curvature in soft matter systems with a focus on active matter, and the interplay between out-of-equilibrium conditions and curvature, with a focus on biological systems. These discussions aimed to deepen the understanding of the physical mechanisms underlying these phenomena and their implications for biological and artificial systems.

Nonreciprocal interactions, which violate Newton's third law, were a central theme. These interactions are crucial in various biological processes and phenomena such as predator-prey dynamics, velocity alignment, and opinion spreading. The event highlighted how these interactions lead to spontaneous currents and non-equilibrium patterns, which are not typically observed in reciprocal systems. By exploring particle and spin models, as well as effective continuum descriptions, the discussions contributed to a better grasp of how nonreciprocal systems operate and how to potentially control and exploit them.

Another significant topic was the role of curvature in soft matter systems, particularly active matter. Curvature and topology are essential in shaping the growth and functionality of cells, tissues, and organs. The event shed light on how curvature influences morphogenic processes and the formation of complex three-dimensional structures, such as those seen during embryonic development. It was noted that topological defects, which act as organizing centers for stress within the material, interact with curvature and topology, thereby playing a crucial role in shaping biological processes.

The event also focused on understanding how out-of-equilibrium conditions, when coupled with curvature, affect biological systems. Active matter systems are inherently out-of-equilibrium, as they convert stored or ambient free energy into directed movement. This characteristic is prevalent in many subcellular, cellular, and tissue-scale processes. The discussions aimed to elucidate the challenges and opportunities in modelling these systems to gain insights into the physics underlying living systems.

In summary, the discussions on nonreciprocal interactions, the role of curvature, and the impact of out-of-equilibrium conditions on biological systems have contributed to a deeper understanding of these complex phenomena. The insights gained are expected to propel the scientific community towards new discoveries and applications in both biological and artificial systems.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop significantly advanced the state of the art by bringing together experts from various fields to share ideas, techniques, and data. The collaborative environment fostered dialogue and solution-oriented discussions, which are crucial for overcoming the challenges in understanding nonreciprocal interactions, curvature, and their interplay in active matter. The collective expertise of the attendees not only pushed the boundaries of current knowledge but also helped create a roadmap for tackling future challenges.

From talks and discussions, it has emerged that the study of nonreciprocity in effective, coarse-grained models provides powerful tool for understanding nonequilibrium phenomena, with its relevance being both widespread and significant. Nonreciprocal models have proven to be particularly useful for simplifying and capturing the essence of complex dynamics that arise in many systems out of equilibrium.

Curvature is another critical feature that is ubiquitous in biological systems, and we believe it has profound implications for how these systems develop and function. However, the effects of curvature on collective behaviour in active systems are still not fully understood. Delving deeper into this aspect may reveal crucial insights into the organizational principles underlying biological processes and could potentially lead to novel applications in material design and biophysics.

One of the most intriguing questions in this context is the role of topological defects in non-equilibrium systems. These defects, which are disruptions in the regular pattern of a system, might hold the key to guiding biological systems toward specific functionalities. Understanding whether and how topological defects influence biological systems could open new avenues for controlling and manipulating these systems for desired outcomes.

To effectively study nonreciprocal systems, the development of efficient simulation techniques is essential. Just as Monte Carlo methods serve as a generic tool for equilibrium systems, we seek to establish similar methodologies for nonreciprocal systems. Such techniques would enable more accurate and comprehensive simulations, helping us to uncover the generic routes through which nonreciprocity contributes to the functionality of complex systems.

A critical area of investigation is identifying the coarse-grained rules that allow nonreciprocal interactions to emerge from fundamentally reciprocal ones. By understanding these rules, we can bridge the gap between microscopic interactions and macroscopic behaviours, providing a clearer picture of how nonreciprocity influences system dynamics.

## 3. What was the take-home message for the participants?

he take-home message for the participants was multifaceted. We need to develop a thermodynamic-like theory of nonreciprocity and identify the minimal rules for self-replication. Experimental verifications and test systems are crucial to validate these theories. Understanding the overarching questions in the field is essential, as nonreciprocity could be a key mechanism in disassembling complex systems, offering insights into fundamental biological processes.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop hold potential for societal benefits in several areas.

**Dynamics of Pedestrians and Animal Groups**

The insights gained from studying nonreciprocal interactions can be directly applied to understanding the dynamics of pedestrians and animal groups. This can enhance urban planning and public safety by improving crowd management strategies and evacuation plans. Furthermore, understanding animal group behaviours can inform conservation efforts, ensuring better protection and sustainability of wildlife populations.

**Targeted Drug Delivery and Robotic Surgery**

The role of curvature and active matter in biological systems has profound implications for medicine. By leveraging these principles, advancements in targeted drug delivery systems can be achieved, allowing for precise delivery of therapeutic agents to specific sites in the body, thereby increasing efficacy and reducing side effects. Additionally, the insights into nonreciprocal interactions and active matter can lead to innovative approaches in non-invasive surgery, such as using micro-robots that navigate through the body's complex environments.

**Alternative Computation and Sustainability**

The workshop's discussions on nonreciprocal systems and active matter also extend to the field of alternative computation. These can inspire the development of new computational models that mimic the efficiency and adaptability of biological systems. Such advancements can contribute to more sustainable computing technologies, reducing energy consumption.

**Ecological Models**

Understanding that many ecological models are inherently nonreciprocal opens new avenues for studying and managing ecosystems. By incorporating nonreciprocal interactions into ecological models, one can better predict and manage complex ecological dynamics, such as predator-prey relationships, resource distribution, and species interactions. This improved understanding can lead to more sustainable management of natural resources.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The main outcome is that we managed to get researchers working on disjoint areas such as nonreciprocity and curvature to meet each other and share their ideas and expertise. This was very fruitful since it became evident that those two research areas share a lot in common, yet many of the results were not widely known across the fields. As a result, this may lead to new collaborations.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

When selecting participants and speakers, considerable effort was put into retaining the gender balance of the field while not affecting the theme of the workshop, with 6/18 invited talks and 4/15 contributed talks delivered by women. Significant effort was made to balance between senior and early-career researchers for invited talks (3/8/7 early/mid/senior). A similar approach was used for contributed talk (6/15 by PhD students), with slight preference to more senior postdocs keeping in mind that they are likely on the job market, thus needing increased visibility.
The workshop also featured a poster session allowing students to actively contribute and present scientific results at a very early stage of their careers.
In close collaboration with the CECAM admin team, the Organiser made sure that the workshop used a hybrid approach allowing remote participation. This also helped geographic diversity, e.g. a speaker was able to present their work from Mexico.

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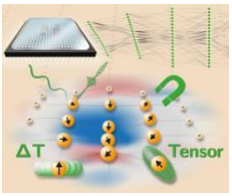


# Machine Learning of first principles observables

**Location: Zuse Institute Berlin, Germany**
**Webpage : https://www.cecam.org/workshop-details/machine-learning-of-first-principles-observables-1322**
**Dates: Jul 8, 2024 - Jul 12, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This year's workshop on "Machine learning of first principles observables" was aimed at addressing the growing need for models, workflows, and databases which go beyond the established methods of producing ML inter-atomic potentials (MLIPs), and instead serve to predict experimentally observable quantities. During the event, we therefore held several subject-specific sessions which aimed at bridging these two communities, from "Thermodynamic observables" to "Long range interactions" and "Spectroscopy", where we invited speakers both from theory and experiment. Additionally, after each set of talks we then held a 45 minute panel discussion on how that specific field was advancing, with respect to ML for observables. There were several recurrent topics throughout the week including:

**Data sharing and management**: In almost every discussion section, the importance of effective data sharing, meta-data utilization, and the creation and maintenance of curated databases was discussed. It was also emphasized that these databases should include negative results, which aid ML models to learn what not to do, and are critical for experimentally relevant ML models for the future. Code documentation and reproducibility was also a feature of these discussions.

**Bridging Experiment and Simulation**: This workshop itself served as a springboard for facilitating exchange between theoreticians and experimentalists. By encouraging discussion between both groups, the speakers and participants identified several areas where these two groups could bridge the complexity gap from both ends. This involves theoreticians reconsidering the approximations and simplifications in their models to make them more realistic by incorporating factors such as interfaces and defects. At the same time, experimentalists were encouraged to conduct simplified, idealized benchmarking experiments. This dual approach aims to bring theory and experiment closer, bridging the complexity gap from both ends.

**Metrics for Evaluating Predicted Data**: A final topic discussed at the event was the need for better metrics for evaluating the accuracy of predicted data beyond simple scalar values. This included discussing metrics which allow for tolerance in

variations in spectra shifts, peak width, and spectral intensities. Additionally, the importance of foundational ML models such as MACE-MP-0, ChargeNET and GenAI models were highlighted.
By addressing these topics, the workshop has not only pushed the boundaries of current methodologies but also fostered a collaborative environment that bridges theoretical and experimental approaches, ultimately contributing to more robust and applicable scientific advancements.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop produced several outcomes and open questions surrounding our three key topics of data sharing, bridging the gap between experiment and theory, and evaluation metrics for databases and models. Throughout the week there was a general consensus on the necessity of better software documentation and the availability of comprehensive databases. Several solutions and ongoing projects were presented, which include Alexandria materials database (alexandria.icams.rub.de), OPTIMADE API for database comparisons (optimade.org), NOMAD data management platforms (nomad-lab.eu/nomad-lab/), and atomate2 workflow manager (github.com/materialsproject/atomate2). All of these databases, and more can be found at (github.com/JuDFTteam/best-of-atomistic-machine-learning) which is hosted by J. Wasmer.
In addition, there was a major focus in the second half of the workshop especially, on the need to bridge the gap between experimental data and simulations. It was generally agreed that the future of science is AI and that experimentalists also need to find a way to format data in a “future proof” method for use with AI models, but also that formatting data in a way that is usable for both experimentalists and theoreticians requires extensive communication and adjustments. For example, the inclusion of metadata was highlighted as essential for making the recycling and reuse of old datasets easier, whether they originate from experiments or simulations. This is particularly important for the longevity and utility of databases. The above database examples in particular, only highlight the use cases for computed data, and do not take into account incorporating experimental data, which is a gap in the current state-of-the-art databases and workflows.
Finally, many of the large discussion sessions commented on the lack of “quality control” in online datasets. There were intense discussions about the data gaps in large, widely popular databases such as the Open Catalyst Database, which does not include any surface structures, for example. Later in the week, there was also a discussion that many databases become unused over time, and that there should be a way for organic updates of metadata over time, in order to preserve data quality. Yet, identifying best practices for this process remains an open question. Finally, given the diversity of databases now being established, including spectroscopy data, experiment and theory data, and Hamiltonian or electron density data, it was concluded that we need to establish standardized metrics to evaluate the quality of databases.

In summation, the workshop successfully identified the critical areas for improvement within the fields of predicting observables from first principles and established a network for future research efforts.

## 3. What was the take-home message for the participants?

The workshop underscored the importance of sharing well-documented data following FAIR principles. It highlighted the necessity of maintaining code and promoted collaboration between experiment and theory. Participants gained an improved understanding of the different requirements from both experiments and theorists, and gained new knowledge of the available datasets (OCD, Alexandria, OPTIMADE, Materials Project) and cutting-edge ML models (MACE-MP-0, Jacobi-Legendre, AIMNet2).

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The “hype” of machine learning and artificial intelligence certainly effects not just the small community of computational materials scientists, but the entirety of the scientific, and ultimately societal communities as well. Our workshop, with its interdisciplinary nature and focus on openness and discussion, highlighted the importance of exchange across disciplines. This is true not just between experimentalists and theorists, but also between scientists from other countries and continents, who may not have had the chance to speak directly without the catalyst of a week-long workshop and large discussion sessions. Furthermore, all participants at the workshop learned about the importance of data responsibility and the FAIR principles of data sharing. Especially for researchers at the start of their careers in science, their ability to bring these principles back to their own labs will have a knock-on effect for the future of science.
More broadly, the ability to use ML models for materials screening by targeting observables directly, instead of simply using potential energy surfaces (especially those at 0K which are not experimentally relevant) represents a significant advancement. This approach enables efficient and cost-effective materials design, and will have effects further down the utility pipelines, especially in industries such as energy, healthcare, and technology where rapid innovation is crucial. Having a workshop in which a large number of people came together and agreed to realize this goal is an important step in promoting the future of novel materials.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

There were several tangible outcomes of the workshop, especially with regards to the dissemination of open-source codes, new collaboration between experimentalists and theorists, and discussion of publications with joint material. Most notably, Johannes Wasmer (DE) shared a very useful github repo on the “Best of Atomistic Machine Learning”. This is a repository designed to highlight the latest open-source codes being actively developed within the machine learning materials science community. There were several other participants, including Janine George (DE), Kulbir Gusman (CAN), and Jonathan Schmidt (CH) who also shared their groups’ codes and databases and expressed active interest in further collaboration. Schmidt presented the OptiMADE API for Database Integration, which all participants viewed as a step in the right direction for smoother data upload and sharing.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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We are proud to report that we took several steps to promote inclusivity at our workshop with an intersectional approach covering disabilities, gender, diverse career stages, and geographic inclusion. A key focus was our hybrid format, allowing online participation for presentations and discussions, accommodating those constrained by university budgets, visa requirements, or geographical distance. We actively sought non-male, international, and early-career speakers in our initial selection, in order to promote gender and age diversity in a typically male-dominated field. During the workshop, we offered "no photo" stickers for people or their posters, allergen-aware dining, and mobility assistance: all of which were actively used by participants! Overall, we had great feedback especially from women participants, who said they were encouraged to attend this workshop specifically because they saw the organizing team was formed of all non-men which was especially motivating.

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**Schmidt, Jonathan** - ETH Zurich, Switzerland
**Selim, Taha** - IMM, Radboud University Nijmegen, Netherlands
**Sharma, Himanshu** - Seth G. L. Bihani Sd Pg College, India
**Siddiqui, Gohar Ali** - Technical University of Munich, Germany
**Simoncelli, Michele** - University of Cambridge, United Kingdom
**Song, Yihua** - Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany
**Sugathan Nair, Akhil** - Fritz-Haber Institute of the Max-Planck Society, Germany
**Susan Abraham, Christina** - Ruhr-Universität Bochum, Germany
**Tang, Zeyuan** - Hainan University, China
**Tomae, Ritu** - University of Bonn, Germany
**Tukadiya, Namrataben Arjan** - The Maharaja Sayajirao University of Baroda, India
**Uranga Pina, Llinersy** - Université Paul Sabatier, France
**Van De Ven, Roel** - Radboud University Nijmegen, Netherlands
**Van Veerdeghem, Jenne** - KU Leuven, Belgium
**Vinod, Vivin** - University of Wuppertal, Germany
**Vitartas, Valdas** - University of Warwick, United Kingdom
**Vondrák, Martin** - Fritz Haber Institute of the Max Planck Society, Germany
**Walker, Matthew** - UCL, United Kingdom
**Wang, Zhenyu** - Jilin University, China
**Wasmer, Johannes** - Forschungszentrum Jülich, Germany
**Willimetz, Daniel** - Charles University, Czech Republic
**Wolffs, Jop** - Radboud Universiteit, Netherlands
**Wu, Chuntian** - JILIN UNIVERSITY, China
**Yaman, Murat** - City University of New York, United States
**Zakary, Ouail** - NMR Research Unit - University of Oulu, Finland
**Zanca, Federica** - STFC, United Kingdom
**Zarrouk, Tigany** - King's College London, United Kingdom
**Zhang, Ruiqi** - Binghamton University, United States
**Zhao, Heng** - University of Fribourg, Switzerland

# Summer School on molecular dynamics for material science, nanotechnology and biophysics

**Location: CECAM-IT-SISSA-SNS**
**Webpage : https://www.cecam.org/workshop-details/summer-school-on-molecular-dynamics-for-material-science-nanotechnology-and-biophysics-1329**
**Dates: Jul 8, 2024 - Jul 19, 2024**

## 1. What were the major topics presented in the School?

The school was organized into three blocks, each one lasting 4, 3, and 3 days, respectively.
Block 1: July 8–11
Fundamental principles and practical tools for molecular simulations using classical statistical mechanics, including:
- Programming foundations using Python for scientific computing.
- Statistical ensembles
- Core molecular dynamics and Monte Carlo techniques
- Hands-on labs involved implementing simulations with simplified models (simpleMD), analyzing phase transitions (e.g., melting and hysteresis), and estimating statistical errors.
Block 2: July 12, 15–16
Electronic structure of molecules and multiscale approaches, covering:
- Quantum chemistry fundamentals (Hartree-Fock, DFT)
- Molecular properties, normal modes, and the effect of solvation
- Multiscale methods for linking quantum and classical regimes
- Laboratory sessions included practical quantum chemistry calculations on small molecules such as water and the Zundel ion, as well as simulations of solvation effects.
Block 3: July 17–19
Data-driven approaches to molecular modeling with an emphasis on physical interpretability:
- Linear models and dimensionality reduction, including PCA and regularization
- Introduction to neural networks, including neural-network potentials and their evolution in the field
- Chemical representations and equivariance.
- Hands-on ML labs, focused on predicting material properties, building invariant and equivariant models, modeling dipole moments in ionic systems
The full program is available at https://github.com/GiovanniBussi/CecamSchool2024.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

In addition to the lectures and hands-on sessions, students had the opportunity to attend four afternoon seminars that expanded on the material covered in the mornings. These seminars, while structured as regular research talks, were delivered by the same instructors who had led the corresponding lectures, fostering an informal and engaging environment. This continuity encouraged active participation from the students, who were well-prepared to ask informed and critical questions. The seminars were particularly effective in highlighting the practical applicability – as well as the inherent limitations – of the theoretical methods discussed during the school. These sessions underscored how many of the most powerful techniques in molecular modeling remain under active development, and helped students recognize where critical thinking and methodological innovation are still needed.
A questionnaire was sent to the student using a Google Form. For each lecture and lab, students were asked about the level and the usefulness of the lecture. 22 students over 24 filled the questionnaire. Results for the individual lectures will be instrumental in reshaping the next editions of the School. Results for the general questions are reported below. It can be seen that, for the majority of the students, the school was very useful in creating a network of contacts. Marks are between 1 (worse) and 4 (best).
- How effective have the school been in facilitating networking with other students: 3 (4 replies), 4 (22 replies)
- How effective have the school been in facilitating networking with PhD students and post-docs: 2 (5), 3 (9), 4 (8)
- How effective have the school been in facilitating networking with professors: 2 (2), 3 (10), 4 (10)
- How did you know about the School: CECAM website (4), Mailing list (5), My advisor (13)
- Would you recommend the school to a friend of yours: 3 (2), 4 (20)

## 3. What was the take-home message for the participants?

The school highlighted how molecular simulations, quantum chemistry, and machine learning provide complementary tools to explore complex systems across scales. Participants learned both the theoretical foundations and practical skills needed to critically apply these methods, gaining awareness of their strengths, limitations, and open challenges.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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- https://github.com/GiovanniBussi/CecamSchool2024
- Lecture materials was shared with the students using a Google Drive: https://drive.google.com/drive/folders/1ilOfF7v4Oh4gkGbkZWNfezuQVxFANWn6

Please note that the google drive folder above contains the solutions to the exercises that were shared with the students in the following days. As we plan to reuse some of these exercises in the next editions of the school, **they are not expected to be made openly available.**

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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Most of the speakers and lecturers were either professors or students affiliated with the organizing institutions (SISSA and SNS) and with the CNR unit hosted at the SISSA campus.
24 students were selected from 11 countries (Czech Republic, Denmark, France, Finland, Germany, Italy, Netherlands, Slovakia, Spain, Turkey, United Kingdom), with a strong female representation (16 female, 8 male). All participants were at the undergraduate level, ensuring equal access to early-stage training opportunities.

## 6. Participant list

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### Organisers

**Brancato, Giuseppe**
Scuola Normale Superiore, Italy
**Bussi, Giovanni**
Scuola Internazionale Superiore di Studi Avanzati, Italy
**Laio, Alessandro**
SISSA, Italy

**Alisler, Ceren** - Izmir Institute of Technology, Turkey
**Barley, Jonathan** - King's College London, United Kingdom
**Bellinzona, Chiara** - King's College London, United Kingdom
**Ben Abdelajoued, Ameni** - Paris Cité, France
**Čančinová, Vanessa** - Czech Academy of Sciences, Czech Republic
**Ceriotti, Michele** - EPFL, Switzerland
**Ciancaleoni, Giorgia** - University of Rome Tor Vergata Italy
**Da Piedade Vieira, Alicia** - Université Gustave Eiffel, France

**Eble, Franziska** - University of Konstanz, Germany
**Gkargolan1@gmail.com, Antonín** - UCT Prague, Czech Republic
**Grisanti, Luca** - Consiglio Nazionale Delle Ricerche, Italy
**Hill, Hannah** - King's College London, United Kingdom
**Idiaquez Valbuena, Ana** - LMGC, France
**Kiuru, Julius** - University of Helsinki, Finland
**Manoza, Ivan** - Queen Mary University of London, United Kingdom
**Mazo, Laura** - University of Barcelona, Spain
**Mtwana, Khanyiso** - Heriot-Watt University, United Kingdom
**Nadison, Josh** - Kings College London, United Kingdom
**Olsen-Green, Oliver** - Heriot-watt University, United Kingdom
**Petti, Stella** - Kings College London, United Kingdom
**Semanaj, Sindi** - Queen Mary University of London, United Kingdom
**Stegani, Bruno** - Università degli Studi di Roma "La Sapienza", Italy
**Tamer, Hilal** - Hochschule Offenburg, Germany
**Trolle, Anna Ida** - University of Copenhagen, Denmark
**Vrba, David** - Comenius University, Slovakia
**Zancanaro, Elena** - Groningen University, Netherlands

# L2M3: Large language models for materials, molecules and beyond

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/l2m3-large-language-models-for-materials-molecules-and-beyond-1291**
**Dates: Jul 9, 2024 - Jul 12, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on the transformative potential of large language models (LLMs) in chemistry and materials science. Participants explored how these tools could transform research processes, from literature review and hypothesis generation to data analysis. While recognizing LLMs' potential to accelerate discovery, the discussion also highlighted challenges in adapting these models to domain-specific tasks and the need for chemistry-specific benchmarks and datasets.

A key topic was the evolving landscape of research organizations, comparing academia, industry, and emerging models like Focused Research Organizations (FROs). The perceived lack of ambition in academic settings was discussed, potentially stemming from structural issues, funding models, and the conflicting objectives of being both a "learning institution" and a "producing institution". In addition, there is an imbalance in engineering and computing resources between academia and industry.

Benchmark design problems were extensively debated. The community recognized the need for more challenging and relevant benchmarks that truly test the capabilities of state-of-the-art models in chemistry and materials science tasks. Current benchmarks, such as MoleculeNet, were considered too easy and inadequate for challenging frontier models. Participants discussed developing benchmarks centered around specific research questions, potentially partnering with journals and industry to create tasks based on real-world chemical problems, and withheld experimental data.

Data generation and quality were central themes. The workshop explored various data generation methods, including high-throughput experimental techniques, computational simulations, and the concept of "black-box data". The importance of negative data - e.g., failed experiments - was debated, acknowledging its current underrepresentation in shared datasets while questioning the cost-benefit ratio of actively pursuing such data.

The limitations of current robotics technology in chemistry were addressed, highlighting the need for setups that don't merely mimic human operations but exploit the unique advantages of automation.

The dual-use nature of advanced AI in chemistry and related biosafety concerns formed a crucial part of the dialogue. Participants grappled with the ethical

implications of AI systems capable of designing novel molecules or materials, emphasizing the need for robust governance frameworks and international collaboration.
Overall, the workshop set the stage for more targeted research efforts, emphasizing the need for better data curation, benchmark development, and organizational structures to advance the field.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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A key outcome was the identification of a critical gap between the current capabilities of Large Language Models (LLMs) and the specific needs of the chemistry domain. While LLMs show promise in tasks like literature review, their ability to perform chemical reasoning remains limited. This realization underscored the urgent need for chemistry-specific AI models and training approaches.
The workshop made substantial progress in outlining requirements for improved chemistry AI benchmarks. Participants agreed that future benchmarks should be significantly more challenging, reflect real-world problems, and assess models' adaptability to new tasks. A novel proposal emerged to partner with journals and industry to create benchmarks based on withheld experimental data, though the implementation details remain to be worked out.
A major outcome was the recognition of the unique data challenges in chemistry AI. A key metric proposed was the "lowest cost per reproducible datapoint," reflecting the need for efficiency in data generation. However, questions persist about the optimal balance of data at different fidelity levels (computational vs. various experimental setups).
The limitations of current robotics and automation in chemistry were brought to light. Participants proposed a paradigm shift in designing automated systems, suggesting they should not merely mimic human operations but exploit unique automation advantages.
Several open questions emerged from the discussions:
- What is the optimal composition of different fidelity levels in chemical datasets?
- How can we create effective synthetic data in chemistry?
- What are the most effective strategies for encoding numerical and structural chemical data for AI models?
- How can we implement "self-play" or similar techniques in the context of chemical AI systems?
- What is the "tacit knowledge" in chemistry that cannot be easily captured in datasets, and how might we incorporate it into AI systems?
In conclusion, the workshop made significant strides in mapping out the landscape of AI applications in chemistry and materials science. It provided a roadmap for future research and development efforts while also highlighting the complexity of the challenges ahead.

## 3. What was the take-home message for the participants?

The workshop focused on the crucial yet challenging task of developing effective AI benchmarks. This difficulty stems from the field's unique characteristics, particularly the tension between open-ended scientific discovery and the need for clear evaluation metrics. Participants agreed that future benchmarks must transcend simple predictions to evaluate a model's chemical reasoning, adaptability, and hypothesis generation.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop outcomes hold significant potential for societal benefits, primarily through accelerating chemical research and materials discovery. As our whitepaper emphasizes, chemistry and materials science represent some of the most impactful applications of AI, with the potential to address pressing global challenges. These advancements could contribute substantially to several UN Sustainable Development Goals, particularly those related to health, clean energy, innovation, and climate action.

However, the workshop also underscored critical dual-use concerns. The same AI systems capable of designing beneficial molecules could potentially be misused to create harmful substances. This reality underscores the urgent need for robust governance frameworks and international cooperation, as detailed in our whitepaper.

