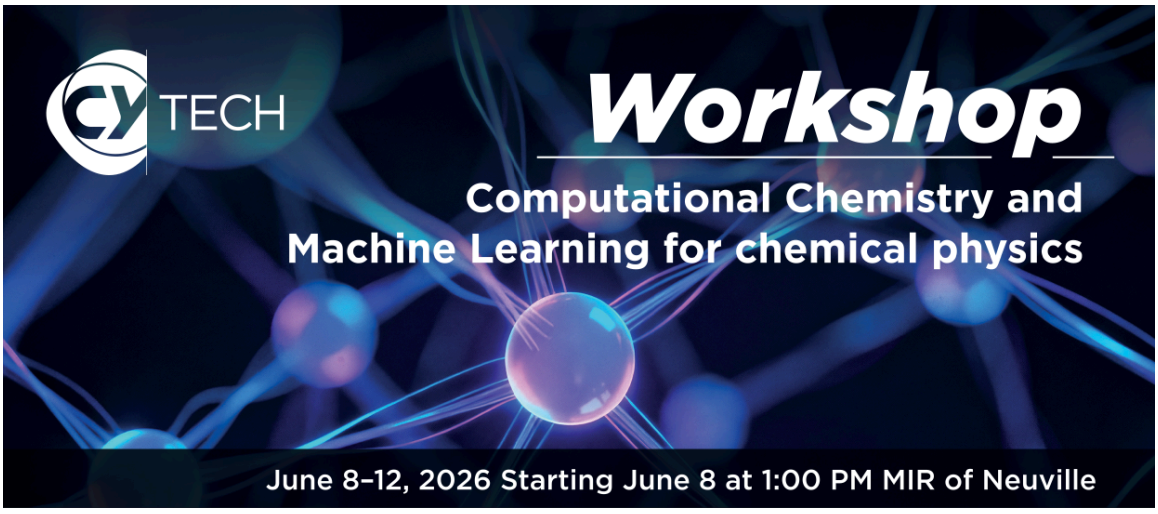
CY ADVANCED STUDIES

WORKSHOP HANDBOOK



Welcome Message

Dear Colleagues,

On behalf of the organising committee, it is our great pleasure to welcome you to the Workshop on Computational Chemistry and Machine Learning for Chemical Physics, held at CY Cergy Paris Université from 8–12 June 2026.

Recent advances in computational chemistry, chemical physics, and artificial intelligence are rapidly transforming our ability to understand, predict, and design complex molecular and material systems. From quantum-chemical simulations and reaction dynamics to machine-learning-assisted discovery and data-driven modelling, these developments are creating unprecedented opportunities for scientific innovation across disciplines.

This workshop has been organised to bring together researchers, educators, and students from diverse scientific backgrounds to explore the emerging synergies between computational methods and machine learning approaches. Through invited lectures, scientific discussions, and hands-on practical sessions, participants will have the opportunity to exchange ideas, share recent developments, and discuss future challenges and opportunities in the field.

The scientific program features speakers from leading research institutions, covering topics that span electronic structure theory, molecular dynamics, spectroscopy, reaction mechanisms, astrochemistry, materials science, and artificial intelligence for scientific discovery. The practical sessions aim to give participants hands-on experience with modern computational and machine learning tools that are becoming central to current research.

Beyond the scientific content, we hope this workshop will foster new collaborations, strengthen existing partnerships, and encourage interactions among researchers at different career stages and across disciplines. We believe that such exchanges are essential for addressing the complex scientific challenges of the future.

We would like to express our sincere gratitude to all invited speakers, participants, and sponsors for making this workshop possible. We wish you a stimulating, productive, and enjoyable workshop, and we look forward to the scientific discussions and collaborations that will emerge during this week.

The Organising Committee.

CY Cergy Paris Université