To maximize societal benefits while mitigating risks, the workshop highlighted three key priorities:

1. Developing comprehensive guidelines for responsible AI use in chemistry
2. Fostering broad interdisciplinary collaboration across multiple institutions to prevent power centralization and to anticipate and address potential negative consequences
3. Implementing staged release approaches for new models, including monitored API access, to ensure safety and control

In conclusion, the roadmap outlined in our workshop provides a framework to harness AI's power to accelerate chemical discovery for the benefit of society while minimizing potential harm.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

1. Whitepaper in Preparation: A draft whitepaper has been written (https://lmy.de/nUAdj) and is currently being refined.
2. New Research Collaborations: The workshop fostered new collaborative relationships across different career stages. Connections were formed not only

among Principal Investigators (PIs, e.g., Andrew White, Philippe Schwaller, Kevin Jablonka) but also between PhD students (e.g., Marta Skreta and Adrian Mirza).
3. Curated Dataset List: Participants compiled a valuable list of existing datasets.
4. Established Community Platform: A shared Slack channel was created to facilitate ongoing discussion and collaboration among workshop participants.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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Our workshop implemented several measures to promote inclusivity:
- Diverse Participant Selection: We used our networks and targeted searches to assemble a diverse group.
- Career Stage Balance: We mixed junior and senior participants to foster mentorship and diverse perspectives.
- Gender Diversity: We actively approached female researchers, securing seven female participants.
- Geographical Diversity: We invited speakers from various regions and offered remote participation options.
- Inclusive Discussion Format: Panel discussions included people from different career stages, genders, institutions, and backgrounds.

## 7. Participant list

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### Organisers

**Jablonka, Kevin**
Helmholtz Institute for Polymers In Energy Applications, Germany
**Pieler, Michael**
OpenBioML.org, Austria
**Smit, Berend**
EPFL, Switzerland
**White, Andrew**
University of Rochester, United States

**Affinito, Fabio** - CINECA, Italy
**Alampara, Nawaf** - Friedrich-Schiller-Universität Jena, Germany
**Altoe, Piero** - NVIDIA, Italy
**Baghaee Ravari, Sepideh** - Interdisciplinary Centre For Advanced Materials Simulation, Ruhr-Universität Bochum, Germany
**Banerjee, Debarshi** - ICTP - International Centre for Theoretical Physics, Italy
**Borisova, Anna** - EPFL, Switzerland
**Caldas Ramos, Mayk** - University of Rochester, United States
**Chen, Junwu** - EPFL, Switzerland
**Chen, Chi** - Microsoft, United States

**Collison, Christopher** - Rochester Institute of Technology, United States
**Crossan, Steven** - Dayhoff Labs, United Kingdom
**De Fabritiis, Gianni** - University Pompeu Fabra, Spain
**Deb, Jyotirmoy** - CSIR-North East Institute of Science and Technology, India
**Elahi, Seyed Amirmohammad** - EPFL, Switzerland
**Foster, Ian** - University of Chicago & Argonne National Laboratory, United States
**Gil, María Victoria** - Spanish National Research Council (CSIC), Spain
**Golkar, Siavash** - Polymathic AI, United States
**Goswami, Rohit** - University of Iceland, Iceland
**Gressling, Thorsten** - Bayer, Germany
**Hanson, Sonya** - Flatiron Institute, United States
**Jena, Nityasagar** - IFM, Linköping University, Sweden
**Kazimi, Bashir** - FZ Jülich, Germany
**Kim, Seongmin** - Seoul National University, Republic of Korea
**Korotkevich, Alexander** - University of Amsterdam, Netherlands
**Lederbauer, Magdalena** - ETH Zurich, Switzerland
**Lei, Ge** - Imperial College London, United Kingdom
**M Bran, Andres** - EPFL, Switzerland
**Madzhidov, Timur** - Elsevier, United Kingdom
**Malbranke, Cyril** - EPFL, Switzerland
**Manica, Matteo** - IBM Research Europe, Switzerland
**Martinc, Matej** - Jozef Stefan Institute, Slovenia
**Meshhal, Moyassar** - Universität Rostock, Germany
**Messaada, Mariem** - University of Tunis El Manar, Tunisia
**Michael, Ikechukwu Henry** - Ahmadu Bello University, Nigeria
**Miret, Santiago** - Intel Labs, United States
**Mirza, Adrian** - Helmholtz Institute for Polymers In Energy Applications, Germany
**ODonoghue, Odhran** - Oxford University, United Kingdom
**Ojeda, Pedro** - Umeå University, Sweden
**Petersen, Martin** - Technical University of Denmark, Denmark
**Ríos-García, Martiño** - INCAR-CSIC, Spain
**Roy, Aritra** - London South Bank University, United Kingdom
**Schwaller, Philippe** - EPFL, Switzerland
**Seidl, Philipp** - Johannes Kepler University JKU, Austria
**Seifert, Konrad** - Simon Institute for Longterm Governance, Switzerland
**Skreta, Marta** - University of Toronto, Canada
**Tshimula, Jean Marie** - Université de Sherbrooke, Canada
**Van Gerwen, Puck** - EPFL, Switzerland
**Van Herck, Joren** - EPFL, Switzerland
**Wellawatte, Geemi** - EPFL, Switzerland
**Xie, Tong** - University of New South Wales, Australia
**Zhang, Hongbin** - TU Darmstadt, Germany

# CCP5 Summer School

**Location: Newcastle University**
**Webpage : https://www.cecam.org/workshop-details/ccp5-summer-school-1347**
**Dates: Jul 14, 2024 - Jul 25, 2024**

## 1. What were the major topics presented in the School?

School is an introductory intensive and comprehensive training program for early-career researchers, primarily new PhD students, in the field of molecular simulation. The curriculum is designed to provide a solid foundation in the theoretical underpinnings of simulation techniques, complemented by extensive hands-on practical sessions. Main topics are

- **Statistical Mechanics:** The theoretical framework upon which molecular simulation is built. Students are introduced to key concepts such as ensembles, partition functions, and the relationship between microscopic states and macroscopic thermodynamic properties.
- **Molecular Dynamics (MD):** A powerful simulation technique that models the time evolution of a system of interacting particles. Lectures cover the basic algorithms for integrating the equations of motion, the implementation of thermostats and barostats, and the analysis of trajectories to calculate various properties.
- **Monte Carlo (MC) Methods:** This section explores a range of stochastic simulation techniques based on random sampling. Participants learn about the Metropolis algorithm, different Monte Carlo moves for various ensembles.
- **Force Fields:** A critical component of classical simulations, lectures on force fields delve into their parameterization, validation, and the different types available for various systems.
- **Free energy methods**: usage of rare events methods for modelling.

Advanced topics discussed:

- **First-Principles (Ab Initio) Methods:** An introduction to quantum mechanical simulation techniques, such as Density Functional Theory, which allow for the study of electronic structure and chemical bonding without empirical parameters.
- **Mesoscale Methods:** This module focuses on simulation techniques that bridge the gap between the atomic and macroscopic scales, such as Dissipative Particle Dynamics and the Lattice Boltzmann method, which are essential for studying complex fluids.
- **Biomolecular Simulation:** Tailored for those interested in biological systems.
- **Machine Learning for Interatomic Potentials:** Reflecting the latest trends in the field, this increasingly popular module explores how machine learning techniques can be used to develop highly accurate and efficient interatomic potentials from quantum mechanical data. In addition to these students, get to attend research seminars, present their research during a poster session with prizes and selected few present during a student research seminar.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

In general school is very well received with students appreciating the breadth of the subjects discussed. This is very important since there is a modern tendency for early specialisation. Limitations noticed by lecturers in general relate around variable level of mathematics showed by participants. This can make courses around statistical mechanics or advanced Moleculard Dynamics and Monte Carlo challenging. During hands on sessions there are few problems reported mainly due to the movement to cloud environments which allowed us to remove previsible issues. Some students prefer more in depth exercises with writing the code, however this is not a time effective solution for all the cohort who in general are not very well versed in programming.
Advanced course are positively received since they align much better with current research topics of the students. One issue raised is related to the fact some students expect to learn how to use a code, rather than the methodology underpinning.

## 3. What was the take-home message for the participants?

Molecular and Materials modelling is a diverse field that can model very diverse systems with various levels of accuracy.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

all material for the school is available online for students to study independently. https://ccp5.gitlab.io/summerschool/
Lectures are circulated separately into electronic format.

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

75 students from UK and oversees took part this year with a roughly 50/50 split. Gender split was approximately 45% female and 55% male , with the first two days being dedicated to computer programming classes, Fortran and Python, which students choosing one of them. No real need other than blind review of applications was needed to achieve this. By choosing students from different fields means we need to accommodate to different levels of hard skills in computing and mathematics.

## 6. Organizers list

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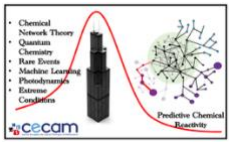
**Allan, Neil**
School of Chemistry, University of Bristol, United Kingdom
**Dawson, James**
Newcastle University, United Kingdom
**Elena, Alin**
Science and Technology Facilities Council - Scientific Computing, United Kingdom
**Freeman, Colin**
University of Sheffield, United Kingdom




# Frontiers of computational reaction prediction

**Location: University of Chicago**
**Webpage : https://www.cecam.org/workshop-details/frontiers-of-computational-reaction-prediction-1348**
**Dates: Jul 15, 2024 - Jul 17, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The event was focused on methods and applications of chemical reaction prediction. Several new or recently developed workflow tools for reaction exploration were presented, including the nanoreactor, Chemoton, YARP, and AutoMech. There were also new approaches aiming to extend the more well developed discovery frameworks for isolated molecular species in their ground states to materials systems with periodic boundary conditions or photochemistry involving excited electronic states and surface-crossings. All of the reaction discovery workflows depend critically on the description of reactive potential energy surfaces. Thus, there were also presentations focused on improved efficient electronic structure methods (including semiempirical methods) and machine learned interaction potentials (MLIPs). Another key enabling technology for reaction discovery is the automated identification of minima representing reactants and products and minimum energy paths (MEPs) connecting them. Several presenters discussed the latest advances in the robust determination of MEPs. Finally, a number of applications of reaction discovery methods were presented, including the design of recyclable polymers and transition metal catalysts.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop achieved substantial knowledge exchange among leading researchers, facilitating direct comparison of unpublished results and methodologies across different research groups. This created valuable networking opportunities between methods developers and practitioners applying reaction prediction tools, fostering cross-pollination of ideas and identifying complementary research directions.
A key outcome was the sharpened resolution of existing disagreements within the field, particularly regarding whether reaction coverage versus computational

efficiency represents the primary bottleneck for practical applications. Some groups emphasized the need for more comprehensive reaction space exploration, while others prioritized developing faster, more scalable algorithms. This debate sharpened the understanding of areas for further methods development.
Several limitations and open questions emerged from discussions. The scalability of current methods to industrially relevant systems remains challenging, with most demonstrations limited to relatively small molecular systems. The transferability of machine-learned potentials across different chemical spaces requires further investigation, as does the development of robust uncertainty quantification methods for reaction predictions. Integration of reaction prediction workflows with experimental validation protocols was identified as an underexplored area requiring attention.
The workshop also revealed gaps in handling complex reaction mechanisms involving multiple steps, competing pathways, and solvent effects. Participants noted that while significant progress has been made in single-step reaction prediction, multi-step synthetic route planning and catalyst deactivation mechanisms remain largely unaddressed. These discussions have already sparked new collaborative efforts aimed at tackling these challenges.

## 3. What was the take-home message for the participants?

The field has reached a critical turning point where multiple practical algorithms are now available for non-practitioners to perform actionable chemical reaction predictions. The transition from research tools to accessible computational platforms enables broader adoption across industry and academia, democratizing advanced reaction prediction capabilities.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The maturation of computational reaction prediction holds transformative potential for addressing global challenges through accelerated chemical innovation. In sustainability, these tools can expedite the discovery of recyclable polymers and biodegradable materials, reducing plastic waste and environmental impact. For energy applications, automated catalyst design can accelerate development of more efficient fuel cells, batteries, and solar energy conversion systems.
In pharmaceutical development, reaction prediction methods can streamline drug discovery by identifying novel synthetic routes and predicting potential metabolic pathways, potentially reducing development timelines and costs. This is particularly valuable for rare disease treatments where traditional trial-and-error approaches are economically prohibitive.
The tools also promise to revolutionize chemical manufacturing by enabling the discovery of greener synthetic pathways that minimize waste and reduce environmental footprints. Automated exploration of reaction space can identify

previously unknown routes to important chemicals using more abundant or less toxic starting materials.
Beyond specific applications, these methods can democratize chemical innovation by making sophisticated computational tools accessible to researchers and companies without extensive computational chemistry expertise. This broader accessibility could accelerate scientific discovery across diverse fields, from materials science to biochemistry, ultimately benefiting society through faster innovation cycles and more sustainable chemical processes.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Several concrete outcomes have emerged from the workshop. Multiple new collaborations were initiated between participants, already resulting in joint preprints and publications that combine different methodological approaches. Several groups have begun developing interoperable software interfaces to enable seamless integration of different reaction prediction tools (e.g., machine learning potentials with new TS search algorithms).

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

For invited speakers efforts were made to ensure that researchers working on all aspects of reaction prediction were represented (e.g., those applying existing methods to specific areas, as well as those developing new algorithms). From this pool efforts were also made to ensure geographical and career stage diversity based on publicly available information. Over half of workshop participants were invited.

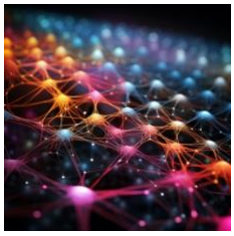
## 7. Participant list

### Organisers

**Jackson, Nick**
University of Illinois, Urbana-Champaign, United States
**Lindsey, Rebecca**
University of Michigan, Ann Arbor, United States
**Martinez, Todd**
Stanford University, United States
**Savoie, Brett**
University of Notre Dame, United States

**Bannwarth, Christoph** - RWTH Aachen University, Germany
**Bonella, Sara** - CECAM HQ, Switzerland
**Broadbelt, Linda** - Northwestern University, United States
**Calcagno, Francesco** - University of Bologna, Italy
**Cavalli, Andrea** - CECAM HQ, Switzerland
**Clark, Aurora** - University of Utah, United States
**Curtin, Gregory** - University of North Carolina at Chapel Hill, United States
**Della Libera, Andrea** - Politecnico di Milano, Italy
**Ghidini, Alessia** - EPFL - CECAM, Switzerland
**Goswami, Rohit** - University of Iceland, Iceland
**Grimme, Stefan** - University Bonn, Germany
**Haug, Graham** - Colorado State University, United States
**Isayev, Olexandr Isayev** - Carnegie Mellon University, United States
**Jakhar, Rishika** - University of Chicago, United States
**Jorner, Kjell** - ETH Zurich, Switzerland
**Kalita, Bhupalee** - Carnegie Mellon University, United States
**Kim, Changhae** - University of Illinois Urbana-Champaign, United States
**Kim, Seonghwan** - University of Illinois, United States
**Klippenstein, Stephen** - Argonne National Laboratory, United States
**Koegel, Jadon** - University of Utah, United States
**Kopp, Wassja** - Heinrich Heine University, Germany
**Kozarekar, Shivani** - Northwestern University, United States
**Kuboth, Philipp** - Heinrich Heine Universität, Germany
**Kulik, Heather** - MIT, United States
**Li, Zhao** - Purdue University, United States
**Liu, Xiaoyang** - Northwestern University, United States
**Luo, Siwei** - Univeristy of Chicago, United States
**Manoj, Uday Sankar** - Pennsylvania State University, United States
**Mayagoitia, Alvaro** - Argonne National Laboratory, United States
**Meisner, Jan** - Heinrich Heine University, Germany
**Meissner, Jan** - Heinrich-Heine-Universität Düsseldorf, Germany
**Miller, Ericka** - Case Western Reserve University, United States
**Mohanakrishnan, Rohith Srinivaas** - UCB, United States
**Parker, Shane** - Case Western Reserve University, United States
**Paton, Robert** - Colorado State University, United States
**Peters, Baron** - University of Illinois, United States
**Pieri, Elisa** - UNC Chapel Hill, United States
**Qin, Andrew** - University of Chicago, United States
**Rodriguez Ropero, Francisco** - Procter & Gamble, United States
**Seal, Aniruddha** - University of Chicago, United States
**Shaw, Alex** - Northwestern University, United States
**Shen, Chen** - TU Darmstadt, Germany
**St. Michel, Roland** - Massachusetts Institute of Technology, United States
**Stirnemann, Guillaume** - Ecole Normale Superieure and CNRS, France
**Strachan, Alejandro** - Purdue University, United States
**Toney, Jacob** - Massachusetts Institute of Technology, United States

**Troni, Federica** - CECAM HQ - EPFL, Switzerland
**Wardzala, Jacob** - University of Chicago, United States
**Wei, Yihui** - University of Utah, United States
**Weymuth, Thomas** - ETH Zurich, Switzerland
**Wititsuwannakul, Taveechai** - University of Michigan, United States
**Wood, Mitchel** - Sandia National Laboratory, United States
**Wu, Jason** - University of Illinois Urbana-Champaign, United States
**Zhang, Quan** - Northwestern University, United States
**Zhu, Ray** - University of Chicago, United States
**Zimmerman, Paul** - University of Michigan, United States



# Frontiers in many-body excited-state dynamics from first principles

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/frontiers-in-many-body-excited-state-dynamics-from-first-principles-1278**
**Dates: Jul 15, 2024 - Jul 17, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Extensive research is dedicated to studying excited-state phenomena when materials are exposed to light. Our workshop involved research that provides valuable insights into the relationship between material's structure and functionality for a range of applications, from energy conversion to quantum information storage.

Recent advances in ultrafast pump-probe spectroscopy have led to the discovery of emergent transient quantum phenomena and new capabilities to track excited-state dynamics at unprecedented temporal and spatial resolution. These spectroscopic measurements encode complicated signatures of lattice, electronic, and multiparticle dynamics, occurring on different time and energy scales and in different regions of momentum space, which are beyond the capabilities of standard first principles theories to unravel. Consequently, in parallel with advances in spectroscopy, there has been a concerted effort to develop new predictive first-principles theories and computational tools that can rigorously account for time-dependent many-body correlations and their coupling with the lattice.

Green's function approaches based on many-body perturbation theory represent the state-of-the-art for calculating excited-state spectra in the low-field linear response regime. Recent advances in the field include the development of Green's function based nonequilibrium and perturbative approaches allowing for accurate simulations of processes such as transient absorption, time-resolved angle-resolved photoemission (TR-ARPES), two-photon absorption spectra, and nonlinear spectroscopies and supply insights into the interactions of a zoo of quasiparticles, like electrons, excitons, phonons, polarons, etc.

These topics were wonderfully and pleasantly discussed in our workshop.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

Our workshop focused on new advances in the development and application of first-principles non-equilibrium many-body dynamics in emerging materials for quantum science. While the workshop was primarily aimed at discussing the theoretical aspects, we covered a rich diversity of materials, methods, and applications, in connection with recent experimental advances. Through the presented research and discussions, we accomplished an updated view of state-of-the-art approaches to first-principles computations of excited-state dynamics in quantum materials, as well as challenges and new and emergent directions in the field.

All participants were engaged, gave wonderful talks and conducted fruitful discussions in between. Leading theoreticians and experimentalists in the field were involved, as well as young faculty, students, and postdocs. Mist of the participants were theoreticians from different communities, who are using a variety of models and computational methods to describe dynamics of excited states in functional materials. We also included leading experimentalists in the field, who are exploring time-resolved phenomena in materials. Such diversity encouraged discussions, generated common ground and collaboration opportunities, and identified emerging questions for future research directions.

The role of light-induced and phonon-assisted quantum interactions in the many-body description and its relation to quantum data science was discussed, as it is studied in recent years from analytical and many-body perturbation theory perspectives. In addition, several talks discussed new insights into associated non-equilibrium dynamics. Both the experimental and theoretical tools involved are new and ongoing, making this topic fundamental in the near-future development of quantum dynamics studies in materials.

From the theoretical perspective, newly developed approaches based on Green's function methods and time-dependent density functional theory, as well as density-matrix and other approaches, were presented; other theoretical directions include the merging of phenomenological methods with ab initio understanding when accounting for phonon coupling. Associated studies discussed related developments and applications.

## 3. What was the take-home message for the participants?

New numerical techniques, such as ab-initio data-driven methods and quantum embedding theories, mark a new era in which many-body predictive approaches can be merged with data analysis, opening the door to accurate predictions of quantum state evolution in realistic materials.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The theoretical approaches and method development presented in this workshop represent new computational horizons of non-equilibrium and time-resolved dynamical excited-state phenomena, including explicit time propagation methods as well as perturbative approaches. The vast majority of these new theoretical directions are based on ongoing code development within existing packages, most of which are publicly available. It is of growing interest to connect such different codes for optimal application, and related efforts are forming these days through mutual grant applications and cross-methodological collaborations. The networking aspect within this community is, however, not trivial. Most of the related scientific meetings typically consider either specific methods - e.g. electronic structure methods, wavefunction-based approaches, or phenomenological models- or specific materials and applications, limiting the scope of the discussed underlying phenomena.
The main goal of this workshop was to bring together researchers and students from different backgrounds and identify common interests primarily associated with the underlying phenomena. Our aim was to generate an open and diverse environment for all participants to familiarize themselves with a variety of relevant theoretical and computational methods on the one hand, and a collection of materials and applications on the other. The fruitful and enriching scientific discussions that emerged during and after the workshop are evidence of such common interests and will hopefully lead to future interactions in the field.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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The workshop was funded by both CECAM and psi-K. Possible funding sources for related collaborations include personal Europe- and US-based funding grants of individual participants (ERC starting and consolidator, NSF), as well as common grants, such as a Horizon-DN networking recently-submitted grant applications, including a number of participants. Joint research is already being performed by many of the participants. One of the main goals of the workshop is to establish pathways for new collaborations, as well as new connections between theoretical and computing approaches that do not trivially merge. Despite the online format, the workshop included stimulating discussions that can potentially lead to such new interconnections.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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Our field includes highly talented researchers of all genders and forms. Gladly, our workshop reflected this in gender diversity as well as participants coming from various countries and scientific cultures.

## 7. Participant list

### Organisers

**Filip, Marina**
University of Oxford, United Kingdom
**Qiu, Diana**
Yale University, United States
**Refaely-Abramson, Sivan**
Weizmann Institute of Science, Israel

**Ahammed, Raihan** - Indian Institute of Technology Kanpur, India
**Amit, Tomer** - Weizmann Institute of Science, Israel
**Calandra, Matteo** - University of Trento and CNRS, Italy
**Caruso, Fabio** - University of Kiel, Germany
**Chan, Yang-Hao** - Academia Sinica, Taiwan
**Chatterjee, Banhi** - Faculty of Physics, University of Duisburg-Essen, Germany
**Cohen, Galit** - Weizmann Institute of Science, Israel
**Esteve-Paredes, Juan José** - Autonomous University of Madrid, Spain
**Giustino, Feliciano** - The University of Texas at Austin, United States
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**Leoni, Luca** - University of Bologna, Italy
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**Monserrat, Bartomeu** - University of Cambridge, United Kingdom
**Neaton, Jeffrey** - University of California, Berkeley, United States
**Paleari, Fulvio** - National Research Council, Italy
**Perfetto, Enrico** - University of Roma Tor Vergata, Italy
**Quek, Su Ying** - National University of Singapore, Singapore
**Reho, Riccardo** - University Of Utrecht, Netherlands
**Reining, Lucia** - CNRS-Ecole Polytechnique, France
**Sangalli, Davide** - Istituto di Struttura della Materia (ISM - CNR), Italy
**Steinitz-Eliyahu, Rachel** - Weizmann Institute, Israel
**Verdi, Carla** - University of Queensland, Australia
**Vosco, Guy** - Weizmann Institute of Science, Israel
**Wiktor, Julia** - Chalmers University of Technology, Sweden

# International guest student programme on computational science

**Location: CECAM-DE-JUELICH**
**Webpage : https://www.cecam.org/workshop-details/international-guest-student-programme-on-computational-science-1320**
**Dates: Aug 5, 2024 - Oct 11, 2024**

## 1. What were the major topics presented in the School?

A total of 10 students (9 male, 1 female) were selected for this year's program, representing 7 different countries. This diversity provided an enriching international environment for all participants. The number of applications increased compared to the previous year, reflecting growing interest; however, further outreach efforts are planned to boost applications for next year, with the goal of reaching 12–15 students and achieving a better gender balance.
The program began with two weeks of intensive training in parallel programming. Students received instruction in both fundamental and advanced concepts using OpenMP, MPI, and CUDA. Additionally, they were introduced to the Jülich Supercomputers, learning how to access and effectively use these powerful systems to develop and execute their codes.
Research topics addressed this year included evaluation of computer architectures, molecular dynamics, data analysis, lattice QCD, and the fast multipole method for electrostatics. These provided a broad and challenging platform for the students' learning and development.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Following the initial course phase, each student was individually assigned to a research group within the Jülich Supercomputing Centre (JSC). These assignments allowed students to become directly involved in ongoing scientific projects, fostering close interaction with experienced researchers. Research topics were either proposed by the group leaders based on current scientific priorities or were brought in by the students themselves, allowing for a degree of personalization and alignment with individual interests.
Due to the limited duration of the program, the scope of research projects had to be adjusted accordingly. While this timeframe allowed for meaningful engagement with complex topics, it also meant that some questions and challenges remained open at the program's conclusion. Despite this, the students were able to make notable progress and gain a substantial understanding of the subject matter.

The experience provided the participants with valuable exposure to real-world scientific research and advanced computational methods. The insights gained are expected to significantly influence the students' academic trajectories, helping them refine their interests and potentially guiding their decisions regarding future studies, including master's theses or even doctoral research.

### 3. What was the take-home message for the participants?

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The students gained high-level programming experience with MPI, OpenMP, and CUDA, working on state-of-the-art CPU and GPU architectures. They benefited from valuable peer interaction, supporting each other through challenges. Additionally, they developed skills in scientific communication by writing a report and presenting their work in a professional research setting.

### 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

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The students prepared and delivered presentations as part of a colloquium held at JSC. In addition, they gained experience in writing scientific and technical reports, with each student required to document their project in a written report. There are plans to publish these individual reports as a collected volume in the form of a JSC technical report.

### 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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Candidate selection is based solely on the quality of applications and the applicant's interest in the program. Every effort is made to avoid bias related to nationality or gender during the evaluation process. The program is advertised in a neutral and inclusive manner, giving no preference to any specific group. When candidates have similar qualifications for a given topic, priority may be given to achieve a more balanced gender distribution among participants.

### 6. Organiser list

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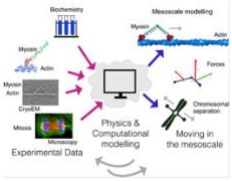
**Kabadshow, Ivo**
Research Centre Jülich, Germany
**Sutmann, Godehard**
Forschungszentrum Juelich, Germany




# Biomolecular Simulations at the Mesoscale

**Location: University of Trento, Italy**
**Webpage : https://www.cecam.org/workshop-details/biomolecular-simulations-at-the-mesoscale-1330**
**Dates: Aug 26, 2024 - Aug 29, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop "Biomolecular Simulations at the Mesoscale" provided a unique opportunity for researchers to focus on the challenges and opportunities in the rapidly evolving field of mesoscale simulations. The event brought together experts from various disciplines, fostering discussions around key themes of the workshop: (1) defining the biological mesoscale, (2) addressing experimental questions and challenges, and (3) exploring computational methods, both in terms of their successes and limitations. The workshop began by tackling the question of what exactly constitutes the biological mesoscale. Unlike the atomic or molecular scales traditionally explored in biophysics and structural biology, the mesoscale deals with structures and processes that bridge the gap between molecular and cellular dimensions. This scale often includes assemblies of molecules that play crucial roles in cellular function. Participants debated how best to define and model these complex systems, emphasizing the importance of connecting molecular interactions with larger-scale biological phenomena. The discussions underscored that mesoscale simulations must account for both the physical properties of molecules and the emergent behaviors that arise from their collective interactions. These models can provide insights into crucial processes such as signal transduction, intracellular transport, and molecular crowding. The second major topic of the workshop focused on the experimental challenges of studying biological systems at the mesoscale. While advances in experimental techniques, such as cryo-electron microscopy and super-resolution imaging, have made it possible to visualize structures at the mesoscale, there remain significant hurdles in linking these experimental observations with the dynamic behaviors of biomolecules. One of the recurring themes was the need for better integration of experimental data with computational models. Workshop participants emphasized the importance of developing hybrid approaches that combine experimental data with computational methods to achieve a more comprehensive understanding. The workshop's final theme centered around the computational methods used for simulating mesoscale biological systems. These include coarse-grained modeling, molecular dynamics (MD) simulations, and advanced algorithms for simulating large biomolecular complexes. Participants highlighted several success stories

where computational methods have provided significant insights into mesoscale systems. At the same time, the limitations of current computational methods were openly discussed. In particular, there were concerns about the scalability of certain algorithms and the difficulty of accurately modeling long timescales, which are often crucial for understanding mesoscale processes. A key point of the discussion was the role of machine learning and artificial intelligence in advancing computational techniques.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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One of the most significant outcomes of the workshop was the realization that the challenges posed by mesoscale biological simulations require a collaborative effort from multiple disciplines, including biology, physics, chemistry, and computer science. The event fostered an environment of cooperation, with researchers expressing a strong desire to form a more integrated community that can tackle these complex problems together. The workshop organizers and participants committed to promoting inclusivity, ensuring that early-career scientists and researchers from underrepresented groups are actively involved in future collaborations. There was also a consensus that future initiatives should focus on creating shared resources, such as open-access simulation tools, databases, and platforms for sharing experimental and computational data. By building a cooperative and inclusive community, the participants believe that they can collectively address the outstanding questions and advance the field more effectively.

## 3. What was the take-home message for the participants?

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By focusing on the definition of the biological mesoscale, exploring the experimental challenges, and critically evaluating the successes and limitations of current computational methods, the event provided valuable insights into future directions. The commitment to fostering a collaborative and inclusive research community is a major step forward in addressing mesoscale biological systems, ensuring that future progress is made in a cooperative and open scientific environment.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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The outcomes of the "Biomolecular Simulations at the Mesoscale" workshop hold significant potential for societal benefits. By advancing our understanding of complex biological systems at the mesoscale, the insights gained could lead to

breakthroughs in health and medicine. For instance, mesoscale simulations could provide crucial information about cellular processes involved in diseases, enabling the development of more effective treatments or therapies, especially for conditions like cancer or neurodegenerative diseases. Moreover, the integration of advanced computational methods with experimental techniques could streamline drug discovery, reducing both the time and cost of bringing new medications to market. The workshop also emphasized the importance of collaboration and interdisciplinary research, fostering a community that can tackle pressing global health challenges. Overall, the knowledge and strategies developed from this workshop could directly impact human health, biotechnology, and pharmaceutical industries, offering widespread societal benefits.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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The workshop identified key steps to make mesoscale simulations FAIR (Findable, Accessible, Interoperable, Reusable). The first challenge is the diversity of methods and scales, which makes usability difficult. To address this, the community should learn from fields like atomistic MD, weather models, and aerospace. A roadmap was suggested: build a common repository for codes, ensuring they are findable with supplementary materials (papers, movies), and accessible by being free for academics with clear instructions. Community building through workshops and collaborations will promote interoperability, while comparisons of complementary codes will improve reproducibility. Future goals include creating experimental data sets for validation and making codes user-friendly to encourage reuse. Practical actions involve writing a community paper, identifying collaborators, and organizing a future meeting, with the aim of advancing mesoscale modeling more efficiently.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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To promote inclusivity at the "Biomolecular Simulations at the Mesoscale" workshop, we ensured diverse representation across multiple dimensions. Speakers and participants were selected with attention to gender balance, ensuring strong female representation. We also made efforts to include individuals from various geographical regions, including under-represented countries in both Europe and beyond. Early-career researchers were encouraged to participate and present, fostering an inclusive environment across career stages.

## 7. Participant list

### Organisers

**Amaro, Rommie**
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**Beaules, Lea** - Sorbonne Université, France
**Beccaria, Riccardo** - Heidelberg Institute for Theoretical Studies - HITS, Germany
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**Bravo Vidal, Adrià** - University of Copenhagen, Denmark
**Breoni, Davide** - Università di Trento, Italy
**Brown, Chelsea** - University of Groningen, Netherlands
**Calza, Alessandro** - University of Bologna - UNIBO, Italy
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**Cocking, Ryan** - University of Sheffield, United Kingdom
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**Coshic, Kush** - Max Planck Institute of Biophysics, Germany
**Covino, Roberto** - Frankfurt Institute for Advanced Studies, Germany
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**Henrich, Oliver** - University of Strathclyde, United Kingdom
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**Leva, Federico** - COMSOL SrL, Italy
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**Martzel, Nicolas** - MFPM, France
**Mazza, Fabio** - Università di Trento, Italy
**Micheloni, Manuel** - University of Trento, Italy
**Monticelli, Luca** - CNRS, France
**Morand, Jules** - University of Trento, Italy
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**Paternoster, Costanza** - University of Trento, Italy
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**Trovato, Antonio** - University of Padova, Italy
**Van Der Hoek, Pieter** - SISSA, Italy
**Voth, Gregory** - University of Chicago, United States

# Machine Learning potentials: from interfaces to solution

**Location: Ruhr University Bochum**
**Webpage : https://www.cecam.org/workshop-details/machine-learning-potentials-from-interfaces-to-solution-1318**
**Dates: Aug 27, 2024 - Aug 29, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on the simulation of liquids (mostly water) at interfaces with machine learning potentials. This involved five major topics:
- Access to accurate and robust reference data, in particular beyond DFT quality
- Improving the accuracy, transferability, and speed of MLPs
- Efficient large-scale simulations with accurate electrostatics employing variable charges
- More accurate incorporation of non-bonded long-range interactions
- Improved training strategies for interfaces and molecular solutions covering a large configuration space

These five topics are critical for advancing the state of the art in the field. Accordingly, we had invited selected, eminent speakers that were able to represent cutting edge research in this area. In addition, we had organized three discussions that were led by leading scientists: 1. The role of workflows for the development of machine learning interatomic potentials, including data beyond density functional theory and including charge transfer. 2. Coarse graining and its role for the development of accurate machine-learning based methods that enable the simulation of biomolecules in water. 3. A discussion on accuracy and transferability of current machine learning interatomic potentials and ways forward.

It was recognized by the attendees that the leading edge of research in machine learning potentials for water and interfaces was presented and discussed at the workshop. Many participants actively contributed to the discussion sections, with many questions and answers between participants, which partly extended also into the coffee breaks. The close and fruitful exchange between the scientists at different levels of experience also contributed to the further development of the field.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The simulation of water and interfaces with machine learning interatomic potentials is a fast moving field with many exciting developments. The community undertakes efforts to build machine learning interatomic potentials on databases of reference calculations from post Hartree Fock methods, such as the coupled cluster method. Furthermore, charge transfer is still challenging for most of the machine learning potentials to date. This workshop highlighted that this is another important area that the community needs to focus on for more reliable and transferable simulations. Furthermore, while great progress in the field has been made, the structure and format of machine learning potentials is far from settled. Potentials are required that can be parameterized efficiently, that are accurate and that are fast. To date none of the available potentials matches all these criteria.
Therefore, in summary the primary outcome of the workshop was that tremendous progress was made in the field during the past few years, but significant efforts for the topics training data beyond density functional theory, charge transfer and format of the potentials still need to be made. Possible ways how the field can move forward in that direction were discussed.

## 3. What was the take-home message for the participants?

The key message was: At this workshop the cutting edge of machine learning potentials for water and interfaces was presented and discussed. The workshop identified open questions and gave directions for new research.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Progress in the simulation of water, interfaces and solvation can have benefits in many fields with a societal impact, for example, medicinal chemistry, improvements in catalysis, and materials science.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

We had feedback from several participants that the workshop should be repeated annually as the field needs a platform to meet and to discuss, to coordinate activities, to demonstrate progress and to generate research ideas. We therefore plan to establish a regular workshop in the area of machine learning potentials for

water, interfaces and solvation. Furthermore, as far as we are aware, several researchers have initialized collaborations with specific plans for funding.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Offering the workshop in hybrid mode enabled the participation of many researchers that otherwise could not have attended. In fact, about 250 participants from nearly all over the world participated online. Furthermore, among the onsite participants, we ensured a balance between early career and experienced researcher. We further ensured that different genders were represented accordingly. All invited speakers came from Europe and the United States of America.

## 7. Participant list

### Organisers

**Alibakhshi, Amin**
SISSA, Italy, Italy
**Behler, Jörg**
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**Drautz, Ralf**
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***, Anmol** - Indian Institute of Technology Delhi, India
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**Afolabi, Inioluwa** - University of Cambridge, United Kingdom
**Aghamolapour, Hossein** - Khatam University, Iran
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**Ammothum Kandy, Akshay Krishna** - Sorbonne University, France
**Anand, Gautam** - Indian Institute of Engineering Science and Technology, India
**Aouina, Ayoub** - Ruhr University Bochum, Germany
**Apergi, Sofia** - INSA Rennes, France

**Avula, Nikhil** - Jawaharlal Nehru Centre for Advanced Scientific Research, India
**Azar, Said** - Assistant Professor of Physics, Jordan
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**Banafsheh, Mojdeh** - Academielab, Switzerland
**Banerjee, Debarshi** - ICTP - International Centre for Theoretical Physics, Italy
**Batalović, Katarina** - VINCA Institute, University of Belgrade, Serbia
**Ben Abdelajoued, Ameni** - Paris Cité, France
**Bhasker Ranganath, Suman** - Stanford University, United States
**Bidoggia, Davide** - University, Italy
**Biswas, Tanmay** - Technische Universität Wien, Austria
**Bochkarev, Anton** - Materials Center Leoben Forschung GmbH, Leoben, Austria
**Bose, Sankhadeep** - Vellore Institute of Technology, India
**Boujnah, Mourad** - CINVESTAV, Mexico
**Brauer, Jakob** - University of Bremen, Germany
**Bro-Jørgensen, William Dilys** - University of Copenhagen, Denmark
**Buchmueller, Kai** - University of Bonn, Germany
**C. Lourenço, Tuanan** - University of São Paulo, Brazil
**Camposano, Anthony Val** - University of Oslo, Norway
**Casalini, Elio** - University of Duisburg - Essen, Germany
**Casar, Ziga** - Durham University, United Kingdom
**Castelli, Lorenzo** - Università di Trento, Italy
**Chalykh, Olga** - No, Russian Federation
**Chattopadhyay, Rajorshi** - University of Cologne, Germany
**Chaudhuri, Simran** - UCSD, United States
**Chico, Frank** - National University of Trujillo, Peru
**Choutipalli, Venkata Surya Kumar** - Temple University, United States
**Clavier, Germain** - CIMAP, Unicaen, France
**Clementi, Cecilia** - Freie Universität Berlin, Germany
**Csanyi, Gabor** - University of Cambridge, United Kingdom
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# Peptides in biology and materials: bridging simulation and experimental data

**Location: CECAM-IT-SIMUL - University of Florence, Italy**
**Webpage : https://www.cecam.org/workshop-details/peptides-in-biology-and-materials-bridging-simulation-and-experimental-data-1333**
**Dates: Aug 30, 2024 - Aug 31, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop was held as an independent satellite alongside the 37th European Peptide Symposium – 14th International Peptide Symposium. The program featured four key thematic sessions: Peptide-Membrane Interactions, Peptide Design & Methods, Peptide-Based Materials, and Peptide-Protein Interactions. A keynote lecture opened each session by presenting cutting-edge research in a different area of peptide science: Robert Vácha showed a novel strategy for the development of de-novo pore-forming peptides based on computational design and experimental verification; Ora Schuler-Furman brought to the audience her experience in methods for the prediction of peptide-protein interactions, showing the advantages for the study of protein-protein interfaces; Carole Perry elucidated the key role of combined computational-experimental approaches in gathering insights into the interactions between peptides and inorganic materials; finally, Martin Zaccharias, provided a striking presentation of promising results in the investigation of peptide-protein interactions in the context of amyloid fibrils. Inspiring talks were provided, among others, by Themis Lazaridis, Richard Pastor, Alexandre Bonvin, Inanc Birol, Massimiliano Bonomi, Alessandro Contini, Carlos Aleman, and Attilio Vargiu.

The event underscored the expanding scope of peptide science, discussing its pivotal role in biological and material applications and highlighting the remarkable and specific challenges involved in in-silico studies of peptides. In particular, the main difficulties in simulating the dynamics of peptides that arise from their intrinsic flexibility and the importance of kinetic effects were addressed. Peptides represent a sort of “middle ground” between small, often rigid, molecules and well-ordered bio-macromolecules (such as proteins). Consequently, integrated approaches where experimental data and computations are used synergistically have emerged as the main route to follow.

Several presentations discussed recent developments aimed at increasing the efficacy of sampling of conformational spaces by using “low-resolution” approaches, such as coarse-grained force fields and enhanced sampling techniques. On the other hand, the increasing feasibility of using higher-resolution descriptions of the systems, such as titrable and polarizable force fields, has also

been addressed. Both fields will represent the frontiers of computations in peptide science, together with the possibility of improving experiment-guided computational techniques.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

Before this event, the community of computational peptide science lacked opportunities to meet in a workshop environment that would bring together experts from related but still different fields and allow them to tackle problems also using expertise unrelated to peptide science.
The primary outcome of the workshop was to stimulate the discussion about the application of known techniques developed in other contexts to the specificity of peptides. The consciousness of the necessity of a tight integration between experimental and computational methods emerged in all the thematic sessions.
Being held as an independent satellite event of the European Peptide Symposium, provided the workshop with an invaluable opportunity to gather scientists from different fields, including those less focused on peptide research, and to foster interaction with experts attending the main symposium. By promoting collaboration between researchers from different disciplines, the workshop has fostered the development of novel therapeutic strategies, biomaterials with enhanced properties, and innovative approaches to address health-related societal challenges.

## 3. What was the take-home message for the participants?

The key takeaway from the workshop highlighted the significant role of long-time scales in understanding peptide activity, particularly in relation to kinetic effects involved in pore formation. In this context, integrative modeling and coarse-grained approaches are recommended to effectively address the large conformational variability of peptides over long-time scales. These methods have already demonstrated their effectiveness and offer a promising avenue for future research.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop covered topics such as membrane-active peptides as promising antimicrobials, peptide inhibitors of protein-protein interactions as potential drugs, and innovative peptide-based materials. By deepening the understanding of peptide behavior, structure-function relationships, and design principles, the workshop has paved the way for future breakthroughs in drug discovery, targeted therapies, and high-performance materials. The societal benefits from these topics

are extensive, including advances in healthcare, biotechnology, and the development of environmentally friendly materials. These innovations can positively impact various sectors. These advancements hold the potential for significant economic impact by attracting investments, fostering innovation, and creating opportunities for commercialization and market growth in related industries.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The limited size of the workshop, along with social events such as the social dinner and coffee breaks, fostered an informal atmosphere conducive to networking and collaboration – one of the event's primary goals. Indeed, during the concluding remarks, participants expressed interest in making this kind of workshop a regular event, further strengthening the community of researchers working at the interface of experimental and computational peptide studies.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop welcomed a diverse group of participants, with 50 attendees selected from a large pool of prospective candidates. The selection emphasized gender equality (two women out of four keynote speakers) and geographical diversity, featuring scientists from various countries, including the United States, Canada, Israel, India, Singapore, and several European nations. Inclusivity across career stages was ensured by having early-career researchers deliver most of the short talk (20 minutes each) presentations. Two poster sessions provided further opportunities for contributions across all workshop topics. To support younger participants, the Italian Society of Pure and Applied Biophysics (SIBPA) provided three bursaries covering travel and accommodation costs for early-career attendees.

## 7. Participant list

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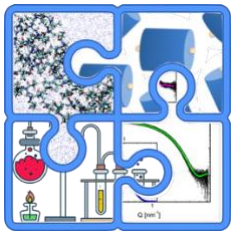

# Exploring bio-inspired systems: a synergy between multiscale experimental and computational approaches

**Location: CECAM-AT**
**Webpage : https://www.cecam.org/workshop-details/exploring-bio-inspired-systems-a-synergy-between-multiscale-experimental-and-computational-approaches-1295**
**Dates: Sep 4, 2024 - Sep 7, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The conference focused on the study of systems at the nanoscale both experimentally and by modelling. It covered the study of bio-inspired materials, ranging from polymeric or colloidal materials to very complex systems such as epithelial sheets and viruses. The major topic discussed is the hierarchical/directed self-assembly of nanoparticles with the goal of designing and/or characterising new materials. It emerged that self-assembly can be exploited for a plethora of technological applications such as self-healing materials, materials with tunable optical or electronic properties, materials that can be used for drug delivery, monitoring systems and purification devices. Another relevant topic is the functionalisation of building blocks that are of interest in all those systems that exhibit anisotropic interactions such as molecules, proteins and viral capsids. It emerged that the assembly behaviour is mainly driven by the anisotropy of effective interactions as it favours some local particle arrangements over others. From a methodological point of view, the strong need for reliable multi-scale procedures for tackling different length and time scale problems was largely discussed.
Finally, the conference served the purpose of bringing together the experimental and theoretical communities, and the productive discussions that followed the talks between the participants highlighted the importance of continuing the close collaboration and exchange of expertise between these communities.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The workshop demonstrated the community's ability to tackle the challenging problem of studying bio-inspired materials, both experimentally and through

modelling. One of the most important outcomes of the workshop is the demonstration that mimicking natural behaviour is a promising strategy to develop advanced materials for a wide range of applications, from energy storage to drug delivery. The discussions highlighted the importance of overcoming some of the current limitations, which are mostly methodological. On the one hand, it emerged the need to build robust bridges between different levels of theory in modelling. In particular, it would be very important to insist on the development of multiscale approaches that have to be strongly bound to both atomistic descriptions and mesoscopic properties. On the other hand, the scarcity of knowledge exchange between different scientific communities seemed to be a major limitation, which can be overcome by increasing the opportunities to meet as a community.

### 3. What was the take-home message for the participants?

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The most important messages that the participants were able to bring back home are related to the development of materials:
1. the self-assembly is a vivid field of study that can be still exploited for advancement in the technological field;
2. nature behaviour can be a source of inspiration for the design of such materials;
3. multiscale procedures, from both experimental and computational point of view, are shown to be the methods of choice for their study.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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Amongst the many topics discussed, possible applications emerged in the field of cancer treatment, drug delivery, water remediation and development of smart materials that can be a benefit for society.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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A wide number of collaborations originated from the discussions. In particular, new collaborations have been born between groups working on a common scientific question but tackled with different methods (e.g. experimentalists with theoreticians, chemists with physicists). The newborn collaborations will likely produce both publications and submissions of joint proposals.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The organising committee was composed by five women out of six members. Among the invited speakers, people from many different geographical areas and different career stages (from PI to PhD students) have been included.

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# Machine Learning interatomic potentials and accessible databases

**Location: Grenoble**
**Webpage : https://www.cecam.org/workshop-details/machine-learning-interatomic-potentials-and-accessible-databases-1313**
**Dates: Sep 9, 2024 - Sep 11, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop successfully brought together researchers from two complementary scientific communities: the development of machine learning interatomic potentials (MLIPs) and the curation and advancement of materials databases. A range of cutting-edge developments in MLIPs were presented, including recent progress in the integration of foundation models, which are expected to enhance the accuracy and generalizability of interatomic potential predictions. The diverse array of talks and posters offered participants the opportunity to delve deeply into technical aspects of the field, while also providing a broader perspective on future directions and research opportunities. In addition, the workshop served as a platform to introduce and discuss several significant European initiatives focused on digital infrastructure and numerical platforms, such as DIADEM, PDSI, Marvell, and OPTIMADE. These efforts aim to foster interoperability and accessibility across computational materials science. A variety of MLIP applications were showcased, spanning metallic and molecular systems, as well as energy-relevant materials such as batteries, illustrating the broad impact and versatility of machine learning techniques in materials modeling.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The primary outcomes of this workshop include successfully bringing together researchers from the machine learning interatomic potentials (MLIPs) community and materials database curators, fostering vital interdisciplinary collaboration. Significant technical advances were highlighted, such as the integration of foundation models to improve accuracy and generalizability, pointing toward promising future research directions. Additionally, the workshop laid the groundwork for new collaborations and the development of interoperable infrastructures aimed at automating and modularizing MLIP creation, enhancing reproducibility and efficiency across the field. Key database initiatives – including DIADEM, PDSI, Marvell, and OPTIMADE – were also introduced, underscoring the

importance of accessible, standardized, and interoperable digital platforms in supporting these efforts.
Although promising, the full realization of interoperable, automated workflows for MLIP construction remains an ongoing challenge, requiring further development and coordination across different tools and platforms. In addition, ensuring adherence to FAIR principles and avoiding redundant computations demand continuous community effort, clear standards, and infrastructure support.

## 3. What was the take-home message for the participants?

A key takeaway from the workshop was the growing recognition of the need to align research efforts with pressing environmental and societal challenges. As the field of materials modeling advances, it becomes increasingly important to ensure that scientific progress contributes to sustainable and responsible technological development. Emphasis was also placed on best practices in the construction and deployment of MLIPs. This includes the careful selection and use of existing databases, as well as the importance of transparent and reproducible data practices. In particular, adherence to FAIR data principles was highlighted as essential for fostering collaboration, accelerating discovery, and ensuring long-term impact.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The anticipated impact of the research discussed at the workshop is substantial, spanning both societal and environmental dimensions. From a societal perspective, the increasing ability to scale up simulations and tackle more complex systems using machine learning interatomic potentials (MLIPs) offers clear advantages, including accelerated discovery and more efficient technological development. On the environmental side, the construction of accurate surrogate models – such as MLIPs – can significantly reduce computational time and energy consumption. This, in turn, supports more sustainable research practices. However, a cautionary note was raised regarding the potential rebound effect: as computational tools become more efficient and accessible, there is a risk that overall computational demand may actually increase, offsetting some of the anticipated sustainability gains. To mitigate this, the community must remain vigilant in promoting responsible use of resources, alongside the adoption of best practices such as FAIR data principles and collaborative data sharing, which can help avoid redundancy and unnecessary computations.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

One of the major outcomes of the workshop was the in-depth discussion on future directions for automating the construction of machine learning interatomic potentials (MLIPs), particularly through the integration of streamlined workflows with accessible materials databases. A key focus was the potential for developing interoperable workflows across different workflow management systems – such as AiiDA, PsiFlow, and PyIron – enabling more flexible, modular, and scalable approaches to MLIP generation. This vision of interoperable infrastructure not only enhances reproducibility and efficiency but also lowers the barrier to entry for new users in the field. Importantly, these discussions have opened the door to potential new collaborations among workshop participants and stakeholders involved in the development of numerical platforms, marking a promising step toward a more connected and coordinated computational materials science ecosystem.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop was organized with a strong emphasis on inclusivity and accessibility. Participants were selected solely on the basis of scientific merit, ensuring an open and equitable selection process. The resulting group was diverse, with approximately 30% women and 70% men, and affiliations spanning ten countries – including the United States, Switzerland, France, Germany, the United Kingdom, Armenia, Belgium, Italy, and Iran – reflecting the international and collaborative nature of the field. To maximize accessibility, the workshop was conducted in a hybrid format, allowing remote participants to fully engage in the scientific discussions. Notably, about one-third of the attendees were current PhD students. The structure and format of the presentations were carefully designed to encourage their active participation, fostering an environment where early-career researchers could contribute meaningfully alongside more senior scientists.

## 7. Participant list

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# Failure in soft materials: from yielding to fracture

**Location: Erwin Schrödinger Institut Vienna, Austria**
**Webpage : https://www.cecam.org/workshop-details/failure-in-soft-materials-from-yielding-to-fracture-1298**
**Dates: Sep 9, 2024 - Sep 13, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on a comprehensive range of topics relating to the mechanics and rheology of both soft matter and biological systems. A key outcome was the opportunity to bridge the knowledge gap between these two areas, and the progress made in creating a common language to connect concepts in rheology of soft materials to the questions in biophysics and biology. Below is a summary of the key points discussed in no particular order:

- **Quantitative Definition of Glassy and Jamming States**: A need to better define glassy and jamming states from a quantitative perspective was identified, particularly in biological systems. Several concepts and questions related to that were clarified.
- **Yield Stress and Tissue Physical Properties**: Yield stress was highlighted as a crucial factor in determining the mechanical properties of biological tissues, influencing the relationship between elastic and plastic deformation. The response to reversing deformation and flows was extensively discussed, and recent progress in its quantification was analyzed for both inert and active systems.
- **Rheology of Soft and Biological Materials**: Topics such as recoverable versus unrecoverable deformation, ductility versus brittleness, yielding and shear banding, as well as length scales, correlations, memory, and relaxation mechanisms, were discussed. The relevance of these concepts and topics to the questions for biological systems and tissues was also analysed.
- **Mechanical Response and Failure:** Understanding the mechanical response and failure modes of soft and biological materials, including yielding, gelation, fracture, and shear banding, was a central theme. Participants exchanged ideas on how these systems respond to large deformations and microscopic precursors to failure can be identified.
- **Biological Systems and Glassy/Disordered Systems**: Connections between biological and disordered systems were explored, with several participants presenting work on how these systems relate. The discussion helped clarify connections and important differences.

**- Bridging Passive and Active Systems**: A major discussion point was the need to bridge the knowledge gap between passive systems, which have been extensively studied, and active, living systems, which remain less understood in terms of their rheological properties and how activity influences mechanical behavior.
**- New Experimental and Theoretical Tools**: Participants discussed recent developments in experimental techniques and theoretical modeling that could help advance the study of complex biological and soft systems, highlighting the need for better tools to describe both active and passive systems.
**- Analogy Between Soft Matter and Biological Systems**: The workshop raised important questions about the analogies and differences between soft jammed systems and biological systems, particularly in terms of rigidity, yielding, fluidization, and structural dynamics.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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A key takeaway from the workshop was the need for both communities - those studying living systems and those focused on passive soft materials - to work together to make meaningful progress. While the presentations and discussions were stimulating, the connection between biological and non-biological systems is still tenuous, and more research is needed to develop a comprehensive framework. For example, questions remain about how well existing models capture the heterogeneity and the multi-functionality of living systems, and whether theoretical approaches from passive systems can be extended to account for the length and time scales relevant to active, living matter.
Several open questions have been raised, such as the role of active forces in the yielding of biological systems, and the extent to which soft matter concepts such as aging in colloidal and protein gels apply to biological materials. Morphogenesis and plastic mechanisms certainly play a key role in the failure dynamics of biological materials, but it remains unclear what useful concepts can be imported from the study of passive systems such as amorphous solids.
The workshop highlighted recent advances in theoretical and experimental tools, but also pointed out persistent limitations in both computational models and experimental approaches. The discussions revealed many open questions, such as the interface between passive and active systems, how to improve two-dimensional vertex models to capture three-dimensional properties of biological monolayers, and in general how to better connect theoretical models with experimental data.
Ultimately, the primary outcome of the workshop was the recognition that bridging the gap between the two communities will be critical to the development of a unified framework. While significant progress has been made in the understanding of passive systems, the application of these findings to living systems - particularly with respect to their rheological properties - requires further development. A few recent experimental techniques, theoretical concepts, and computational approaches were identified as promising for such development. The discussions

laid the groundwork for potential future collaborations, and many new research directions were identified that will advance the state of the art in both biological and soft matter physics.

## 3. What was the take-home message for the participants?

- Despite progress in passive systems, a significant gap remains in connecting these insights to living systems, particularly in understanding their rheology and the impact of activity on their response.
- In this growing fields, it is crucial to have scientists doing experiments, simulations and theory to discuss.
- Accessing simultaneously different length scales and different quantities (stress, strain) is critical for understanding yielding and fracture.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The primary scope of the workshop was definitely in the domain of basic science, however the kind of scientific questions that have been discussed do have a societal impact. In fact, the idea when putting together the program was a genuine effort to bridge the gap between biologists and physicists in the domain of mechanical yielding and failure. Developing a common language and exchanging expertise in experimental/simulation techniques and data analysis could significantly enhance how we advance research in both biology and medicine. At the same time, participants from fields less exposed to medical questions have had the opportunity to engage with problems of significant medical relevance, such as the study of phase transitions in pathological collective entities like carcinomas. For example, the interplay between these two communities could lead to insights into the mechanical properties of malignant cell collectives, which may help identify potential vulnerabilities in cancer progression.
In general, understanding the principles governing biological and pathological phenomena, beyond specific systems, may lead to better control of these phenomena. The development of (bio)physical characterization tools with predictive power can have a significant impact at both industrial and biomedical levels.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop was held at the Erwin Schrödinger Institute (ESI) as part of the six-week program "Linking Microscopic Processes to the Macroscopic Rheological Properties in Inert and Living Soft Materials Description" that also included the two-

week summer school "Non-equilibrium Processes in Physics and Biology". We believe that the CECAM workshop was the highlight of this event, promoting many new collaborations and discussions. Most of the teachers at the school also participated in the workshop, and this allowed the participants to devote a considerable and distributed amount of time to discussion. In addition, several workshop participants stayed an extra week at ESI the week after the workshop to continue the discussions. As a result, writing a review, roadmap article, or special issue on the topic is currently being considered. Several new collaborations across theory, computational approaches, and experiments have been discussed, with the possibility of joint proposals.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The workshop has seen the attendance of 47 participants, from European (34), North American (9) , and Asian (4) institutions, with a very diverse ethnicity. Among them, we counted 34 male participants, and 13 female participants. Restricting the analysis to the 39 workshop invite and contributed speakers, the ratio of female speakers was 31%. Among the contributed talks, 60% was reserved to early career stage researchers, and the invited talks ensured a balanced contribution from tenure-track and tenured researchers at various career stages. Another measure to promote inclusivity was to make use of the audiovisual facilities provided by ESI to professional record all the presentations, which have been made available (for the speakers who agreed), publicly on the ESI's Youtube channel.

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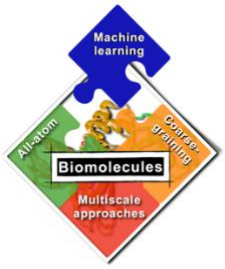


# Leveraging Machine Learning for sampling rare events in biomolecular systems

**Location: CECAM-DE-SMSM**
**Webpage : https://www.cecam.org/workshop-details/leveraging-machine-learning-for-sampling-rare-events-in-biomolecular-systems-1325**
**Dates: Sep 17, 2024 - Sep 19, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

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Main topics:

**- Machine learning (ML) force fields, from quantum-accurate atomistic molecular dynamics (MD) to coarse-grained descriptions for (bio)molecular simulations.** The current QM-based ML force fields can enable the simulation of challenging systems in materials sciences, as well as large biomolecules solvated in explicit water This approach offers a more efficient and accurate way to explore reactive systems (e.g. bond breaking) and subsequent conformational changes. However, several challenges are still present: i) describing intricate QM long-range interactions, ii) developing efficient and transferable ML force fields, ii) accounting for QM description of complex biomolecular systems composed by a heterogeneous environment such as lipids, post-translational modification, etc.

- **Machine learning enables the study of the thermodynamics and kinetics of complex molecular systems.** Brute force MD faces limitations in sampling long-time scales required for rare events. However, transition path sampling (TPS) addresses this by collecting unbiased trajectories, capturing critical transitions. By integrating ML, the process of sampling can be enhanced and also learning the committor function in a complex system hints to the likelihood of transitioning from one state to another. This novel method provides an efficient and data-driven approach to not only sample rare events, but also estimate mechanisms, free energies, and rates at a lower computational cost.

**- Combination of machine learning (ML)** with **path reweighting** and **Markov state models (MSMs**). The integration of path reweighting with ML methods, particularly for optimising reaction coordinates and improving molecular potentials, represents a forward-looking direction in this field. Also, the memory kernel minimization based Neural Networks (MEMnets), a novel method that is specifically designed to account for non-Markovian dynamics was presented.

**- Generative models for molecular simulations.** It was demonstrated how to tackle the sampling of rare events, which are difficult to address using plain MD. One can predict molecular trajectories by training generative models on existing

MD data. Also, it was discussed the high efficiency in timescales. Generative models can bypass MD limitation by learning the CVs or configurations directly, enabling faster exploration of the conformational space.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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**Primary outcomes:** The workshop has integrated a well-established biomolecular simulation community with the current state-of-the-art ML method development and its applications for the exploration of the so-called rare events in biomolecular systems. Similar ML communities mainly focus on problems related to model systems and near equilibrium conditions. Nowadays, most computational biophysical applications involve several length and time scales, which are typically beyond the reach of all-atom MD simulations. To address this, the MD community has developed advanced techniques, such as enhanced sampling and coarse-grained methods, to improve sampling efficiency in biophysical applications. In this regard, ML force fields offer an alternative tool to enhance MD simulations by providing quantum accuracy, thereby improving the overall description. Such a description is key when chemical processes are involved, particularly in the formation or dissociation of bonds.
**Limitations:** ML force fields are still limited by system size, the need for a dedicated and efficient MD engine, and their complexity. In rare cases, they have been used to study other biomolecular systems, such as RNA systems or biomolecular complexes (e.g., protein-sugar interactions). To improve the pseudo-transferability commonly associated with classical force fields, ML force fields should embark on the journey to parameterize other biomolecules, as is done in popular classical force fields (e.g., AMBER, CHARMM36c, etc.).
**Open questions:** The workshop has opened several possibilities for the use of ML force fields and generative models to study longer chains in proteins and flexible biomolecules. However, the flexibility associated with nucleic acid chains requires the development of more efficient data-driven methodologies for parameterizing ML force fields. In particular, the effect of water in ML force fields remains poorly explored, and the improvement of ML force fields for describing large solute-water complexes has yet to be achieved. ML force fields for proteins need to be carefully validated on e.g. NMR data reporting on conformational equilibria. The computational cost required for the ML-assisted MD simulation is a key factor, if we plan to achieve large length and longer timescales. Therefore, new methodologies still need to be explored to bridge the gap in the study of rare events. The systematic comparison between experimental free energy (FE) such as in binding processes and FE methods using ML force fields is still not fully provided. New methods that take advantage of the current ML architectures should be developed to facilitate and reduce the computational cost of the calculation.

## 3. What was the take-home message for the participants?

Participants with partial to moderate understanding of ML actively engaged in the workshop, while those with less expertise gained key insights into novel methods applicable to their biomolecular research, with an emphasis on rare event sampling. They were introduced to a new field that requires further integration of MD and ML expertise. Tthe workshop demonstrated that the gap between these two fields is closing through ongoing information exchange.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The CECAM workshop explored how ML can be integrated with biomolecular simulations, particularly in the study of rare events. These events are critical for understanding diseases, drug design, and the behavior of biological systems. While conventional MD simulations are resource-intensive and require significant computational power to model long timescales, ML-based simulations have the potential to significantly reduce both computational costs and energy consumption associated with these investigations. This advancement has broader implications for sustainable computing in scientific research, as it makes ML-based methodologies more accessible to various institutions, simultaneously reducing energy consumption and its environmental impact.

The workshop emphasized the convergence of the ML and biomolecular simulation communities. This cross-disciplinary collaboration is crucial for addressing global challenges, as it promotes knowledge exchange between fields. By integrating expertise in biomolecular science and machine learning, the potential for innovative solutions to health, environmental, and technological issues is significantly increased. Additionally, the workshop offered valuable educational opportunities for young researchers, equipping them with the skills to apply cutting-edge ML techniques to their work in biomolecular simulations. This initiative fosters a new generation of scientists ready to tackle interdisciplinary challenges, further expanding the workshop's positive societal impact. In summary, the workshop advances the state of the art in biomolecular simulations through the integration of ML methods, with wide-ranging implications for health, technology, and sustainability. By enhancing collaboration and encouraging new ideas, it helps pave the way for future breakthroughs in medicine and biomolecular systems.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

As a result of the workshop and the extensive range of methodologies presented, we are now planning to write a comprehensive review on machine learning methods for biomolecular simulations.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote inclusivity, the CECAM workshop aimed for diverse representation across gender, geography, and career stages, including participants from both academia and industry. Although cancellations affected the initial invited speaker's balance, finally 38% of contributors were female. The event included 89 participants from 21 countries, ensuring geographical diversity. Early-career scientists and PhD students were encouraged to present posters and give contributed talks (CT), 6 CT were selected among all participants fostering networking and mentorship. The workshop was organized in the Staudinger Lecture Hall, which was accessible to individuals with disabilities. However, participation was limited to on-site attendees due to local constraints. To further promote networking and integration, a gala dinner was held at the Wasem Kloster Engelthal restaurant in Ingelheim, contributing to a welcoming and inclusive environment.

## 7. Participant list

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**Huang, Xuhui** - University of Wisconsin-Madison, United States
**Isayev, Olexandr Isayev** - Carnegie Mellon University, United States
**Janoš, Pavel** - Consiglio Nazionale Delle Ricerche, Italy
**Kalita, Papu** - University of Bristol, United Kingdom
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**Khanshaghaghi, Bahar** - University of Stavanger, Norway
**Kremer, Kurt** - Max Planck Institute for Polymer Research, Germany
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**Künze, Georg** - University of Leipzig, Germany
**Lazzeri, Gianmarco** - Goethe University Frankfurt, Germany
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**Lutsyk, Valery** - Polish Academy of Sciences, Poland
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# Understanding the function of G-Protein coupled receptors by atomistic and multiscale studies

**Location: CECAM-Lugano, Aula Magna, USI Lugano, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/understanding-the-function-of-g-protein-coupled-receptors-by-atomistic-and-multiscale-studies-1288**
**Dates: Sep 23, 2024 - Sep 25, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

CECAM support enabled us to organize the second edition of the workshop entitled "*Understanding the Function of G-Protein Coupled Receptors by atomistic and Multiscale Studies*". Held in Lugano, Switzerland, the event attracted world-leading scientists and promising young researchers from Europe, North America, and Asia. The workshop consisted of several talks given by experts involved at various levels in different fields of GPCR research, both experimental and computational, as well as short oral communications to enhance the visibility of promising young scientists.

The scientific program included thematic sessions dedicated to the latest discoveries in GPCR functional dynamics and allostery, the influence of the cellular environment, ligand binding modes, mechanisms, and kinetics, as well as novel approaches, methods, and algorithms for sampling GPCR movements. Several talks were reserved for recent discoveries with notable potential for translational and clinical applications. In particular, the characterization of activation mechanisms and the capabilities of certain ligands to induce interaction with specific effectors upon binding, a phenomenon known as "biased signalling", were the highlight of this workshop's edition. Another emerging topic was the elucidation of homo- or hetero-oligomerization processes involving two or more GPCRs, another allosteric mechanism that regulates the receptor signalling cascade.

As in the previous edition, particular attention was dedicated to the exchange of data and expertise between computational, structural, and experimental researchers. Industries, such as Novartis and SandboxAQ, were also involved to foster interaction between the academic and corporate fields and to enhance the networking capabilities of both young and established researchers. A brainstorming session was held to illustrate the collaborative grants available in the Swiss, European, and international scenarios and discuss potential synergies between the participants.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The following topics emerged as focal points of future research:
**- Functional dynamics of GPCRs and their signalling partners.** NMR, Cryo-EM, and time-resolved x-ray crystallography have enabled a more detailed characterization of how G-Protein-Coupled Receptors (GPCRs) interact with G proteins, arrestins, and other signalling partners. Such a wealth of information enabled the performance of novel studies on the GPCRs' activation mechanism and how these receptors interact with their ligands.
**- GPCRs allostery.** Precise control over the GPCRs' activation mechanism enables the enactment of specific transduction patterns, potentially resulting in drugs with reduced adverse effects and increased potency. Recent evidence has shown that two particular classes of molecules, known as biased ligands and allosteric modulators, can achieve such results and thus have the potential to become the next generation of GPCR drugs.
**- Novel computational methods.** Recent developments in the fields of machine learning and artificial intelligence are empowering research on GPCRs, paving the way for novel possibilities and applications in drug discovery, structural characterization, and functional dynamics.
The following open questions were discussed:
**- Complete characterization of the biased signaling mechanism.** Different ligands can elicit specific interactions between GPCRs and their signaling partners. While some advances have been made, a comprehensive elucidation of the driving forces behind this phenomenon has yet to be achieved.
**- Investigation of new GPCR classes.** While class A GPCRs have been the research focus of the last decades due to their pharmacological implications, recent advances with experimental techniques (NMR, CryoEm, etc.) have unlocked the possibility of characterizing previously difficult-to-obtain structures of Taste and Class D GPCRs. Preliminary evidence showed that these receptors have a slightly different activation mechanism with respect to A class GPCRs.
In the following, we report the primary outcomes of the discussion:
**- Investigation of GPCRs requires increasing collaborative research efforts.** While new approaches and methods have been developed to address the mechanistic aspects of GPCR activation, their study requires increasing amounts of resources, cutting-edge technologies, and specialized expertise. Opportunities for collaboration, including funding options for joint projects, were thus discussed.
**- Roadmap for next generation drug design.** Biased ligands and allosteric modulators represent the next generation of drugs in the GPCR field. However, the underlying principles and mechanisms are not entirely understood. Their clarification represents a priority target for both basic and translation research.

## 3. What was the take-home message for the participants?

Future efforts in GPCR research require collaborative, coordinated projects that cover structural, computational, and experimental analyses of GPCR activation and protein-ligand interactions to pave the way for the next generation of GPCR drugs with increased potency and reduced side effects.
The employment of artificial intelligence and machine learning techniques in current studies is recommended to enhance data analysis and research capabilities.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

GPCRs are the single most important drug target in the human proteome. Approximately 35% of marketed drugs target a GPCR, and the global GPCR market size is estimated to be USD 3.0 billion. While many medications targeting GPCRs have already been brought to market, numerous additional targets remain to be explored. An emerging theme focuses on more selective GPCR activation – not targeting the protein level, but rather the biochemical signaling pathway. Many distinct signaling pathways converge through a single GPCR, and different native ligands and drugs couple into distinct pathways. Furthermore, allosteric modulators offer the opportunity to regulate the efficacy, efficiency, or potency of a drug in a specific and time-dependent manner, thereby avoiding cross-interactions with other molecules.
Rationally designing these kinds of functional modulation is a major current challenge in the GPCR field with significant societal implications. Efforts underway leverage massively scaled molecular simulations to learn how exactly distinct drugs preferentially activate different pathways. Success would open new and promising therapeutic strategies for safely treating many pathologies and conditions. In this context, the workshop facilitated knowledge transfer that will significantly enhance the quality of present and future research in the field, thereby increasing its success rate. Collaborations and joint research projects fostered by the scientific exchange will also allow the enacting of plans otherwise difficult to realize individually. The participation of industries will also facilitate the translation of findings from preclinical to clinical settings.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Several collaborations are ongoing or in the planning phase with multiple groups from Europe and North America. The attendees are currently writing a report on the workshop, which will be published in specialized journals. An example of the scientific output achievable by this event is a review written by the speakers of the

workshop's first edition and published in the prestigious journal Nature Reviews Drug Discovery: https://www.nature.com/articles/s41573-024-01083-3

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Speakers and attendees were selected based on merit while also considering factors such as gender distribution, geographical origin, career stage, and other societal aspects to promote inclusivity.
We achieved a 40% gender ratio among the speakers and attendees, who came from 15 countries, including India, Nigeria, and Japan.
More than half of the participants were early career researchers. We supported the participation of people from outside Europe by providing the necessary documentation for the release of the Swiss visa.

## 7. Participant list

### Organisers

**Conflitti, Paolo**
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# Bridging the atomic-mesoscale gap for complex interfaces

**Location: CECAM-FR-GSO, Laboratoire de Mécanique et Génie Civil, France**
**Webpage : https://www.cecam.org/workshop-details/bridging-the-atomic-mesoscale-gap-for-complex-interfaces-1316**
**Dates: Sep 25, 2024 - Sep 27, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop has gathered researchers from two different areas of multi-scale modelling: reaching large systems and reaching long simulation times. Gathering both communities created an interesting field for discussions about how to push the state of the art in order to be able to reach both large systems simulations and long simulations times, in the view of doing simulations that are close to the scales that can be reached experimentally. Many different methods have been discussed (thermodynamics integration, metadynamics, machine learning potentials, diffusion models, brownian dynamics, etc.) and applications in different fields have been presented (phase coexistence, polarized systems such as supercapacitors, amorphous materials such as cement or polymers, biomaterials, etc.).
There was interesting discussions to bring the state of the art forward, in particular on the force fields, that governs both atomistic simulations and coarse grain models. Many discussions were about how to develop better force fields, in particular using machine learning approaches, and in particular how to keep the information on what are the contributing forces in a given interaction. For instance, stress was put on the fact that MLPs can indeed reproduce ab initio results but it's not sufficient to predict the value of the energy or of the forces, it's also key to understand the origin of such a force. Therefore, efforts should be put to develop MLPs that are also outputting the contribution of each force (van der Waals, electrostatic, bonding, non-bonding, etc.).
In the same time, it has been revealed clearly by many contributors that the simple models at the coarse grain level (such as Martini, Lennard Jones) can do very well in reproducing the physics of the systems. Therefore, going for more complex force fields is not always a good strategy. We had an interesting discussion in the round table about how to retain the scales that matter. Multi-scale simulations are often sold as a way of simulating everything but rather than doing this, one outcome of the workshop was that it is much more relevant to use multi-scale modelling to find what is relevant in the system. For instance, cracks appear in a materials: is it due to a phase transformation (molecular level), to ion transport

(meso scale), or perhaps to both where phase transformation modifies local stress and forces matter transport.
Overall, we had fruitful and lengthy discussions. We asked in advance to the speakers to prepare any question they would like to ask the audience. This has trigged interesting discussions and has kept the whole audience active during the three days of the workshop.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The primary outcomes are that there exist a number of very efficient methods for doing multi-scale modelling (starting from the atomic scale). If we want to do multi-scale simulations that are both multi-time-scales and multi-lengths-scales, we need to figure out how to simplify the interactions between molecules / atomic clusters without losing the important contributions.
Future directions of research for researchers working on multi-scale problems might be to integrate not only a bottom-up approach, as it is often done for multi-scale simulations including the atomistic simulations, but also a top-down approach. In particular, there is a need for implementing experimental data in the models not only to compare with the simulations but also to inform the models.
A great limitation seem to be on the transferability. For instance, in MLPs, it has been shown that they can perform extremely well on a specific system but fail on related systems.
There is also an open question on how to deal with flexibility that exists at the molecular level (atomic vibrations). In a coarse grain approach, the internal vibrational modes are ignored but this might be a shortcoming. In particular, for studying adsorption properties (capacitance, depollution, gas recovery, etc.) the local flexibility is key for the adsorption and transport mechanisms.
In the concluding discussions, we found out that there are still great challenges in both time-scale and length-scale approaches.
Another important aspect of the discussion was about FAIR data management and how to make our research available and reusable. This appeared to be important, in particular for machine learning approaches that requires a high number of good quality data. Despite the importance of FAIR approaches, only about ~15% of the audience was fully involved in it.

## 3. What was the take-home message for the participants?

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The take-home message for the participants is to find what is the relevant scale in a multi-scale simulation, what are the relevant forces, what can be cut-out without losing the key aspects of the system so that computations become time-efficient and still full of information for understanding a system.

A secondary take-home message is that we need to adapt our research to environmental and societal concerns (FAIR data, carbon footprint, etc.).

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The workshop was about multi-scale methods and was focusing mostly on the methods. Nonetheless, we can highlight the fact that many presentations were about applications for socially important topics : lower the CO2 emissions for cement production, optimize supercapacitors, gas storage, PFAS removal, etc. Multi-scale simulations find applications in fields that are important for the public: energy production, greener construction materials, water treatment, air depollution, etc.
Topics of the workshop were mostly on materials sciences applications but the methods that were discussed can also be applied in other fields such as health-related science, environmental science, economy, etc. Simulations have proven to be impactful in research to help accelerate the discovery of materials and find solutions to environmental, industrial, and societal problems.
We had discussions about the carbon footprint of research in our laboratories but also on the carbon footprint of molecular simulations and how we could reduce this carbon footprint by reusing the data and raising awareness. This implies a better management of the data, availability of the data. Students were particularly interested and concerned about lowering the carbon footprint of research. For solutions, we had a presentation of the NOMAD project by Joseph Rudinzki and an example of use by Tristan Bereau showing also the usefulness of these approaches.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop has been the grounds for opening new collaborations, researcher and student exchange.
We had initial discussions about making this a periodic event (by-yearly) in order to gather the two communities (time-scale and length-scale) and share about progress and future directions.
After the workshop, we are discussing about writing a perspective / positioning paper on the topics of the workshop.
Paola Carbone, chair of CCP5, encouraged the participants of the workshop to apply in future CECAM/CCP5 calls for joint projects.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We have based our selection of all participants only based on scientific aspects which means being totally inclusive. The proportion for the participants is about 40% women and 60% men. We had participants affiliated from Canada, Spain, Norway, Germany and students currently doing their studies in Europe but originally from all over the world (Asia, Africa, South America, etc.).
In terms of career stage, we have invited speakers from all carrier stage: young researchers, senior researchers, well-recognized researchers in the field. Moreover, about 1/3 of the participants are currently PhD students and we ensured they participate in the discussions.
Everyone was welcome to participate in the discussion and eventually, everyone participated in discussions during the workshop. Particularly the round table was the place for discussion from nearly all participants (students included).

## 7. Participant list

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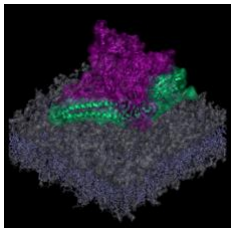

# Understanding peripheral protein-membrane interactions: membrane recognition, dynamics, function and therapeutic opportunities

**Location: CECAM-HQ-EPFL, Switzerland & online**
**Webpage : https://www.cecam.org/workshop-details/understanding-peripheral-protein-membrane-interactions-membrane-recognition-dynamics-function-and-therapeutic-opportunities-1289**
**Dates: Sep 25, 2024 - Sep 27, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on the mechanistic and functional roles of peripheral membrane proteins (PMPs), exploring how they recognize, interact with, and are regulated by cellular membranes. Major topics included the biophysical underpinnings of PMP-membrane interactions, computational modeling of protein-membrane dynamics, the influence of membrane curvature, and the role of lipids in protein association and signaling.

One key theme was Ras/MAPK signaling, particularly the importance of membrane microdomains and nanoclusters, the influence of effector interactions like Raf, and phase transitions in protein signaling. These insights are reshaping how signal transduction at the membrane interface is understood, especially regarding the conformational control of protein complexes. Another key theme was the mechanics of membrane curvature sensing and generation. Through studies on amphipathic helices and caveolin-1, researchers highlighted how curvature-sensing peptides and proteins localize to distinct membrane geometries, playing roles in trafficking, endocytosis, and remodeling. The workshop also explored GPCR dynamics, including receptor activation, dimerization, and ligand bias through time-resolved cryoEM and Bayesian integrative modeling. Such methods bridge experimental data and computational models, offering atomic-resolution views of signal transduction.

In terms of methods, advanced molecular dynamics (MD) simulations and machine learning (ML) approaches were discussed across presentations, enabling new insights into lipid-binding, structural transitions, and membrane deformation. Examples include OneOPES-enhanced sampling, MuMMI frameworks, and ensemble ML algorithms to predict membrane-penetrating residues, facilitating drug discovery at protein-membrane interfaces.

Finally, the workshop dealt with drug discovery targeting PMPs revealed promising avenues for modulating "undruggable" targets via their membrane interfaces. Efforts to design selective peptides, understand binding promiscuity, and simulate

the effects of drugs on neuronal receptors exemplify a paradigm shift in therapeutic development.
In summary, the workshop significantly advanced the state of the art by integrating experimental and computational approaches, highlighting emerging concepts like lipid-mediated allostery, curvature selectivity, and AI-driven modeling in PMP biology.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop described key mechanisms by which PMPs associate with, remodel, and signal through biological membranes. One major outcome was the establishment of shared physical principles, such as hydrophobic mismatch, electrostatic interactions, and curvature-sensing as drivers of PMP function. These principles are critical for designing future experiments and therapies targeting protein-membrane interactions.
The event proposed multiscale molecular simulations (atomistic and coarse-grained MD, enhanced sampling, and machine learning models a tools to study membrane-protein dynamics and guide drug discovery. Several computational pipelines (e.g., DREAMM, MuMMI) were presented, illustrating how predictive modeling can identify therapeutic hotspots on membranes.
Despite this progress, key limitations and open questions remain. One persistent challenge is the contextual variability of PMP interactions, which depend heavily on lipid composition, curvature, and cellular conditions. Experimental systems often fail to replicate this complexity. Furthermore, the transient nature and low affinity of many PMP-lipid interactions make them difficult to capture experimentally or model accurately.
Another open question involves how exactly lipid environments modulate signal specificity and strength, particularly for dynamic assemblies like Ras nanoclusters and GPCR dimers. The fine-tuning of signaling output by membrane composition, curvature, and topology requires further experimental validation.
The workshop also revealed that many computational tools are still limited by timescales and sampling bottlenecks, especially when dealing with large conformational changes in multidomain proteins or long-range allosteric effects. While new ML approaches are promising, they require more robust training sets and validation.
Moreover, the translation of structural insights to pharmacology remains a key hurdle. Although some peptides and small molecules have shown efficacy in modulating PMP interactions, their specificity and in vivo stability need improvement. Better integration of simulations with experimental assays will be needed to validate candidate drugs.

## 3. What was the take-home message for the participants?

Peripheral membrane proteins are master regulators of cellular signaling, remodeling, and trafficking, and their dynamic interplay with the lipid environment represents both a scientific frontier and a therapeutic opportunity. Integrating computational and experimental approaches, especially using AI, MD simulations, and cryoEM, enables deep mechanistic insights that can guide future drug discovery at the membrane interface.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the workshop outcomes hold strong potential for societal benefits, particularly in the areas of drug discovery and precision medicine. By advancing understanding of PMPs (many of which are implicated in cancer, neurodegeneration, and cardiovascular disease) researchers are opening new therapeutic avenues. PMPs have historically been considered "undruggable" due to their transient and lipid-dependent interactions, but the computational and AI-driven strategies discussed in the workshop offer promising routes to overcome this barrier. For instance, targeting protein-membrane interfaces in Ras signaling or GPCR pathways could lead to next-generation inhibitors with high specificity, reduced side effects, and novel mechanisms of action. Several talks showcased pipelines (e.g., DREAMM) that integrate machine learning and molecular dynamics to predict membrane-penetrating regions and design small molecules or peptides for selective inhibition. Additionally, understanding how membrane curvature and lipid composition regulate signaling has implications for metabolic diseases, viral infection, and immune responses, where lipid environment plays a key role. Tools for modeling these effects can be applied to engineer more effective vaccines, diagnostics, and therapeutic delivery systems. The integration of AI and biophysics also supports education and infrastructure development in regions with limited experimental resources. These scalable computational methods democratize access to high-resolution biology, enabling wider global participation in drug development. By facilitating interdisciplinary collaboration, this workshop fostered a community of researchers equipped to tackle diseases at the membrane interface – paving the way for more effective, mechanism-based therapies. In conclusion, the workshop defined a roadmap for addressing several remaining challenges through collaborative efforts in computational modeling, structural biology, and drug design. Continued progress depends on standardizing datasets, improving model interpretability, and fostering interdisciplinary exchange.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Yes, the workshop led to multiple tangible outcomes. Participants initiated new collaborations focused on multiscale modeling of peripheral membrane proteins and AI-assisted drug discovery. Several research groups reported plans to co-author publications on topics such as RAS/RAF membrane interactions and curvature sensing. There were also discussions of joint proposal submissions to Horizon Europe and COST actions. In addition, software tools such as MuMMI, OneOPES, and DREAMM were presented, refined through feedback, and will be made openly available or further developed as community resources.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The organizers ensured inclusivity by inviting a balanced mix of male and female speakers and prioritizing early-career researchers and postdoctoral fellows in oral presentations. Participants represented over 10 countries across Europe, North America, and Asia, with strong representation from underrepresented regions in Southeastern and Eastern Europe. Hybrid participation via Zoom allowed involvement from those unable to travel due to personal or financial constraints.

## 7. Participant list

### Organisers

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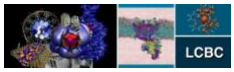


# Computational chemistry across scales and disciplines: celebrating the 60th birthday of Ursula Röthlisberger

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/computational-chemistry-across-scales-and-disciplines-celebrating-the-60th-birthday-of-ursula-rothlisberger-1290**
**Dates: Oct 1, 2024 - Oct 3, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The topics discussed at the symposium reflected the width and inter-disciplinarity of the scientific interests of Prof. Ursula Rothlisberger, spanning from fundamental physics through material science and chemistry to biology and medicine. Physics and material science-oriented presentations about quantum computing, the modeling of rare events, open-shell systems, phase transitions, crystal structure prediction, nanomaterials, and absorption spectroscopy were complemented with a focus on the simulation of dye sensitized and perovskite solar cells. Chemistry-related topics included homogeneous catalysis, photochemistry, light-driven molecular motors, and quantum machine learning in chemical space. Many biological questions such as enzymatic mechanisms, pore formation, synthetic metabolism, DNA redox chemistry, photosynthesis and allostery were discussed. Finally, method development and applications of computational tools for precision medicine, protein design, and cancer immunotherapy were presented.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The goal of the symposium was to bring together mentors, alumni, and longstanding collaborators of Prof. Ursula Rothlisberger to celebrate her achievements as an outstanding scientist and to discuss open questions in the field. Many of the invited participants were happy to participate in the symposium and to share both an overview of their current work and of their work done together with Prof. Rothlisberger. The presentations highlighted the instrumental role that Prof. Rothlisberger played in the careers of numerous scientists, as well as her function as a role model and a friend for most participants. In addition, the workshop highlighted the transformation of computational chemistry over the last 25 years, and provided a discussion platform for what's ahead.

## 3. What was the take-home message for the participants?

Over the course of the symposium, it became clear that Prof. Rothlisberger succeeded to create a vibrant research environment in her group over many years and that she influenced and mentored a great number of prolific scientists.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The symposium highlighted the role of computational chemistry for many diverse fields and showed the benefit of its applications for society. Examples discussed at the symposium include computational studies for clean energy production, the treatment of viral infections, and the prediction of cancer-causing mutations.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

We are not aware of tangible outcomes in the sense of this question. However, this was not the primary goal of the symposium.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To ensure diversity and inclusivity among the workshop participants it proved to be sufficient to rely on the personal network of Prof. Ursula Rothlisberger, which mirrors her mindfulness to these questions. Presenters came from all over Europe, North America, South America, and Asia, and included early career scientist, established researchers, and retired professors. About 25% of presentations were given by women.

## 7. Participant list

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# Green's function methods: the next generation 6

**Location: CECAM-FR-GSO, Toulouse, France**
**Webpage : https://www.cecam.org/workshop-details/greens-function-methods-the-next-generation-6-1286**
**Dates: Oct 2, 2024 - Oct 4, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The Green's functions formalism is a general framework to tackle the many-body problem. For instance, the one-body Green's function (GF) delivers a wealth of information about a physical system, such as ground-state energy, excitation energies, densities and other measurable quantities. Other observables, like optical properties, might require the knowledge of the two-body Green's function, or higher level in the many-body hierarchy. Another class of observables, namely time-dependent processes, require non-equilibrium Green's functions. The development of approximate methods to calculate GFs has been an active research topic in many-body physics since the 60's, and many routes have been explored in order to find increasingly accurate GFs. A prevalent class of methods is based on the iterative solution of an integral equation for the GF containing an effective potential, the so-called self-energy, which needs to be approximated. In this framework, called Many-Body. Perturbation Theory (MBPT), one of the most successful approach was the well-known GW approximation, which permits one to obtain accurate band structures. The GW approach, however, presents also several shortcomings, such as the wrong description of satellites in photo-emission spectra, particularly in so-called strongly-correlated materials. Therefore more refined levels of approximations are needed to keep pace with the advances made in experiments. In recent years several paths have been proposed to overcome these shortcomings: i) going to second order; ii) introducing effective interactions that resume the perturbation at all orders; iii) proposing alternative approaches, non-perturbative, via Cumulant Expansion (CE) or Dynamical Mean Field Theory (DMFT); or iv) by trying to use approximations to contractions of the GF, like in the reduced Density Matrix Functional Theory (rDMFT). Pioneering developments and results have been presented at this workshop for all these new frontiers approaches, for both equilibrium and non-equilibrium GFs.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

Going beyond today's state-of-the-art GF approaches is absolutely necessary if one wants to tackle complex electronic properties, like metal-insulator transitions, half-metallicity, or unconventional superconductivity. New strategies emerged during the workshop which revisit fundamental equations, introduced novel approximations and exploited connections among different approaches. Following this, the workshop has shown three big axes of development, promising to tackle the new challenges in material science:
1) Many novel approaches and pure theoretical developments have been proposed that span from second order expansion of GW (GWGWG), to vertex corrections via effective resummation; from combinatorial diagrammatic expansion to the introduction of novel representation of the GF (anomalous GF and 4-particle GF).
2) The workshop has been the ideal platform to present GF approaches for spectroscopies and observables that are typically tackled within single-particle approximations, due to their intrinsic difficulties: electroluminescence rectifications, magnetic skyrmions, pump and proble in the X-ray regime, thermal conductivity, and fermionic quasi-condensation. 3) GF approaches are notoriously cumbersome, from the computational point of view, with respect to standard single-particle or mean field approaches. Several talks were devoted to simplification and proposition of new algorithms. Among them: efficient treatment of the continuum in the spectroscopy of finite systems, matrix-product states for cluster solvers, and Monte-Carlo sampling of the dielectric matrix irregularities.

## 3. What was the take-home message for the participants?

- going beyond the single-particle approach is crucial (even within the realms where historically simple approximations were considered adequate). Reason are: new experimental features, new regimes, better resolutions.
- today theoretical developments need to become tomorrow's standards: collaboration with mathematicians, computer scientists, algorithms experts is a crucial need that we have to tackle as a community (also considering the ever-changing available hardware, and the spread of novel tools related to machine learning) - increased support of fundamental research is needed. Very often calls give high priority to joint research+industry projects. Perverse ramification of calls is highly inefficient funding procedure.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Besides the obvious points that one might cite (enhancing scientific collaborations and cooperation among people and countries - we had 15 different nationalities

represented at the workshop, 7 of them extra-European; education and knowledge transfer - many of the participants are involved in high-end teaching, including CECAM schools, ICTP, PRACE, Psi-k events), we should also underline long-term innovation (as we know, the fundamental new knowledge might not find immediate applications but, in the long term, always reveal useful, pioneering or eye-opening), and tackling global challenges (though very fundamental, the results discussed in the workshop address physical quantities relevant in energy materials, photovoltaics, optoelectronics, etc.). It is not, in fact, a coincidence that many participants are also involved in industry-related projects, being those linked to software development (like Software for Chemistry & Materials), to start-up in quantum computing (like IQM Quantum Computers), or to national programs for technology (like the TASE, Priority Research Programme on Technologies for Advanced Energy Systems).

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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While any progress in Green's function methods is of great importance to fundamental research, we want to stress the crucial usefulness also for what concerns industrial applications. Many-body Green's functions contain a wealth of information that can be used to develop novel materials for various innovative technological applications. Even though the topics of the workshop were about fundamental research, the target was about a more accurate, fast, and precise description of Green's functions (GF) of the electronic many-body problem. The single-particle GF contains information on the electron addition and removal energies, which allows for an accurate description of band gaps, band alignments, etc. This is critical information in the development of photovoltaic devices.
In addition, since the current density is contained in the single-particle GF, all electron transport-related processes can be described. If we consider the two-particle Green's function instead, we can obtain information about all process involving the electron-hole interaction, which is crucial for developing new photo-voltaic and photo-catalytic devices. Non-equilibrium GF, finally, are crucial to describe pump-probe experiments, pertinent for catalysis research (studying the mechanisms of chemical reactions), ultrafast phenomena (like phase transitions of materials), biomedical applications or even data storage and computing.
In this respect, some collaborations have arisen from the previous editions, that were represented as main topics in this workshop (first talks on G3W2 in the first day, excitonic properties and efficiency talks on first and second day). Other collaborations will be born from this edition. Examples are on x-ray spectroscopies between Palaiseau and Berlin, on cumulant expansion between Seattle and Paris.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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Particular attention was given to encouraging the participation of younger scientists, especially those from rapidly developing countries such as Morocco and India. We also maintained a focus on gender balance, despite the predominantly male nature of this community. Additionally, we supported researchers traveling with their families; two participants attended with their spouse and child, and they were invited to all social events (without charge).

## 7. Participant list

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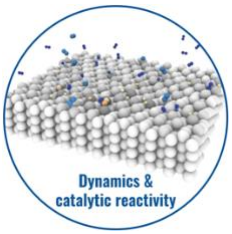


# Advances in catalytic reactivity simulations under operando conditions

**Location: CECAM-IT-SIMUL**
**Webpage : https://www.cecam.org/workshop-details/advances-in-catalytic-reactivity-simulations-under-operando-conditions-1332**
**Dates: Oct 7, 2024 - Oct 9, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on several advanced topics at the intersection of catalytic modeling, machine learning (ML), and molecular dynamics (MD) simulations, with a focus on simulating catalytic processes under operando conditions. A key theme was the evolution from static to dynamic models in catalytic processes. Traditional computational models relied heavily on idealized assumptions, such as static surfaces or single reaction mechanisms. However, recent developments in MD simulations, enhanced sampling methods, and ML-driven potentials are transforming how we can simulate catalytic systems.

One significant topic was the development and application of **machine learning interatomic potentials.** These potentials allow for fast, accurate simulations of catalytic systems with ab initio-like precision, significantly accelerating the study of complex reactions. This shift to data-driven potentials helps overcome the computational bottleneck posed by traditional methods like density functional theory (DFT). The development of new ML models together with strategies to build and validate them for reactive events enable large-scale simulations of catalytic systems, which would be infeasible using conventional methods.

Furthermore, the integration of **enhanced sampling techniques** into catalytic modeling was highlighted. These combined techniques help overcome the timescale limitations of conventional simulations by allowing the efficient exploration of rare events, as well as obtaining insights into transition states for complex catalytic reactions and also serve as crucial ingredients to construct reactive potentials.

Another important topic was the modeling of **dynamic interfaces**. Rather than assuming a static catalytic site, we discussed how different catalysts undergo significant dynamic transformations at the interface (and sometimes also in the bulk) during reactions. This focus on dynamic interfaces challenges previous notions of catalysts as static materials and underscores the importance of considering the catalyst as a whole to understand catalysis.

Finally, a major discussion centered on **realistic simulations under operando conditions**. Many catalysts behave very differently under reaction conditions than in controlled laboratory environments. Realistic modeling requires including many different ingredients such as temperature, pressure, solvent effects, electric fields and other important variables. The workshop participants illustrated how new computational techniques are beginning to bridge the gap between idealized models and actual catalytic behavior.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop highlighted recent progress and persistent challenges in simulating catalytic reactivity under operando conditions. A key outcome was the recognition that accurate modeling must move beyond idealized, static representations and reflect the full complexity of real-world catalytic environments. This includes accounting for temperature and applied bias, realistic scales, the role of promoters and spectator species, structural changes such as catalyst activation or deactivation, and the presence of defects. Crucially, the dynamic structure and location of active sites remain poorly characterized during reactions. Changes in particle shape, surface reconstruction, and local environment introduce structural complexity that limits predictive accuracy. Added to this is the challenge of modeling reactive environments, particularly in liquids where solvent effects, acidity, and ions play key roles. Current methods often struggle to capture the structure and reactivity of such interfaces.

Participants stressed the need to link atomistic simulations to experimentally measurable observables – such as reaction energies, activation barriers, and rate constants – to guide experimental design and catalyst optimization. Achieving this requires tighter integration with mesoscopic and kinetic models. This connection is essential not only for advancing understanding but also for generating actionable outputs for industrial catalysis, including the identification of rate-limiting steps, optimization of conditions, and screening of materials under realistic constraints.

Another important aspect discussed was the influence of time-dependent external conditions – such as fluctuations in temperature, pressure, or composition – which can strongly affect catalytic performance, sometimes beyond equilibrium predictions. Whether such effects cause lasting changes in catalyst behavior remains an open question.

Advances in machine learning were acknowledged as transformative. ML potentials allow efficient sampling of potential energy surfaces and enable large-scale simulations. Yet limitations persist: they rely on high-quality training data – often from quantum methods with limited accuracy for complex systems – struggle with transferability and cannot yet replace high-level electronic structure approaches. Phenomena like non-adiabatic dynamics, electric fields in electrocatalysis, and magnetic effects are often beyond current ML and MD capabilities.

Finally, the workshop highlighted infrastructural gaps such as limited software interoperability, lack of shared repositories, and absence of standards for realistic simulations. While progress is evident, a unified framework for predictive catalyst modeling is still lacking. Overall, the workshop outlined a roadmap for future methodological development and underscored the need for deeper integration between theory, experiment, and application.

### 3. What was the take-home message for the participants?

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The take-home message from the workshop was that the future of catalytic modeling lies in embracing dynamic, real-world conditions. By combining molecular dynamics simulations, machine learning, and enhanced sampling techniques, we can now study catalytic systems more realistically than ever before, providing deeper insights into reaction mechanisms and paving the way for more efficient and sustainable catalysts.

### 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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The outcomes of the workshop have significant potential for societal benefits, particularly in sustainable energy and green chemistry. By improving our understanding of catalytic processes under real-world conditions, these advancements could lead to the development of more efficient and robust catalysts for critical industrial reactions like ammonia synthesis, hydrogenation, and biomass conversion.

### 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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We discussed writing a perspective paper on the evolving role of dynamics in computational catalysis, particularly in the context of recent advancements in molecular dynamics, machine learning, and enhanced sampling techniques. This perspective aims to highlight how these developments are reshaping the field and will likely serve as a foundation for future research collaborations.

### 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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Efforts were made to ensure a balanced representation of gender and career stages in the selection of invited speakers. Out of approximately 25 speakers, 11

were women, and we included 3 postdocs and 4 early-career researchers. The workshop structure, in which everything from accommodation to talks and meals took place in the same venue (a small hotel reserved for the workshop), also promoted inclusivity through shared meals and networking opportunities, which facilitated interactions across different career stages.

## 7. Participant list

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# Pushing the frontiers of molecular dynamics simulations

**Location: CECAM-HQ-EPFL, Switzerland & online**
**Webpage : https://www.cecam.org/workshop-details/pushing-the-frontiers-of-molecular-dynamics-simulations-1275**
**Dates: Oct 7, 2024 - Oct 9, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Meeting was focused mainly on four topics
- Massive simulations in time and especially in size, showing how MD is approaching systems of real biological relevance. Clear advances are shown in the study of dynamic effects in gigantic systems, showing simulations are able to reproduce experimental findings.
- Coarse grain methods appear as an alternative to deal with ultra-gigantic systems, either coupled to multi-resolution models or alone. In some cases, coarse-grained models are tailored to the specific system of interest.
- The need to store and share data to guarantee reproducibility, avoid redundant calculation and helps in improvement of force-field, the training of lower resolution methods (coarse-grained models) and provide data for the training of artificial intelligence (AI) methods.
- Based on the talks and the discussion, AI technologies are gained weight in molecular simulations in different levels: i) as a way to accelerate sapling of complex transitions which are not easy to trace in a reasonable time scale; ii) as a method to make predictions from simulations and available experimental data.
Synergy between simulation and experiments in gaining momentum. Many speakers presents examples of simulations suggesting experiments to do, or experiments validating the simulations. Even more exciting different authors present studies, where medium or low resolution experimental data were used to refine the theoretical calculations.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

I think it has been one of the best meeting I have attended recently, with some of the top speakers in the field and an ultra-rich discussion environment. Different topics have appear, among others:

- Absolute consensus exist on the community about the need to collect simulation data and give them a second live, specially related to training of machine learning approaches.
- The type of systems that are subjected to MD simulations is expanding by increasing the size of the simulation systems (up to the billion scale) and incorporating intrinsic disordered proteins, or single stranded nucleic acids, which were out of focus of MD simulations in the past. We learnt on projects representing nucleopore complex, entire virus, even reduced cell models. Many groups are interested in the dynamic of these gigantic systems, exploring for example genome packing, large ligand-induced transitions on membrane proteins or even translocation machineries.
- Time scales are not scaling so much, and with exception of Athon, which promises $10^2$ microseconds a day, no dramatic increases in simulation times are reported with the multi-microsecond scale being still the state-of-the-art.
- Machine learning techniques are appearing in many areas of molecular dynamics and in general of molecular simulations, with a special impact in accelerating biassing strategies to guide transitions on molecular dynamics simulation of conformational transitions.
- A very large effort is focused on the development of coarse-grained models, including those trained for a single system.
- More and more group are collecting experimental data, from low to high resolution that are in some cases as biasing elements in molecular simulations.

## 3. What was the take-home message for the participants?

We can expect the field approaching to real biological systems at the cell-scale level. We can expect a higher impact of general and in situ parametrize CG models. The interaction between MD, experiments will be of increasing intensity, with simulations suggesting experiments beyond the mere validation of the results. The interaction of MD with data-driven technologies such as AI would re-define the nature of the simulation field.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

- Along a meeting that was centered on simulations, structural data and artificial intelligence techniques. Two Nobel prices were announced (chemistry and physics), that fit into the topics treated in the congress. This reveals how timely was the meeting and the impact that the topics discussed have in current science, and by extension to the society.
- We have treated fundamental problems about the functioning of biological systems, which can provide clues on the way on which genomic alterations affect help. Very intense has been the discussion on systems that might have pharmacological impact, and results highlighted the impact of simulations

techniques, and especially molecular dynamics in rational drug design, finding not only interaction modes, binding free energies, or kinetics of the interaction, but also cryptic cavities, opening the scenario of druggable targets.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Sure new collaborations will emerge. We were invited by the editor in chief of a reference journal in the field to write a review, we will decide in the next weeks whether or not to follow this invitation.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We tried to maintain a good balance. The number of non-speakers in the congress was limited by the size of the room (close to 2000 people were registered), but the excellent remote capabilities of CECAM allowed extensive remote access by people around the work. The cofunding of the initiative by the MDDB consortia allowed us to attract speakers from the US, that attend later to other CECAM meetings.

## 7. Participant list

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# Simulating soft matter across scales

**Location: CECAM-DE-SMSM, University of Stuttgart, Germany**
**Webpage : https://www.cecam.org/workshop-details/simulating-soft-matter-across-scales-1324**
**Dates: Oct 7, 2024 - Oct 11, 2024**

## 1. What were the major topics presented in the School?

This school teaches coarse-grained and lattice-based simulations methods suitable for modeling soft matter systems at mesoscopic length and time scales. We explore topics such as simulating coarse-grained ionic liquids in electrolytic capacitors to measure differential capacitance, simulating coarse-grained liquids with machine-learned effective potentials to match the properties of models with atomistic resolution, polymer diffusion in an implicit solvent, particle coupling to continuum hydrodynamic fields, and diffusion-advection-reaction solvers for electrokinetics and catalysis. Lectures provide an introduction to the physics and model building of these systems as well as an overview of the necessary simulation algorithms. During the afternoon, students practice running their own simulations in hands-on sessions using ESPResSo and waLBerla. Time is also dedicated to research talks, which illustrate how the simulation models and software are applied, and which provide further background on soft matter at different length and time scales.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

Multiscale modeling is concerned with simulations of complex physical systems with emergent properties that resolve different time- or length-scales. As a consequence, conflicting goals have to be met. On the one hand, a detailed description at the small scale is needed, but on the other hand, sufficiently long length- and time-scales have to be covered to capture the problem in its entirety while keeping the computational cost limited. Understanding many soft matter systems requires such a multi-scale approach. Often, a combination of simulation techniques, e.g., particle-based molecular dynamics and lattice-based hydrodynamics are coupled to obtain a satisfactory description of physical phenomena at different scales.

A typical example in fluid dynamics is Kármán vortex streets, which is a repeating pattern of swirling vortices that remain stable over a long distance from the source, which require a simulation environment that supports multi-grid resolution, such that the grid resolution along the path of the vortex street decreases linearly to save memory and computational effort, without sacrificing accuracy.
Another example in energy materials is the atomistic description of ionic liquids inside the porous nanostructure of electrodes, and the coarse-grained description inside the bulk solution in contact with the electrode. This type of simulation requires a adaptive resolution molecular dynamics simulation methods to create overlapping regions with different resolutions, typically atomistic inside the nanopore structure, coarse-grained far away from the electrode material (i.e. one sphere per molecule), and an intermediate region where the molecule is simultaneously resolved as individual atoms and a single coarse-grained sphere, with a weighting parameter that linearly depends on the distance between the fully atomistic and fully coarse-grained domains. In more advanced models, an extra domain is introduced with a grid-based description of the solvent and dissolved salt that is easily calculated using advection-diffusion solvers, but require complex boundary conditions to properly transform the particles momentum and net charge into fluid momentum and solvated charges.
Multiscale simulation software may also benefit from machine learning. One example is machine-learned potentials to re-introduce chemical detail in a specific region of a coarse-grained simulation, for example an electrode nanopore, or a protein catalytic site. Neural networks trained on chemically diverse datasets of quantum chemistry calculations are nowadays readily available for use in molecular dynamics software. They evaluate forces on atoms with accuracy close to density functional theory at a fraction of the computational cost. Alternatively, neural networks can be used for enhanced sampling, e.g. to discover new protein conformations that cannot be easily found by traditional molecular dynamics enhanced sampling methods.

## 3. What was the take-home message for the participants?

Multiscale modeling requires interdisciplinarity and access to heterogeneous computing architectures. Numerical methods developed in one software need to be re-usable in another software with minimal effort. Automated code generation workflows will become essential for research software to leverage future hardware without a big rewrite. Simulation data needs to be made available in open source materials databases to help train robust neural networks and democratize AI-powered research.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

Recorded lectures are available on the YouTube channel ESPResSo Simulation Package. The lecture slides are available in the Documents tab of the school page. Participants brought 11 posters and presented them in lightning talks. A book of abstracts was released on Zenodo under an open source license (doi:10.5281/zenodo.13933147) and advertised on the MultiXscale Cluster of Excellence in a blog post and in the July–December 2024 newsletter (a EuroHPC Joint Undertaking project). Hands-on session worksheets with solutions are available as Jupyter Notebooks in the source code of the ESPResSo software on GitHub. They can be remotely executed in the web browser via the Binder platform or viewed as static pages in the online user guide. The school format was presented in the talk "Organizing successful software community workshops" at the 5th conference for Research Software Engineering in Germany on February 26th 2025 and at the CASTIEL2 Training Coffee Break webinar on April 3rd 2025.

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The participants' career stages are evenly spread out: 3 undergraduate students, 7 graduate students, 11 PhD students, 9 post-docs, 7 professors. Most participants have their home institution in the European Union. A few joined from the United States, India, Pakistan, and Turkey. To promote attendance by graduate students, the event was included in the science curriculum of the University of Stuttgart as an ECTS-granting module and made a pre-requisite of the advanced simulation methods module. No conference fee was charged to make participation fair to everyone; we helped a participant from outside the European Union secure a travel grant via the Erasmus+ programme. The chosen location of the event is barrier-free and wheelchair-accessible. The teaching material of the hands-on sessions is in a file format accessible to visually impaired users.

## 6. Participant list

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**Bat-Erdene, Bat-Amgalan** - Fritz Haber Institute, Germany
**Bereau, Tristan** - Heidelberg University, Germany
**Bertrand, Jérémie** - EPFL, Switzerland
**Beyer, David** - University of Stuttgart, Germany
**Blanco, Pablo M.** - Norwegian University of Science and Technology, Norway
**Brodbeck, André** - University of Stuttgart, Germany
**Colak, Eren** - Hacettepe University, Turkey, Turkey
**Dansuk, Kerim** - Bogazici University, Turkey
**Dapena García, Raquel** - University of Santiago de Compostela, Spain
**Desmarchelier, Paul** - PHENIX, France
**Drotleff, Jannik** - University of Stuttgart, Germany
**Dullak Angeloni, Axel Roberto** - ZHAW, Switzerland
**Felden, Fabian** - University of Stuttgart, Germany
**Gandhi, Yashas Tejaskumar** - University of Stuttgart, Germany
**Gern, Marcel** - University of Stuttgart, Germany
**Hennig, Frederik** - Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
**Hohenberger, Paul** - Universität Stuttgart, Germany
**Hoßbach, Julian** - University of Stuttgart, Germany
**Jonnalagadda, Anirudh** - Istituto Italiano di Tecnologia, Italy
**Kamran Shabbir, Syed Muhammad** - Government College University, Pakistan
**Kobayashi, Hideki** - Georg-August-Universität Göttingen, Germany
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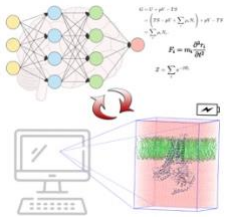
**Kurahatti, Somesh** - University of Stuttgart, Germany
**Lamparská, Veronika** - University of Stuttgart, Germany
**Lehtihet, Moncef** - Laboratoire Du Futur Syensqo, France
**Liberati, Diego** - National Research Council of Italy, Italy
**Maity, Ruma** - Technischen Universität Wien, Austria
**Mondal, Soumya** - IIT DELHI, India
**Müller, Niklas** - Universität Stuttgart, Germany
**Padhee, Ipsita** - Charles University, Czech Republic
**Peter, Christine** - University of Konstanz, Germany
**Peters, Julian** - Universität Stuttgart, Germany
**Praprotnik, Matej** - National Institute of Chemistry, Slovenia
**Rajput, Satyendra** - Indian Institute of Technology Delhi, India
**Reinauer, Alexander** - University of Stuttgart, Germany
**Scheunemann, Jonas** - University of Stuttgart, Germany
**Shojib, MD Mozakker Hosen** - Karlsruhe Institute of Technology, Germany
**Stoev, Iliya** - Karlsruhe Institute of Technology, Germany
**Tovey, Samuel** - University of Stuttgart, Germany
**Vieira, Lourenço** - ZHAW, Switzerland



# Expanding the impact of molecular simulations by integrating Machine Learning with statistical mechanics

**Location: Grand Hotel Vesuvio, Italy**
**Webpage：https://www.cecam.org/workshop-details/expanding-the-impact-of-molecular-simulations-by-integrating-machine-learning-with-statistical-mechanics-1331**
**Dates: Oct 10, 2024 - Oct 12, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The CECAM workshop focused on several major topics that significantly advanced the integration of machine learning (ML) with biosimulations, addressing key challenges and pushing the boundaries of the field.

**1. ML-Readable Representations**

The workshop highlighted methods for converting atomistic data from biosimulations into ML-compatible representations. This is crucial, as the quality of ML predictions relies on how well these representations retain essential physico-chemical properties.

**2. ML-Trained Interatomic Potentials**

A central theme was the use of ML to train interatomic potentials, which can enhance the efficiency of molecular dynamics (MD) simulations. ML potentials allow faster simulations while maintaining accuracy, helping to overcome the longstanding timescale problem.

**3. Dimensionality Reduction and Collective Variables**

The identification of suitable collective variables (CVs) for enhanced sampling methods was a key focus. Discussions centered on using deep neural networks to analyze large MD datasets, which can identify critical physical descriptors that serve as effective reaction coordinates (RCs).

**4. Enhanced Sampling**

Participants explored how ML could enhance sampling methods, such as metadynamics. Novel deep learning path-like CVs were introduced to improve the exploration of free energy landscapes, facilitating the study of complex biological processes.

**5. Coarse-Graining and Backmapping**

The workshop also addressed the challenge of retaining atomistic details in coarse-grained models. ML techniques were discussed as solutions to improve coarse-graining and backmapping processes, enhancing the predictive power of these simulations.

**6. Long-Range Interactions**

Discussions included how ML models could better capture long-range interactions, critical for understanding phenomena like molecular assembly. Self-consistent field neural networks were proposed to include these effects, marking a step forward in model accuracy.

**Contribution to Advancing the State of the Art**

The discussions contributed to advancements in:

- **Accuracy and Efficiency**: Integrating ML leads to more accurate and computationally efficient simulations.
- **New Methodologies**: Novel ML-based techniques address longstanding challenges in molecular simulations.
- **Expanded Applicability**: ML opens up possibilities for studying larger, more complex biological systems.
- **Collaborative Innovation**: The workshop fostered interdisciplinary collaborations, setting the stage for future advancements in methodology and software.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop successfully fostered a brainstorming session on the key applications of ML algorithms in biosimulations, offering a critical assessment of their advantages, current challenges, and future directions. Discussions centered on several main themes:

**- Transitioning from atomistic data to ML-friendly representations**

Various methods were presented for converting atomic configurations from biosimulations into ML-compatible representations. This step is crucial for any ML application, as the accuracy and consistency of ML predictions heavily depend on how well the input preserves the essential physico-chemical properties of the system being studied.

**- ML-trained interatomic potentials**

Applying ML techniques to enhance the speed or performance of classical MD simulations is gaining attention as a potential solution to the timescale issue. Neural networks are being trained using simulation data to compute interatomic potentials more efficiently than traditional force fields based on molecular mechanics or quantum mechanics approaches.

**- Dimensionality reduction and collective variable identification**

One of the major challenges in advanced sampling methods like metadynamics or umbrella sampling is identifying the right RCs (or CVs). ML-based solutions to this dimensionality reduction problem are capturing the interest of many researchers. Specifically, deep neural networks are being developed to process the vast datasets generated by cutting-edge MD simulations, identifying the most relevant physical descriptors. These variables, often combined in non-linear ways, can then be used as reaction coordinates in more accurate enhanced sampling experiments.

## 3. What was the take-home message for the participants?

The take-home message for participants emphasized the transformative potential of integrating machine learning (ML) with biosimulations to overcome current limitations in timescale, system dimensionality, and data analysis. Participants were encouraged to explore ML approaches for accelerating molecular simulations and improving accuracy, while fostering collaborations and innovative software developments to push the boundaries of biological research.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

During the workshop, the social benefits of applying Machine Learning (ML) to biosimulations were emphasized. Biosimulations already serve as a powerful tool for investigating complex biological processes, such as protein folding, conformational changes, and ligand binding and unbinding mechanisms. These advances provide valuable insights into biomolecular behavior and the fundamental mechanisms governing receptor-ligand interactions, ultimately aiding in the design and development of more effective drugs.
By integrating ML with biosimulations, these social benefits could be further amplified, as this combination can help overcome current limitations related to timescale and system dimensionality. Additionally, the development of new ML algorithms tailored to specific research projects could be adapted for use in other fields, as is often the case in scientific research.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

Tangible outcomes from the CECAM workshop are already materializing in several areas:
**1. Publications**: Collaborative papers focused on the integration of ML with biosimulations, such as ML-trained interatomic potentials or CVs identification, are likely in preparation or already being developed.
**2. Collaborations**: New interdisciplinary collaborations have begun forming, particularly between computational chemists, biophysicists, and ML specialists, aiming to address the challenges discussed during the workshop.
**3. Research Proposals**: Plans for joint proposals are likely ongoing to further explore ML-enhanced molecular simulations.
**4. Software Developments**: The development of new ML-based software tools for improving biosimulations, such as better RC identification, is already being pursued by some workshop participants.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The CECAM workshop took significant steps to promote inclusivity across various dimensions, including gender, geographical origin, and career stage:
**1. Geographical diversity**: Participants and speakers represented institutions from multiple countries, including Switzerland, the United States, China, and more, highlighting the effort to ensure a wide global representation.
**2. Career stages**: The workshop featured both prominent figures in the field and early-career researchers, offering opportunities for young scientists to present their work through oral communications and poster sessions, fostering an inclusive environment across career levels.
**3. Gender inclusivity**: Although efforts were made to include female speakers, some invited women were unable to attend, underscoring the workshop's proactive approach toward gender diversity despite these challenges.

## 7. Participant list

### Organisers

**D'Amore, Vincenzo Maria**
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**Bidone, Tamara** - University of Utah, United States
**Bolhuis, Peter** - University of Amsterdam, Netherlands
**Bowman, Greg** - University of Pennsylvania, United States
**Breebaart, Rik** - University Of Amsterdam, Netherlands
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**Carli, Matteo** - University of Italian Switzerland (USI), Switzerland
**Carosella, Laura** - Universita' della Svizzera Italiana, Switzerland
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**Dal Peraro, Matteo** - EPFL, Switzerland

**De Fabritiis, Gianni** - University Pompeu Fabra, Spain
**Di Cristofano, Samuele** - Sapienza University of Rome, Italy
**Diakogiannaki, Isidora** - University of Naples Federico II, Italy
**Dijkman, Jacobus** - University of Amsterdam, Netherlands
**Donati, Greta** - University of Napoli Federico II, Italy
**Ensing, Bernd** - University of Amsterdam, Netherlands
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**Milenkovic, Stefan** - University of Cagliari, Italy
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**Peter, Christine** - University of Konstanz, Germany
**Raimondi, Chiara** - Università della Svizzera Italiana, Switzerland
**Raniolo, Stefano** - Università della Svizzera Italiana, Switzerland
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**Riccardi, Enrico** - University of Stavanger, Norway
**Šimko, Pavol** - Charles University, Prague, Czech Republic, Czech Republic
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**Vaikuntanathan, Suriyanarayanan** - University of Chicago, United States
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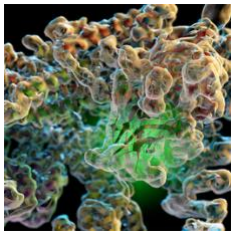
**Zanovello, Luigi** - Istituto Italiano di Tecnologia, Italy
**Zgarbova, Marie** - Palacky University, Czech Republic
**Zhang, Mingyuan** - Zhejiang University, China



# Emerging theoretical approaches to complement single-particle cryo-electron microscopy

**Location: CECAM-IT-SISSA-SNS**
**Webpage : https://www.cecam.org/workshop-details/emerging-theoretical-approaches-to-complement-single-particle-cryo-electron-microscopy-58**
**Dates: Oct 21, 2024 - Oct 24, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Biophysics is undergoing a transformative phase, driven by groundbreaking advancements in cryo-electron microscopy (cryo-EM). The recent CECAM workshop gathered experts to tackle pressing challenges in processing, validating, complementing, and interpreting cryo-EM data.
This meeting brought together leaders in cryo-EM technology and application, as well as computational scientists focusing on data processing methods and the complex dynamics of large biomolecules imaged by cryo-EM. Additionally, the agenda covered cutting-edge work in electron tomography, emphasizing multiscale modeling approaches that capture cellular components in remarkable detail.
We addressed current challenges in modeling cryo-EM data, emphasizing theoretical approaches to refine models within cryo-EM maps. Additionally, we discussed ongoing computational efforts aimed at enhancing cryo-EM data processing. We also examined applications that generate models of large biological systems from cryo-EM maps and integrate all-atom simulations of these systems.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

**Atomic Refinement into Cryo-EM Maps.** We evaluated current methods for model refinement, including docking searches, Monte Carlo, and molecular dynamics (MD), while identifying key challenges, such as resolution heterogeneity. Low-resolution regions can influence the dynamics of neighboring high-resolution areas, complicating refinement. We explored how enhanced sampling techniques could improve the fitting process by avoiding non-physiological local minima. Throughout, we emphasized validation and reproducibility, aiming to answer the open question: “What defines the best fit?”

**Assessing Conformational Heterogeneity from Cryo-EM Maps**. We examined challenges posed by conformational heterogeneity and discussed ways to capture a comprehensive view of conformational states. This included leveraging advanced clustering methods and Bayesian approaches to better characterize protein flexibility and generate representative 3D structures.
**The Future of Cryo-EM and Modeling for Large-Scale Systems**. Finally, we explored recent applications of all-atom MD simulations and cryo-EM processing techniques for investigating large biological systems derived from cryo-EM data. These applications showcased high-impact biological targets, such as the human spliceosome and the Piezo channel, exemplifying the potential of cryo-EM and MD simulations to advance our understanding of complex biological machinery.

## 3. What was the take-home message for the participants?

The goal of this workshop was to identify strategies to maximize the synergy between computational and experimental expertise in single-particle cryo-EM. We achieved this by discussing emerging theoretical approaches and recent applications designed to process, complement, and interpret cryo-EM data. Key methodological advances and challenges in the field were examined, with particular focus on validation and reproducibility

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The characterization of biological systems through cryo-EM and computational modeling is revolutionizing drug discovery and therapeutic development, with profound impacts on society. By providing precise insights into biomolecular structures and their interactions, these tools enable the design of targeted drugs that treat diseases more effectively. This precision medicine approach is accelerating the availability of treatments, especially for complex diseases like cancer and neurological disorders, thereby improving health outcomes and reducing healthcare costs.
Moreover, the predictive power of computational modeling enhances our understanding of how drugs will perform, minimizing costly trial-and-error stages. As a result, cryo-EM and modeling not only drive innovative treatments but also lay the groundwork for preventive and personalized healthcare, ultimately contributing to a healthier, more resilient society.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

This meeting has sparked valuable collaborations between experimentalists and computational scientists, opening pathways for innovative research publications and potential technological advancements. By combining the expertise of experimental cryo-EM practitioners with computational modelers, attendees are positioned to tackle some of the most pressing challenges in structural biology with a more integrated approach.
These collaborations foster a cross-pollination of ideas that can lead to the development of more robust, validated models, enhancing the reproducibility and accuracy of structural interpretations. This synergy not only enriches scientific understanding but also accelerates the timeline for impactful publications and may even pave the way for patents in areas like drug design, novel imaging techniques, or algorithm development for processing cryo-EM data. Ultimately, this meeting has laid the foundation for a collaborative network that can drive advancements in biomedicine and influence the future landscape of scientific discovery.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Over 80 participants from around the globe gathered in the beautiful city of Trieste, a crossroad of Mediterranean, Central, and Eastern European heritage. The city is home to the International School of Advanced Studies (SISSA-ISAS), providing an inspiring location for this event.
The meeting was notable for its geographic, gender, disciplinary diversity, with participants from North and South America, Europe, and Asia. 21 invited speakers, 14 short talks (from submitted abstracts), and 29 posters showcased the creativity of the community, with representation from 17 countries: Australia, Canada, China, Czech Republic, France, Germany, India, Italy, Japan, Poland, Singapore, Slovenia, South Africa, Spain, Sweden, United Kingdom, United States. An outstanding number of women scientists contributed, reflecting inclusivity in the field.

## 7. Participant list

### Organisers

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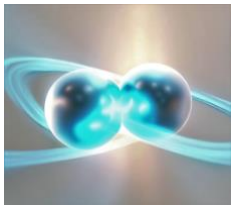
**Fraser, James** - UCSF, United States
**Lapinaite, Audrone** - Arizona State University, United States
**Singharoy, Abhishek** - Arizona State University, United States
**Sugita, Yuji** - RIKEN, Japan
**Tama, Florence** - Nagoya University, Japan
**Vendruscolo, Michele** - University of Cambridge, United Kingdom



# Challenges and perspective in computational modelling for fusion reactors

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/challenges-and-perspective-in-computational-modelling-for-fusion-reactors-1293**
**Dates: Oct 28, 2024 - Oct 29, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

Seven cross-cutting topics emerged:
I) Multiscale radiation-damage modelling. The presentations illustrated a seamless transition from first-principles defect energetics to full-component finite-element and Monte-Carlo transport models. Applied to the MAST-U spherical tokamak and other ITER-class components, this approach delivered robust estimates of stress, swelling and tritium-inventory margins.
II) Design of advanced structural and plasma-facing materials (PFMs). High-entropy and compositionally-complex refractory alloys (Leinenbach, Nguyen-Manh) plus large-scale experimental data-based and DFT-driven screening of PFMs (Fedrigucci) illustrated how machine-learning interatomic potentials and high-throughput workflows are compressing discovery cycles.
III) Plasma–wall interaction & divertor physics. Recent SOLPS-ITER and ERO 2.0 simulations of impurity sources and power exhaust, validated against JET and other metallic-wall tokamak data, are refining ITER predictions and helping to delineate the prospective DEMO operating window.
IV) Beyond-the-wall components. Talks on high-temperature superconductors for stellarators (Riva) and Po-containing chemistry in lead/bismuth blankets (Cottenier) highlighted modelling needs that extend outside the plasma-facing components.
V) High-performance & exascale computing. Case studies ranged from quantum-accurate MD of IFE ablators on the Frontier supercomputer (Oleynik) to randomized linear-algebra kernels for petascale neutronics (Grigori) and the EUROfusion Advanced Computing Hub at BSC (Mantsinen), signaling that exascale resources are becoming integral to fusion materials research.
VI) Uncertainty quantification (UQ). Peterson introduced OpenMC-based workflows that propagate nuclear-data and model uncertainties through reactor designs, converting best-estimate simulations into statistically robust engineering margins.
VII) Experimental infrastructure & validation. IFMIF-DONES (Ibarra) and ion-beam surrogate campaigns (Schäublin) were presented as the imminent bridge between

modelling and 14 MeV fusion-neutron exposure, while Mason showed fully validated cascade-based microstructure predictions.

By chaining these elements - cross-scale physics, data-driven discovery, verified plasma-surface models, exascale computing, quantified uncertainty and purpose-built irradiations - participants outlined a coherent roadmap toward predictive digital twins of fusion components. Such an integrated capability, now moving from concept to practice, represents a decisive advance over the fragmented approaches of only a few years ago.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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Primary tangible outcome:
A common Dropbox workspace storing every slide and supplementary material shared during the two-day meeting, giving all attendees persistent, immediate access and thus speeding up post-workshop cross-checking, reuse of reference data and the launch of joint follow-up studies.
Scientific consensus points.
I) Next-generation alloys.
Talks by Natarajan, Leinenbach and Nguyen-Manh converged on low-activation, refractory, compositionally complex W-based alloys as a credible route to exceed pure tungsten in radiation tolerance and high-temperature strength.
II) Integrated multiscale modelling. Speakers spanning atomistic (Granberg), meso-microscopic (Dudarev, Mason) and reactor-scale transport (Theiler, Brezinsek, Dudarev) agreed that bridging the gap in length and time remains one of the dominant bottlenecks. Reduced-order surrogates were highlighted as the enabling tools
III) Quantifying uncertainty. In transport calculations, the true uncertainties, such as those from nuclear data and model approximations, are often much larger than the inherent statistical errors from Monte Carlo simulations. Addressing these uncertainties is therefore fundamental for robust predictions of key design aspects, such as radiation damage in materials.
Outstanding gaps and limitations
I) 14 MeV neutron exposure. Until IFMIF-DONES begins delivering prototypical fluxes, dose-accumulation and transmutation studies must continue to rely on surrogate irradiation sources whose spectra lack full fidelity to a fusion reactor environment.
II) Plasma-wall interaction fidelity. Current SOLPS-ITER, SOLEDGE-EIRENE and ERO 2.0 workflows still under-predict impurity sources and divertor conditions. Neutron-induced effects and tritium-cycle constraints must be incorporated before reliable DEMO extrapolation is possible.
III) Experimental-computational validation loop. Coordinated campaigns that couple TEM, TDS and NRA diagnostics with high-dose cascade simulations are required to close the present validation gap for irradiated microstructures.

Open questions for future collaboration
I) How can uncertainty-aware, fully coupled neutron-plasma-material simulations be executed at reactor time-scales without prohibitive computational cost?
II) Which irradiation and thermal protocols will provide the definitive screening criteria and data for W alloys and alternative candidates prior to DEMO component down-selection?
III) What data-management architecture that satisfies FAIR principles can act as a persistent benchmark repository for the fusion-materials community?

## 3. What was the take-home message for the participants?

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Exascale HPC, machine-learning - from interatomic potentials to phase- and microstructure surrogates - and rigorously validated multi-physics models (Monte Carlo neutron transport, plasma-wall interaction, cascade-to-continuum mechanics with quantified uncertainties) now enable simulation-led fusion-materials design; impact demands open benchmarks and rapid experiment-model loops.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

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Delivering radiation-resistant, low-activation materials remains a key challenge for fusion energy.
The workshop addressed this through developments in simulation-driven design, combining machine learning with physics-based models to study phase stability, microstructure evolution, defect energetics, and irradiation effects.
Multi-scale simulations linking neutron transport, material response, and damage accumulation were presented, alongside advances in numerical solvers and high-performance computing. These tools support more systematic exploration of candidate materials.
While experimental validation remains essential, the approaches discussed may contribute to broader applications in nuclear materials and extreme environments.
In addition, by involving an emerging fusion-energy start-up the workshop directly connected fundamental modelling advances to eventual commercial deployment, strengthening the pathway toward societal benefits. Proxima Fusion contributes through advanced modelling of HTS magnets - a line of work with potential relevance beyond fusion, including in other high-tech industries.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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A shared Dropbox folder has been created to collect all workshop materials and it is accessible to all participants. The event fostered new interdisciplinary connections between modelling, plasma physics, and materials groups, with early-stage discussions already underway regarding potential follow-up studies.
Furthermore, the workshop enabled fruitful exchanges between academia and industry. Proxima Fusion's presentation on HTS coils generated mutual interest and opened the door to possible collaborations among the invited participants.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Inclusivity was built into the workshop design. A hybrid format (on-site at CECAM-HQ-EPFL plus Zoom livestream) enabled 8 remote and 24 on-site participants, expanding access beyond visa or travel constraints and bringing together researchers from 11 countries across Europe, North America and Asia. Gender balance remains a challenge, but three women took part, two of them (M. Mantsinen, L. Grigori) as invited speakers (10 %).
Beyond gender, geography and career stage, the line-up deliberately included a speaker from the private fusion sector (Proxima Fusion), broadening the professional background represented among participants.

## 7. Participant list

### Organisers

**Fedrigucci, Andrea**
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**Ricci, Paolo**
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**Cottenier, Stefaan** - Ghent University, Belgium
**Dominguez Gutierrez, F. Javier** - NCBJ, Poland
**Dudarev, Sergei** - UK Atomic Energy Authority, United Kingdom
**Er, Suleyman** - DIFFER, Netherlands
**Fasoli, Ambrogio** - EPFL, Switzerland
**Février, Olivier** - EPFL, SPC, Switzerland
**Granberg, Fredric** - University of Helsinki, Finland
**Grigori, Laura** - EPFL & PSI, Switzerland
**Gutierrez, Julio** - Barcelona Supercomputing Center, Spain
**Ibarra, Angel** - IFMIF-DONES España, Spain

**Iglesias, Roberto** - University of Oviedo, Spain
**Leinenbach, Christian** - Empa, Switzerland
**Liberati, Diego** - National Research Council of Italy, Italy
**López Cazalilla, Álvaro** - Barcelona Supercomputing Center, Spain
**Mantsinen, Mervi** - Barcelona Supercomputing Center, Spain
**Mason, Daniel** - UKAEA, United Kingdom
**Masoudi, Ali** - Amirkabir University of Technology, Iran
**Morgan, Dane** - University of Wisconsin - Madison, United States
**Neu, Rudolf** - MPI for Plasma Physics, Germany
**Nguyen-Manh, Duc** - United Kingdom Atomic Energy Authourity, United Kingdom
**Oleynik, Ivan** - University of South Florida, United States
**Palfy Alonso-Alegre, Maria** - Erasmus Mundus Master In Nuclear Physics, Spain
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**Raju Natarajan, Anirudh** - EPFL, Switzerland
**Riva, Nicolo** - Proxima Fusion, Germany
**Ruestes, Carlos** - Polytechnic University of Madrid, Spain
**Schäublin, Robin** - ETH Zürich, Switzerland
**Suárez Recio, Jorge** - Universidad Politécnica de Madrid, Spain
**Tayran, Ceren** - DIFFER, Netherlands
**Theiler, Christian** - EPFL-SPC, Switzerland
**Waagaard, Elias** - EPFL, Switzerland
**Zhang, Lei** - University of Groningen, Netherlands

# Multiscale investigation of bubble-cell interaction mechanisms for enhanced drug delivery

**Location: CECAM-FR-MOSER**
**Webpage : https://www.cecam.org/workshop-details/multiscale-investigation-of-bubble-cell-interaction-mechanisms-for-enhanced-drug-delivery-1305**
**Dates: Oct 28, 2024 - Oct 31, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This CECAM workshop brought together a diverse group of experts at the intersection of computational modeling and experimental studies. The event focused on four major topics, each contributing to advancing the state of the art in the understanding and application of bubble cavitation in fields like drug delivery. Below is a summary of the key topics discussed and how they have contributed to the field:

**1. Bubbles and droplets at equilibrium**

This session focused on the fundamental properties of bubbles and droplets at equilibrium. Understanding these basic principles is crucial for manipulating bubbles in various applications, as it helps researchers predict their stability, size, and behavior in different environments. The discussions provided new insights into the stability of microbubbles, nanobubbles and nanodroplets, and the mechanisms of the bubble nucleation.

**2. Bubble cavitation dynamics**

This topic covered the core principles of bubble cavitation, including the initiation, growth, and collapse of bubbles in response to external stimuli such as ultrasound and laser, and how to image and control the cavitation. Computational models and experimental studies were presented that explore cavitation dynamics at different scales, and how the dynamics is influenced by the bubble properties. The session also highlighted advances in controlling cavitation bubble prevent unwanted tissue damage and improve the efficacy of cavitation therapies.

**3. Effects of bubble cavitation on the surrounding environment**

The session on the effects of cavitation focused on the physical forces generated by bubble collapse, including shock waves, shear forces, and localized heating. Researchers discussed how these effects impact surrounding biological systems

such as solid walls, microfluidics, microvessels, bacteria and amyloid fibrils. Understanding the environmental impact of cavitation is critical for optimizing its use in medical applications and exploring new applications. The insights gained also contribute to the development of non-invasive techniques for material cleaning and surface treatment.

**4. Bubble cavitation-mediated drug delivery**

One of the most promising applications of bubble cavitation discussed during the workshop was its potential to enhance drug delivery. Recent preliminary clinical trials have demonstrated its effectiveness, and discussions focused on methods for large-scale bubble fabrication and the design of prototypes for cavitation-mediated drug delivery devices, particularly targeting pancreatic cancer.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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**1. Primary outcomes:**

Overall, the workshop made significant contributions to advancing the state of the art in bubble cavitation, enhancing our understanding of its fundamental mechanisms and broadening its medical applications. Key outcomes include:

- A deeper understanding of bubble dynamics and their environmental effects, enabling better control over cavitation events.
- Progress in using bubble cavitation for targeted drug delivery, with promising implications for treating diseases such as cancer and neurological disorders.
- Increased interdisciplinary collaboration, fostering more robust models, experimental designs, and clinical applications of cavitation technologies.

**2. Limitations:**

- Many findings presented in the workshop are still at the fundamental and preclinical stages.
- The potential risks and long-term side effects of cavitation-mediated therapies have not been fully explored.

**3. Open questions:**

The following challenges should be addressed:

- The lack of standardized protocols and regulatory guidelines for cavitation technologies may hinder both our understanding of their mechanisms and their applications in clinical practice.
- Greater collaboration between experimental and simulation studies is needed to fully elucidate bubble-cell interactions across various spatiotemporal scales.
- Scaling bubble cavitation techniques from small-scale laboratory research to clinical applications remains challenging due to technical and methodological complexities.
- Enhancing the use of molecular and particle dynamics simulations in bubble cavitation is essential, as these simulations can provide unprecedented insights into mechanisms at short spatiotemporal scales, which are difficult to capture through experiments or traditional computational fluid dynamics approaches.

## 3. What was the take-home message for the participants?

Bubble cavitation holds potential for applications, especially in drug delivery. However, further research is needed to understand the mechanisms across spatiotemporal scales, control cavitation dynamics, enhance safety, and optimize bubble design. Collaboration between molecular dynamics simulations, computational fluid dynamics, and experiments is crucial to overcome these limitations and advance the application of this technology.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the CECAM workshop on bubble cavitation hold potential for societal benefits, particularly in the fields of medicine, biotechnology and environment.

**1. Advancing drug delivery**: One of the most promising outcomes of the workshop was the discussion around bubble cavitation-mediated drug delivery. This technology has the potential how we treat complex diseases such as cancer, neurological disorders, and cardiovascular diseases with advantages such as noninvasive, cost effective, safe, more targeted therapies and minimised side effects.

**2. Enhancing cancer therapy**: The use of bubble cavitation to increase the permeability of tumor tissues could significantly improve the delivery of chemotherapy or immunotherapy agents, reducing the need for systemic drug delivery, which often results in harmful side effects. This targeted approach could increase the success rates of cancer treatments and provide more affordable and accessible healthcare solutions.

**3. Environmental and industrial applications**: Beyond medicine, bubble cavitation has potential applications in material cleaning and water purification. The ability to use controlled cavitation for cleaning surfaces or breaking down pollutants could help reduce the environmental impact of industrial processes and contribute to more sustainable practices in waste management and environmental remediation.

In summary, the workshop's outcomes suggest that bubble cavitation holds the potential for significant societal benefits, from improving healthcare outcomes through more effective drug delivery to supporting environmental sustainability and industrial innovation. However, realizing these benefits will depend on continued research and interdisciplinary collaboration to overcome existing limitations.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

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**1. New collaborations**: The workshop provided a unique interdisciplinary platform that brought together experts from diverse fields, such as molecular dynamics simulations, mesoscale simulations, computational fluid dynamcs, mathematical modeling, bioengineering, nanomedicine, in vivo and in vitro experiments. This could lead to the establishment of new collaborations between researchers who plan to combine their expertise to study the drug delivery and other therapeutic uses.
**2. Software development**: The workshop discussions emphasized the need for improved computational approaches to predict bubble behavior across diverse spatiotemporal scales. Several participants proposed developing new multiscale simulation software that integrates molecular dynamics, particle simulations, fluid dynamics models, and machine learning with experimental data. These tools aim to standardize and enhance the study of bubble cavitation.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

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To promote inclusivity at the CECAM workshop, several measures were implemented:
**1. Gender balance:** We prioritized gender diversity among both speakers and participants. Efforts were made to invite female experts alongside male counterparts, resulting in 5 female speakers and 25 male speakers.
**2. Geographical diversity:** The workshop featured speakers and participants from various regions, including Asia, Europe, and the Americas, ensuring a globally representative exchange of expertise.
**3. Career stage inclusivity:** Researchers at all career stages were welcomed, ranging from early-career scientists and PhD students to senior researchers. This approach enhances opportunities for mentoring, networking, and collaboration.
These initiatives helped create an inclusive and equitable environment for all participants, enriching the overall workshop experience.

## 7. Participant list

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### Organisers

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**Cavalli, Roberta** - Università degli Studi di Torino, Italy
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**Dockar, Duncan** - University of Edinburgh, United Kingdom
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**Hu, Guohui** - Shanghai University, China
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**Taulier, Nicolas** - Sorbonne University, France
**Teshima, Hideaki** - Kyushu University, Japan
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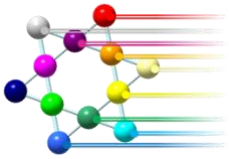

# School on experimental, theoretical and numerical approaches to frustrated quantum magnets

**Location: Ecole de Physique Les Houches, France**
**Webpage : https://www.cecam.org/workshop-details/school-on-experimental-theoretical-and-numerical-approaches-to-frustrated-quantum-magnets-1310**
**Dates: Oct 28, 2024 - Nov 8, 2024**

## 1. What were the major topics presented in the School?

The topics presented in the School covered many experimental, theoretical and numerical aspects of frustrated quantum magnetism in a coherent and complementary way. More precisely, the lectures were dedicated to:
- A general introduction to frustrated magnetism and microscoping modelling (which includes the mechanisms for magnetic exchanges in Mott insulators, the anisotropic interactions, crystal field effects and the quadrupolar and nematic states)
- Low dimensional systems (Luttinger liquids), Kitaev magnets and spin-orbit coupled systems, triangular and kagome systems, pyrochlore systems with classical and quantum spin ice. For all these categories, examples of materials were given.
- Characterisation of quantum and classical spin liquids, classification of topologically ordered phases, projective symmetry groups for Z2 spin liquids, definition of fractional quasiparticles and anyons (exchange statistics, symmetry fractionalization), with examples of solvable models (toric code, resonating valence bond models).
- Experimental probes for frustrated magnets, which includes neutron scattering, neutron magnetic resonance, muon spin resonance, thermodynamics and magnetometry.
- Analytical approaches: dimer models, mean-field theory (Schwinger bosons and Abrikosov fermions), non-perturbative approaches.
- Numerical approaches: Monte Carlo methods (classical and quantum), variational calculations (Gutzwiller projection), TN (tensor networks) and DMRG (density matrix renormalization group).
The applications of numerical approaches have be developed during the tutorials about exact diagonalization, matrix product state, and NMR data analysis.

## 2. What were the limitations and open questions raised during the lectures and the hands-on sessions?

We had planned several practical sessions to go into greater depth on the notions seen in class. We probably should have devoted more slots in the timetable to this, not with the aim of offering more different subjects, but to give students time to follow through on what was proposed. It should be mentioned, however, that a few students regretted the absence of a practical on the specific subject of “spin waves”. A second room equipped with an overhead projector would certainly have been useful. As a result, we had to modify the timetable, being unable to run two sessions in parallel.
With hindsight, we feel that the amount of time devoted to experimental techniques was too small. This would be an area for improvement in a future edition.
Lastly, due to changes in the timetable, we had to concentrate the “project” feedback session on a single 3-hour slot, which was undoubtedly too long! However, we did not notice any particular limitations during the question sessions: students were able to ask their questions in a relaxed way, either during class, or during breaks, meals, walks...

## 3. What was the take-home message for the participants?

The take-home message was the importance of considering experimental, theoretical and numerical approaches all together in the research in frustrated magnetism in order to tackle and solve the important questions that are addressed in the field. For this reason, lectures proposed an interplay between the three elements: Introduction to the main concepts, models and theories, overview of the experimental techniques, introduction to numerical techniques.

## 4. Are there tangible outcomes for the School (e.g., lecture notes, recording of the lectures, GitHub repository, etc.)?

- The lecture notes as well as the material for the tutorials, and bibliographic information are accessible on a cloud.
- A booklet with the summary of the lectures and the projects the student worked on was edited.

## 5. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

Lecturers have been chosen first according to their expertise. Although their geographical provenance was international, a preference was given to European lecturers in order to limit the travels. Special care was then given to gender equilibrium in the choice of lecturers, which was complicated due to the low number of women in the field, and we could reach 25% of woman lecturers (after one withdrawal). The lecturers were at different stages of their career with some of them recruited in the 2010s and some with a long experience.
The selection of the applicants was made in order to keep the repartition in the geographical provenance as emerged from the applications. Reduced and free fees were proposed for certain students. The gender ratio was also respected.

## 6. Organiser list

**Laflorencie, Nicolas**
LPT CNRS, France
**Lhotel, Elsa**
Institut Néel, CNRS, France


# Beyond ground state simulations: navigating challenges in excited states of extended molecules and materials

**Location: CECAM-HQ-EPFL, Switzerland**
**Webpage : https://www.cecam.org/workshop-details/beyond-ground-state-simulations-navigating-challenges-in-excited-states-of-extended-molecules-and-materials-1285**
**Dates: Nov 5, 2024 - Nov 8, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop focused on four central topics identified as key to advancing the modeling of excited states in extended systems:

**1. Non-adiabatic Molecular Dynamics (NAMD)**
**2. Charge Transfer (CT)**
**3. Long-Range Interactions**
**4. Machine Learning (ML) for Excited States**

These areas were examined in depth, including current approaches, existing challenges, and future directions. A major outcome of the workshop is the collaborative drafting of a **living, open-access review and perspective article**, which is currently in progress. This article will be published in a **perpetual format**, meaning it can be continuously updated as new insights, results, and methods emerge.

This flexible structure allows for the addition of newly identified challenges as well as the closure of resolved ones, making it a dynamic and enduring resource for the community. Through this evolving document, the workshop establishes a lasting contribution that will actively support and shape future developments in the field.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

A key outcome of the workshop was the productive exchange between scientists from both the excited-state and ground-state communities. This interdisciplinary dialogue brought together expertise from photochemistry, photophysics (including charge transfer and long-range interactions), non-adiabatic dynamics, and machine learning. The convergence of these diverse perspectives enabled a more holistic understanding of the challenges in modeling excited states in extended systems.

By fostering cross-disciplinary thinking, the workshop pushed the boundaries of conventional approaches and revealed important conceptual and methodological gaps. Discussions uncovered limitations in current methods – such as the difficulty of treating long-range interactions accurately, the challenges in simulating non-adiabatic dynamics in large systems, and the limited transferability of ML models trained on narrow datasets. Importantly, the open and collaborative format of the event allowed participants to identify promising research directions and synergies across fields that are not often in direct dialogue.
One significant open question is how to effectively bridge ground- and excited-state modeling frameworks to enable seamless, multiscale simulations. Another recurring theme was the need for better benchmarking strategies and community-wide datasets to support reproducibility and robust ML applications.
These outcomes will be captured and continuously updated in a living, open-access perspective article – currently in preparation – which will serve as a long-term platform for tracking progress, integrating new developments, and refining research priorities in the field.

## 3. What was the take-home message for the participants?

The take-home message was that **progress in excited-state modeling relies on interdisciplinary collaboration across disciplines**, i.e., electronic structure theory & method development, simulations and machine learning. Bridging ground- and excited-state communities revealed key open questions, such as how to create reliable **benchmark datasets** and how to effectively include **solvation effects**, guiding participants toward shared goals and future research directions.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

Yes, the outcomes of the workshop hold significant potential for societal benefits, particularly by advancing the prediction and design of photofunctional molecules and materials used in solar-light-driven energy conversion, such as in photocatalysis and photovoltaics. Accurate modeling of excited states is crucial for the development of efficient solar cell materials, photochemical systems, and photofunctional components for applications like data storage.
The interdisciplinary discussions and insights from the workshop will directly inform a living, open-access review article. This evolving resource is intended to serve as a long-term guide for future research and innovation in the field.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

A key tangible outcome of the workshop is the collaborative development of a living, open-access review article designed to allow ongoing extensions and updates. This format enables incorporation of new insights and advances over time, potentially involving contributions from researchers beyond the workshop participants. Additionally, by bringing together scientists from diverse backgrounds, the workshop fostered valuable interdisciplinary exchanges that are expected to encourage future collaborations and joint initiatives within the community.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

To promote inclusivity, we actively ensured a balanced representation of gender, career stages, and geographical regions among participants and speakers. Invitations were extended to early-career researchers, e.g. Adil Kabylda (LUX) and Edward Linscott (CHE), alongside senior experts, e.g. Claudia Draxl (GER), Reinhard Maurer (GBR), and Sergei Tretiak (USA), fostering diverse perspectives.

## 7. Participant list

### Organisers

**Kronik, Leeor**
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**Blaskovits, J. Terence** - Max-Planck Institute for Polymer Research, Germany
**Buzsáki, Dániel** - Wigner Research Centre for Physics, Hungary
**Chaudhuri, Shayantan** - University of Nottingham, United Kingdom
**Creed, Isabel** - Imperial College London, United Kingdom
**Curchod, Basile** - University of Bristol, United Kingdom
**Das, Sambit** - Stockholm University, Sweden
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**Draxl, Claudia** - Humboldt-Universität zu Berlin, Germany

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**Kümmel, Stephan** - University of Bayreuth, Germany
**Lieberherr, Annina** - University of Oxford, United Kingdom
**Linscott, Edward** - Paul Scherrer Institute, Switzerland
**Lu, Gang** - California State University Northridge, United States
**Mamusi, Fatemeh** - Universitat De Barcelona, Spain
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**Maurer, Benedikt** - IRIS, Germany
**Meisner, Jan** - Heinrich Heine University, Germany
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**Reuter, Karsten** - Fritz-Haber-Institut der MPG, Germany
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**Salihbegovic, Faruk** - Universität Wien, Austria
**Sodjargal, Tulga-Erdene** - EPFL, Switzerland
**Taghizadeh Rahaghi, Narjes** - University of Graz, Austria
**Tayebi, Zahra** - Leibniz-Institut für Katalyse E.V., Germany
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**Xu, Xun** - EPFL, Switzerland

# Beyond the structural frontier: modeling the dynamics of biomolecular interfaces

**Location: Institut de Biologie physico-Chimique, France**
**Webpage : https://www.cecam.org/workshop-details/beyond-the-structural-frontier-modeling-the-dynamics-of-biomolecular-interfaces-1303**
**Dates: Nov 12, 2024 - Nov 15, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

This workshop aimed to address challenges faced by computational biologists trying to model biomolecular assemblies that include proteins, which are specifically related to the dynamic properties of these systems. These issues can arise from the fact that these complexes comprise active interfaces (where chemical reactivity takes place), or that they involve disordered fragments. But even fully folded partners can present dynamic interfaces. Working on dynamic systems also requires the development of new analysis tools that go beyond classic structural metrics, such as RMSDs, and enable the comparison of complex conformational ensembles.
In this perspective the workshop was organized in six sessions addressing the following topics:
- Protein interfaces for biology
- Protein interfaces with nucleic acids
- Protein interfaces for health
- Experimental data for protein interfaces
- IA and integrative approaches in structural biology
- New methods and analysis tools.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

Apart from addressing the concerns of experts in molecular simulations, the scientific discussions also benefited from the contribution of experimentalist of various fields, since the availability of reliable experimental data is crucial for investigating the structure and activity of macromolecular assemblies at molecular level. Experimental data is also crucial for validating the models developed in the computational research groups, and integrative approaches that take into account data from various experimental techniques are important for improving the

sampling of large systems that might otherwise prove to be too costly from a computational point of view.
Several talks highlighted how quantitative information regarding the binding stability of biomolecular assembly remains difficult to obtain. In particular, when performing numerical simulations, accurate binding free energy calculations rely on the extensive sampling of the system, which can be hard to access for large biomomecular assemblies.
The talks also highlighted the importance of integrative approaches, for example including restraints derived from experimental data in numerical models, for rebuilding large biomolecular assemblies. New approaches including ML steps were also presented. Also one should keep in mind that, while providing precious help for the prediction of starting structure, artificial intelligence remains inefficient for many "unusual" cases that are not sufficiently documented on the PDB.

## 3. What was the take-home message for the participants?

The timing of the workshop, only one month after the 2024 Chemistry Nobel Prize attributed to the Alpha-Fold team for their work on protein structure prediction, appeared to be on spot, as dynamics now appears to be the new challenge to be overcome to properly understand how biomolecules function in the cell.
Liquid-liquid phase transitions and liquid droplets have increasingly raised interest over the last decade and now represent challenging systems for the biomolecular modeling community.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

While dealing mostly with a fundamental issue of structural biology, the workshop also included a session "Protein interfaces for health" specifically devoted to important questions for pharmaceutical research. As numerous pathologies are related to dysfunctional proteins, and in particular proteins that no longer interact properly with their cellular partners (be it other proteins, membranes of nucleic acids), it is fundamental to take into account the dynamics of these interactions.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The discussions highlighted the importance of open science initiatives (such as the MDDataBase), which help making software and raw data accessible. In particular, the need for publicly available, large datasets of MD trajectories was mentioned on several occasions.

Discussions also highlighted the need for more flexible coarse-grain models, which are currently under development within the MARTINI 3 framework, in order to investigate conformational changes in large systems.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

From the start of this project, the organizers were particularly vigilant regarding the gender balance in the workshop program, which resulted in 10 out of the 18 invited talks, and 4 out of the 7 contributed talks, to be given by female speakers. Women accounted for exactly 50% of the 42 registered participants.
Out of the 25 talks that were programed, 7 slots were for contributed talks from junior researchers (either 3rd year PhD students or postdocs). In additions, junior participants also had the opportunity to present their work on posters that were visible from Tuesday evening till Friday morning. Thus giving ample time for discussion, in particular during the lunch breaks on Wednesday and Thursday.

## 7. Participant list

### Organisers

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**David, Lucas** - Université Côte D'Azur, France
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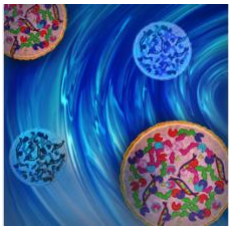


# Physics of mesoscale liquid condensates

**Location: Yangtze River Center in Liyang, China**
**Webpage : https://www.cecam.org/workshop-details/physics-of-mesoscale-liquid-condensates-1277**
**Dates: Nov 18, 2024 - Nov 21, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

We have identified three wide topics related to mesoscale liquid condensates:
1. Mesoscale separation in active soft materials. In particular, the effects of activity and the role of non-equilibrium effects on the growth and stabilization of mesoscale liquid structures constitute a must in order to understand how to control physicochemically multicomponent mixtures and what the essential differences between that control phase separation and arrest in equilibrium and non-equilibrium mixtures.
2. Physical mechanisms for controlling phase separation of biopolymers in non-biological conditions. In order to exploit the phenomenology of biological aggregates and arrested phase separation, we need to advance our understand the fundamental physical mechanisms of driven LLPS in multicomponent systems – combining biopolymers and chemical matter – that undergo phase separation under non-physiological conditions
3. Control and manipulation of phase-separating soft materials in complex environments. The understanding of the fundamental mechanisms and specificities associated to nonequilibrium in arrested phase separation of liquid mixtures must advance in parallel with our ability to control these systems, Soft materials composed by multicomponent mixtures are normally found or handled in complex environments. Therefore, we must advance in our analysis of the impact that nonequilibrium conditions and external driving forces have on liquid formation and manipulation of aggregates in complex environments, geometries and strong confinement.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

The major outcomes of the workshop were presentations of the state of the art in the field, which were of very high quality. The speakers also mostly followed the instructions very well and presented open questions and unpublished work.
1. consequently, the discussions were very active and in-depth.
2. The need for working with simple models - despite the complexity of the systems (or rather because of it) - has emerged as a common denominator in most of the discussions.
3. Several new collaborations emerged, which is a good sign for a discussion-oriented workshop
4. We achieved a good exchange between the soft matter communities in China and Europe. Several overseas participants visited various Chinese institutions after the workshop and started new collaborations...

## 3. What was the take-home message for the participants?

Liquid - liquid phase separation is a well-established mechanism for locally confining macromolecules and initiating / controlling their activity in life processes. However, it is equally interesting and important to exploit this principle in man-made systems, potentially achieving efficiencies closer to those in biology.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The topics of the workshop have in general a huge societal impact and any progress in fundamental understanding of molecular association and LLPS will have downstream effects on the key problems of society.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

One of the outcomes of the workshop is consolidation of a working group of researchers applying for Marie-Curie network funding (DN-MESOLIQ) on mesoscale condensates at non-biological conditions. The network, if eventually successful, will be an excellent medium to collaborate further on these topics, and to educate young researchers in the field.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

We tried hard to achieve a good gender balance. It turned out that for a workshop in China, it was very difficult to attract young female participants from overseas (i.e. Europe, with exception of two, it was practically impossible to attract participants from USA). Eventually, we had two female speakers that we really wanted in the workshop, presenting online (which was not very successful eventually, since the person-to-person contact turns out to be extremely important). We still had roughly 20% female speakers, which is more or less field - typical. We had a good mixture of younger and not so young speakers, and an excellent mixture of Chinese and European participants, which was one of the main objectives for a CECAM-CN workshop.

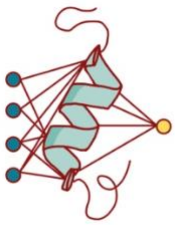
## 7. Participant list

### Organisers

**Dobnikar, Jure**
Institute of Physics, Chinese Academy of Sciences, China
**Mao, Man**
Institute of Physics, Chinese Academy of Sciences, China
**Pagonabarraga, Ignacio**
University of Barcelona, Spain

**Angioletti-Uberti, Stefano** - Imperial College London, United Kingdom
**Barducci, Alessandro** - Centre de Biologie Structurale, France
**Castañeda-Priego, Ramón** - University of Guanajuato, Mexico
**Cheng, Zhengdong** - Zhejiang University, China
**Collepardo, Rosana** - University of Cambridge, United Kingdom
**Curk, Tine** - Johns Hopkins University, United States
**Doi, Masao** - Wenzhou Institute University of Chinese Academy of Science, China
**Fan, Zhaochuan** - Suzhou Institute of Nano-Tech and Nano-Bionics, China
**Fan, Dian** - Southern University of Science and Technology, China
**Fan, Wenyue** - Institute of Physics. Chinese Academy of Sciences, China
**Farrell, James** - Institute of Physics, Chinese Academy of Sciences, China
**Gong, Wentao** - University of Barcelona, Spain
**Guzman, Horacio V** - Consejo Superior de Investigaciones Científicas, Spain
**Horbach, Juergen** - Heinrich Heine University Duesseldorf, Germany
**Jiang, Xiuyun** - SIMIT, China
**Komura, Shigeyuki** - University of Chinese Academy of Sciences, China
**Li, Tao** - Wenzhou Institute, China
**Liverpool, Tanniemola** - Unversity of Bristol, United Kingdom
**Luo, Chengjie** - Max Planck Institute for Dynamics and Self-Organization, Germany

**Ma, Xiaotian** - University of Edinburgh, United Kingdom
**Mognetti, Bortolo M Mognetti** - Université Libre de Bruxelles, Belgium
**Ni, Ran** - Nanyang Technological University, Singapore
**Oğuz, Erdal C.** - Institute of Physics, Chinese Academy of Sciences, China
**Podgornik, Rudolf** - University of Chinese Academy of Sciences, China
**Qi, Kai** - Shanghai Institute of Microsystem and Information Technology, China
**Qiang, Yicheng** - MPI for Dynamics and Self-Organization, Germany
**Saric, Andela** - Institute of Science and Technology Austria, Austria
**Shi, Xiaqing** - Soochow University, China
**Vacha, Robert** - Masaryk University, Czech Republic
**Wang, Xipeng** - Shandong Normal University, China
**Weber, Christoph** - MPI for the Physics of Complex Systems, Germany
**Xia, Xiuyang** - Ludwig-Maximilians-Universität München, Germany
**Xie, Zhaoping** - Johns Hopkins University, United States
**Xu, Limei** - Peking University, China
**Xu, Limei** - Peking University, China
**Yang, Mingcheng** - Chinese Academy of Sciences, China
**Yao, Hanrui** - University of Chinese Academy of Sciences, China
**Ye, Fangfu** - Institute of Physics, Chinese Academy of Sciences, China
**You, Zhihong** - Xiamen University, China
**Zhang, Xianren** - Beijing University of Chemical Technology, China
**Zhang, Zexin** - Soochow University, China
**Zhou, Jiajia** - South China University of Technology, China



# Generative models for classical and quantum matter

**Location: CECAM-HQ-EPFL, Switzerland & online**
**Webpage : https://www.cecam.org/workshop-details/generative-models-for-classical-and-quantum-matter-1274**
**Dates: Dec 2, 2024 - Dec 4, 2024**

## 1. What were the major topics discussed in the event, and how have they contributed to advancing the state of the art?

The workshop "Generative Models for Classical and Quantum Matter" gathered a diverse group of researchers at the forefront of machine learning and molecular science to discuss the rapid developments in generative modeling and their transformative potential for physical and chemical applications. Drawing inspiration from the successes of generative models in domains like text, image, and audio generation, participants explored how similar paradigms can be applied to systems governed by physical laws.

A central theme was the use of generative models to represent and explore molecular conformational landscapes. Several talks and discussions focused on the application of diffusion models to sample protein conformational ensembles, generate realistic molecular structures, and predict transitions across order parameters. This approach offers an alternative to traditional molecular dynamics simulations by learning the underlying distribution of configurations, providing potentially orders-of-magnitude improvements in efficiency.

The design of transferable generative models – capable of generalizing across chemical space and thermodynamic conditions – was another key topic. A key idea is to gather massive training data sets to enable highly versatile foundation models. Here strategies that build models respecting symmetries (e.g., rotational and permutational invariance) were critically compared to non-constrained approaches.

Another area of interest for building highly generalizing model was the integration of multimodal data sources.

More classical topics of machine learning applied to molecular systems were also discussed:

- machine learning force fields both on full-atom configurations and coarse-grained representations
- coarse-graining and back-mapping

The challenge of data scarcity – a common obstacle in these applications of machine learning for molecular science – was addressed through discussions of active learning. Approaches that iteratively select informative samples to maximize

model learning were presented as crucial for training effective models with limited data.
In sum, the workshop highlighted how generative modeling is not merely a tool for representation but a framework for simulation, design, and interpretation. The cross-pollination between disciplines fostered new perspectives on the limitations and opportunities of these methods, laying the groundwork for the next phase of development in computational molecular science.

## 2. What were the primary outcomes of this workshop, including limitations and open questions?

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The workshop yielded several important outcomes that reflect both the promise and the current limitations of generative modeling in molecular and materials science. One of the central outcomes was the identification of **__generalization beyond training datasets__** as a critical bottleneck for the field. While significant progress has been made in training generative models for specific systems, it remains an open question whether truly **__foundational models__** — trained once and deployed across a wide range of molecules, materials, and thermodynamic states — can be developed. The discussions emphasized that large, diverse datasets and symmetry-aware architectures are likely necessary (but not necessarily sufficient) for achieving this level of generalization.
Another central discussion point was the **__balance between targeting dynamics versus thermodynamics__**. While much of the existing work focuses on sampling thermodynamic distributions (e.g., equilibrium structures, free energies), several participants raised the question of whether generative models should also explicitly learn **time evolution** and dynamical pathways. Diffusion models and time-conditioned generative approaches offer promising tools for this, but their performance and reliability in capturing realistic physical kinetics remain active areas of research.
Finally, a recurring open question was **__how to rigorously evaluate__** generative models in this domain. Metrics such as likelihood or visual inspection are often insufficient; physical validation — e.g., reproducing experimental observables or obeying known constraints — is essential but not yet standardized. Establishing **__community benchmarks__** and shared datasets was proposed as a concrete step to help align efforts and foster reproducibility.

## 3. What was the take-home message for the participants?

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The key takeaway was that transferability is the next major challenge for generative models in molecular science — both across different molecular systems and varying thermodynamic conditions. Building models that generalize beyond narrowly defined datasets will be essential for moving from proof-of-concept applications to broadly useful tools.

## 4. Does the outcome(s) of the workshop hold potential for societal benefits?

The outcomes of the workshop hold significant potential for societal benefits. One of the most promising directions discussed was the **acceleration of molecular dynamics simulations**, particularly for biomolecules such as proteins. Generative models that can efficiently sample conformational ensembles or predict molecular transitions could dramatically reduce the computational cost and time required for such simulations. This has clear implications for **drug discovery and personalized medicine**, where understanding protein dynamics is essential for identifying binding sites, designing inhibitors, and predicting the effects of mutations.
Finally, improving the ****transferability and robustness**** of generative models – as emphasized during the workshop – will help bridge the gap between academic research and real-world applications. More reliable and general-purpose models can be integrated into industrial workflows, leading to ****safer, faster, and more cost-effective development of technologies**** in healthcare, materials science, and beyond.

## 5. Are there tangible outcomes of the workshop (e.g., publications, new collaborations, plans for proposal submission, software developments, etc.)?

The workshop fostered an extremely productive and insightful exchange among experts in the field, helping to clarify key challenges and opportunities in generative modeling for molecular science. While no direct tangible outcomes – such as publications, software releases, or formal collaborations – have emerged yet to our knowledge, the discussions laid a strong foundation for future joint efforts and research directions. Several participants expressed interest in follow-up initiatives, which may lead to concrete outcomes in the near future.

## 6. What measures did you take to promote inclusivity (gender, geographical provenance of participants and speakers, career stage, disabilities, etc.)?

The original speaker list included 8 women out of 22 invited speakers; despite 3 declining, we retained 5 female speakers. We prioritized diversity in career stage, with approximately one-third of invited speakers being pre-tenure or recently tenured. To support inclusivity, we featured 6 contributed talks and a poster session, encouraging interaction across all career stages. Speakers came from across Europe and the US; one invited speaker from China unfortunately declined to attend. The hybrid format further broadened accessibility.

## 7. Participant list

### Organisers

**Carleo, Giuseppe**
EPFL, Switzerland
**Gabrié, Marylou**
École Normale Supérieure, France
**Rotskoff, Grant**
Stanford University, United States

**Aghamolapour, Hossein** - Khatam University, Iran
**Albergo, Michael** - New York University, United States
**Aryal, Niraj** - Brookhaven National Laboratory, United States
**Bianciotto, Marc** - Sanofi, France
**Bishnoi, Bhupesh** - Centre National de La Recherche Scientifique, France
**Chapellier, Charlotte** - Ecole Nationale des Ponts et Chaussées, France
**Cheng, Bingqing** - UC Berkeley, United States
**Clementi, Cecilia** - Freie Universität Berlin, Germany
**Cossio, Pilar** - Flatiron Institute, United States
**Cournia, Zoe** - Biomedical Research Foundation, Greece
**Dawid, Anna** - Leiden University, Netherlands
**Dellago, Christoph** - University of Vienna, Austria
**Dinner, Aaron** - Chicago University, United States
**Ferguson, Andrew** - University of Chicago, United States
**Galliano, Leonardo** - ESPCI, France
**Garrahan, Juan P.** - University of Nottingham, United Kingdom
**Gastegger, Michael** - Microsoft Research AI for Science, Germany
**Ghamari, Danial** - ETHZ, Switzerland
**Ghio, Davide** - EPFL, Switzerland
**Gilardoni, Ivan** - SISSA, Italy
**Gomez-Bombarelli, Rafael** - MIT, United States
**Hütter, Michael** - Universität Innsbruck, Austria
**Ibarraran, Sebastian** - Stanford University, United States
**Inack, Estelle** - Perimeter Institute, Canada
**Jena, Nityasagar** - IFM, Linköping University, Sweden
**Kapil, Venkat** - University College London, United Kingdom
**Khaled, Mohammed** – H-BRS Germany
**König, Patricia** - Fritz-Haber-Institut of the Max Planck Society, Germany
**Koza, Adam** - University of Warsaw, Poland
**Langer, Marcel** - EPFL, Switzerland
**Liberati, Diego** - National Research Council of Italy, Italy
**Medvidović, Matija** - ETH Zürich, Switzerland
**Mendels, Dan** - Technion, Israel
**Metz, Friederike** - EPFL, Switzerland
**Michel, Manon** - CNRS, Université Clermont-Auvergne, France

**Mocanu, Felix-Cosmin** - University of Oxford, United Kingdom
**Mondal, Soumya** - IIT DELHI, India
**Morocho, Luis** - Yachay Tech University, Ecuador
**Nguyen, Nhan** - UChicago, United States
**Noe, Frank** - Free University of Berlin, Germany
**Olsson, Simon** - Chalmers University of Technology, Sweden
**Papoian, Garegin** - University of Maryland, United States
**Poletayev, Andrey** - University of Oxford, United Kingdom
**Ponkiya, Zarna D.** - The Maharaja Sayajirao University of Baroda, Vadodara, India
**Schebek, Maximilian** - Freie Universität Berlin, Germany
**Schönle, Christoph** - École Polytechnique, France
**Sobral, João Augusto** - University of Stuttgart, Germany
**Tangsongcharoen, Krit** - Chulalongkorn University, Thailand
**Tiwary, Pratyush** - University of Maryland, United States
**Varela Rosales, Nydia Roxana** - Tohoku University, Japan
**Viguera Diez, Juan** - Chalmers University of Technology/ AstraZeneca, Sweden
**Xie, Yu** - Microsoft Research, Germany
**Youssef, Ahmed** - Smava GmbH, Germany
**Zanders, Pieter** - Barcelona Supercomputing Center, Spain
**Zdeborova, Lenka** - EPFL, Switzerland

# MARY ANN MANSIGH CONVERSATION SERIES

The Mary Ann Mansigh Conversation series focuses of non-strictly technical topics of cultural interest for the simulation and modelling community. The format reflects the informative and informal nature of these sessions, with talks introducing the subject followed by a conversation between the speakers and the audience.

The lecture series "Mary Ann Mansigh Conversation series" is co-organized by CECAM (https://www.cecam.org) and MARVEL (http://nccr-marvel.ch/) at EPFL.

# Science writing and science editing - from journals to journalism

***Dates:*** **Apr 23, 2024**
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Science editors and writers play an essential role in the ecosystem of scientific information. Research journals rely on editors who assess manuscripts, shepherd them through peer review, prepare them for publication and create secondary content around them. Journalistic media rely on science writers who can recognize newsworthy scientific stories and bring them to their readers, while applying critical scrutiny to the work of scientists.
Learning how journal editors and science journalists work, and how to relate with them, is an important skill for young scientists. Journal editing, journalism and communication also represent potentially interesting career paths for anyone who has scientific training.
In this conversation, a senior editor for a major physics journal and a science journalist with a long experience in major outlets – respectively with a physics and chemistry research background - will describe how their job plays out, how an editorial team is organized in publications such as Nature, Nature Physics or Chemistry World, and how both science publishing and science journalism are being transformed by new technologies and market dynamics.

**The journal editor's perspective**
**Nina Meinzer, Nature Physics**

*Nina Meinzer is Senior Editor and Team Leader, Nature Physics. They obtained their PhD from the Karlsruhe Institute of Technology, where they studied plasmonic metamaterials and their interaction with semiconductor quantum heterostructures. They also carried out postdoctoral work at the University of Exeter, working on hybrid systems that combine plasmonic structures and emitters as well as studying microwave metamaterials. In 2016 they joined Nature Communication as Associate Editor, and in 2019 moved to Nature Physics as Senior Editor. They are editorially responsible for the full range of optical physics content the journal publishes, and also oversee the secondary content produced by all editors.*

**The science journalist's perspective**
**Mark Peplow, Journalist**

*Mark Peplow is a science journalist and editor with over 20 years of experience. He has a masters degree in chemistry from the University of Oxford, a PhD in organometallic chemistry from Imperial College London, and spent a year as a post-doctoral fellow at McMaster University, Canada, studying the chemistry of technetium radiotracers. He also holds an MSc in Science Communication from Imperial. He was the editor of Chemistry World magazine from 2006 to 2008, and then became chief news editor at Nature magazine, where he ran the global news team. He turned freelance in January 2013 and is now a regular contributor for Nature, Chemical & Engineering News and many other publications, writing on chemistry and materials, astrophysics and planetary sciences, Earth and environmental science.*


# CLASSICS IN MOLECULAR AND MATERIALS MODELLING

In this lecture series, we take a different look at fundamental developments of simulation and modelling. Milestone conceptual steps, methods and algorithms are presented by their originators. These technical lectures are followed by an interview in which the speakers recall for us the period, problems, people and circumstances that accompanied these developments, providing important and unusual insight in the birth and growth of tools that we now take for granted.

The lecture series “Classics in molecular and materials modelling” is co-organized at EPFL by CECAM (https://www.cecam.org/) and MARVEL (http://nccr-marvel.ch/).

# Methods for computational biology and drug discovery

***Dates:*** **Jun 5, 2024**
View full video

In this series, methods that have become fundamental tools in computational physics and chemistry are presented by their originators at a level appropriate for master and graduate students. The lectures are followed by an interview: we ask our guests to recall for us the period, problems, people and circumstances that accompanied the creation of milestone methods and algorithms that we now routinely use.
Join us to share this exciting opportunity to learn first-hand from our pioneers and get to know better the genesis of work that is now recorded in books!

**Evolution of Free-Energy Calculations from Butane to Drug Discovery**
**Bill Jorgensen, Yale University**

Free-energy calculations have had a revolutionary effect on computational chemistry. In conjunction with molecular dynamics and Monte Carlo simulations, they have enabled the calculation of free energy changes for wide-ranging phenomena including fundamental solution thermodynamics, solvent effects on equilibria, activation barriers for reactions in solution, host-guest binding, and drug lead optimization. An overview of our free energy efforts starting in 1981 with umbrella sampling for conformational equilibria, continuing to the FEP calculations in 1985 for the ethane to methanol mutation, and leading to recent discoveries of extraordinarily potent inhibitors of the main protease of SARS-CoV-2 will be presented.

*Since 1990* ***Bill Jorgensen*** *has been on the faculty at Yale, where he is the Sterling Professor of Chemistry. Bill's research has covered both computation and experiment. He has combined quantum, statistical, and molecular mechanics to model chemistry in solution. He has been a leader in computational studies of organic and enzymatic reactions in solution, molecular recognition, protein-ligand binding, and molecular properties. His OPLS force fields and TIPnP water models are widely used. Bill's research group has also pursued de novo drug design, synthesis, and protein crystallography, particularly for anti-infective, anti-proliferative, and anti-inflammatory agents. He pioneered the use of free-energy perturbation calculations for widespread applications including efficient drug lead optimization.*

*Among honors, Bill has received the ACS Award for Computers in Chemical and Pharmaceutical Research, the ACS Hildebrand Award, AAAS and ACS Fellowships, the ISQBP Award in Computational Biology, the Sato International Award from the Pharmaceutical Society of Japan, the Tetrahedron Prize, and the Arthur C. Cope Award. He has been elected to membership in the International Academy of Quantum Molecular Science, American Academy of Arts & Sciences, and US National Academy of Sciences. He was the Editor of the ACS Journal of Chemical Information and Modeling during 2004-2013 and the Journal of Chemical Theory and Computation from its founding in 2005 through 2021.*

**Modeling Protein-protein interactions: then and now**
**Shoshana Wodak, Flemish Free University of Brussels**

I'll describe the birth of protein-ligand and protein-protein docking methods developed in 1974-1978 and their application to the elucidation of the quaternary structure change in hemoglobin ten years later. This will be followed by an overview of the progress achieved in modeling protein-protein interactions during the last 5 decades. This overview will highlight the important role of community-wide blind prediction experiments in nurturing the field. It will discuss the recent breakthrough in the accurate prediction of single protein chains driven by deep learning methods, illustrating the advances this enables for the prediction of protein-protein interactions, and outlining important remaining challenges.

***Shoshana J. Wodak**, earned her PhD at Columbia University, New York, under the supervision of Cyrus Levinthal, who was developing what were then the first and most powerful computational and graphics tools for modelling proteins and protein interactions. Importing and implementing many of these tools to Belgium and France in the late seventies (with crucial support from CECAM (Centre Européen de Calcul Atomique et Moléculaire) in Paris and EMBO), she developed, in collaboration with Joel Janin, the first docking algorithms for the prediction of protein-protein interactions and one of the first procedures for defining structural domains from the atomic coordinates of proteins. With her team at the Free University of Brussels she then used molecular simulations and bioinformatics approaches to investigate the role of local interactions in stabilizing the native state of proteins, protein structure prediction, protein folding, and fold recognition. Together with her teams at the Free University of Brussels, the European Bioinformatics Institute in Hinxton, UK, and at the Hospital for Sick Children in Toronto, she developed efficient procedures for computational protein design, for simulating protein interactions and conformational changes, and for analyzing protein interactions networks and cellular pathways.*

*Between 1986-1993, Dr. Wodak was the Scientific Director of the protein engineering team at Plant Genetic Systems, Belgium (now part of Bayer CropScience). Among their success stories was the engineering of more thermostable versions of the xylose (glucose) isomerase enzyme, changing its metal specificity, and pH profile.*
*Dr. Wodak founded and co-directed the Centre for Structural Biology and Bioinformatics and headed a Master's program in Bioinformatics. She has been a member of the European Molecular Biology Organization (EMBO) since 1990. She held a Tier 1 Canada Research Chair in Computational Biology and Bioinformatics from 2005-2012 and was elected an ISCB fellow in 2016. She is a member of F1000 since 2017.*
*Dr. Wodak has been a member of numerous expert panels and Advisory Committees in Europe (ERC, Horizon 2020), US (DOE) and Canada (CIHR), and is on the Editorial Boards of several journals her field.*
*Since 2001, Dr. Wodak serves on the Management Committee of CAPRI (Critical Assessment of Predicted Interactions), a community-wide international initiative for fostering the development of methods and algorithms for the prediction of protein interactions and complexes, and has been coordinating this effort, since 2013.*
*Dr. Wodak is currently a Visiting Group Leader at the VIB-VUB Structural Biology research Centre, at the Flemish Free University of Brussels, Belgium. She is a member of the Executive Committee of the Elixir 3DBioInfo Community and serves on the Scientific Advisory Board of Cyclica Inc. in Toronto Canada.*


# CECAM WEBINARS

Webinars are a new adventure for CECAM. We hope that you will enjoy experimenting with us on the possibilities offered by this tool to share exciting science with the community.

This format offers an interesting opportunity to facilitate access to our activities for a broader community.

While our love of the informal and productive environment of face-to-face meetings is unchanged, we plan to explore its potential as a complementary tool to our workshops and schools, being an alternative format to the CECAM Flagship program.

# Lhumos training portal

***Dates:*** **Jan 15, 2024**
View full video

The novel e-learning platform Lhumos enters the material sciences realm to ease knowledge sharing and capacity building within the material sciences community and beyond.

As the demand for coding skills rises in the technology industry, it is imperative to increase code usage and training on different methods in HPC environments.

Supported by **MaX, CECAM, MARVEL, MultiXscale,** and **DOME4.0**, Lhumos (Learning HUb for MOdeling and Simulation) is a novel educational platform developed to facilitate the upskilling of students, scientists, and industrial users in HPC applications in the material sciences domain.

Targeted at early-career and more advanced scientists, the e-learning platform gathers videos, lectures, codes, tutorials, seminars, and exercises that cover a wide range of subjects including electronic structure calculations, molecular dynamics, high performance computing, and code optimization.


# TREX - CECAM WEBINAR: Quantum Monte Carlo HPC applications in condensed matter, quantum chemistry and materials science

***Dates:*** **Jan 25, 2024**
View full video

Join us for a deep dive into the cutting edge of quantum materials research and quantum chemistry at the upcoming webinar on "Quantum Monte Carlo HPC Applications in Condensed Matter, Quantum Chemistry, and Materials Science" on January 25, 2024, from 09:30 to 12:00 CET. The webinar is a collaborative effort between the Targeting Real Chemical Accuracy at the EXascale (TREX) project and CECAM (Centre Européen de Calcul Atomique et Moléculaire).

The webinar will be exploring the frontiers of quantum materials research and quantum chemistry, by means of Quantum Monte Carlo (QMC) calculations, owing to their unique suitability in solving complex many-body problems as well as in harnessing the parallelism offered by upcoming exascale supercomputer architectures.
The agenda covers a spectrum of key topics, including magnetism, surface physics, layered materials, energy excitations, and high-pressure hydrogen. Participants will gain a deeper insight into high-performance computing applications via quantum Monte Carlo simulations.

# MDDB webinar series: “MDDB project and MDPosit: a prototype of distributed MD database”

***Dates:*** **May 17, 2024**
View full video

**Modesto Orozco & Daniel Beltrán**

The Molecular Dynamics Data Bank (MDDB) project is an European-scale repository for biosimulation data, which harnesses decades of cutting-edge computational resources to build a unified database that compiles and organises all data generated by molecular dynamics (MD) simulations.

MDDB is a collaborative initiative, bringing together some of Europe’s leading institutions to transform the handling of MD data and facilitate its sharing within the scientific community. The partners involved in this exciting project are IRB Barcelona, Barcelona Supercomputing Center, their joint spin-off Nostrum Biodiscovery, along with the Royal Institute of Technology (KTH), the European Molecular Biology Laboratory, the University of Oxford, and CECAM (EPFL).

If you would like to learn more about MDDB, please visit the project’s website.

With this series of webinars, MDDB aims to engage the MD community and discuss the importance of data sharing, the methodological and technological issues involved, and present how they are addressing these challenges, with examples taken from recent projects such as the Covid19-related MD simulations database.

During this first webinar, Modesto Orozco and Daniel Beltrán from IRB Barcelona will introduce the MDDB project and discuss their ongoing efforts to establish a distributed MD database, an approach where different research groups have their own local data repositories while contributing to a global database.

# MultiXscale - CECAM webinar: supporting the development of multiscale methods via the European environment for scientific software installations (EESSI)

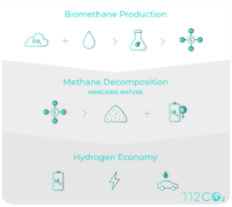
***Dates:*** **Oct 17, 2024**
View full video

This webinar provides an introduction to EESSI and demonstrates how it supports the development of the key MultiXscale application codes – **LAMMPS, waLBerla,** and **ESPResSo**. Discover how EESSI accelerates scientific software installations and development, enabling cutting-edge research in multiscale modeling across various scientific domains. Perfect for researchers, developers, and engineers looking to enhance their software efficiency. This webinar is a joint effort between the CoE MultiXscale EuroHPC and CECAM.

The goal of the MultiXscale EuroHPC Centre-of-Excellence is to enable the simulation of hydrodynamics at different length scales, from atomistic to continuum models, on large scale HPC resources like those provided by EuroHPC systems. It will do this via 3 scientific showcases:

- Supercapacitor systems for battery applications
- Biomedical applications of ultrasound
- Simulation of turbulent flows for rotor aeroelastic analyses

The webinar will explore how the European Environment for Scientific Software Installations (EESSI) can accelerate scientific software installations and support multiscale research. This session will provide an introduction to EESSI, followed by in-depth discussions on how the powerful multiscale simulation codes – LAMMPS, waLBerla, and ESPResSo – are being developed via the EESSI framework.




# 112CO2 - CECAM Webinar: simulation assisted steps in research and technology in the hydrogen ecosystem

***Dates:*** **Oct 17, 2024**
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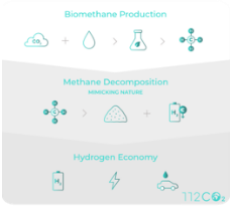
112CO2 is an EU H2020 Future and Emerging Technologies (FET) project (H2020-EIC-FETPROACT-2019 GA no. 952219), renamed into Pathfinder within Horizon Europe and now part of the portfolio of the recently established European Innovation Council (EIC) funding schemes. FET (and Pathfinder) are projects starting from TRL 1-2 and finishing at TRL 3-4; they are meant to explore the applicative potential of fundamental research ideas. Concerning 112CO2, the objective is to promote the methane splitting process into COx-free hydrogen and graphitic carbon with high added-value. 112CO2 project aims at developing a low temperature methane splitting Ni-based catalyst, easy to regenerate and very active, and stable for at least 10 000 h. Why methane splitting technology to obtain cost-competitive hydrogen? This is to ease the clean energy transition at the core of EU objectives: methane is an abundant fossil fuel that is easier to transport and to distribute than hydrogen (using the existent natural gas infrastructure networks); if biomethane is used, negative CO2 footprint hydrogen is produced. Moreover, methane can be produced by several renewable sources (e.g., solar energy), and valorizing byproducts of other industries (e.g., bioCO2 contained in biogas). The vision is that one can transport biomethane locally, to some suitably large geographical area for which it is economically relevant to split it into hydrogen for the decentralized applications.

The methane splitting reaction at low-temperatures, bringing to different byproducts (e.g., carbon nanotubes, graphenic sheets, amorphous carbon, etc), and the problem of catalyst deactivation/regeneration are difficult, if not impossible, to investigate experimentally, or without a suitable combination of simulations and experiments. Thus, simulations are key in this context and, more in general, in the study of industrially-relevant chemical processes. We identified several challenges: i) techniques for rare events to study chemical reactions, ii) computing accurate interatomic interaction at an affordable computational cost, iii) the modeling of processes in electronic excited states, for, e.g., photo-assisted reactions. This is what we want to discuss in this webinar. The webinar is addressed to non-specialists in the field of simulations, thus it is key to identify the main issues and explain, with a language accessible to experimentalist and engineers, challenges that have been already addressed and those that are still open.




# 112CO2 - CECAM Webinar: methane splitting in Europe: how to promote swift and low-cost energy decarbonization?

***Dates:*** **Oct 24, 2024**
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Methane splitting is an emergent technology in the quest for the production of clean and cost-competitive hydrogen and solid carbon products. In this second webinar organized within the scope of EU project 112CO2 (H2020-EIC-FETPROACT-2019 GA no. 952219), different European initiatives, political and the academic and industrial sectors, will be discussed.

Our goal is to foster a conversation with the research community, policymakers and relevant stakeholders, in particular in the experimental and engineering communities participating in the 112CO2 project and other EU-funded projects.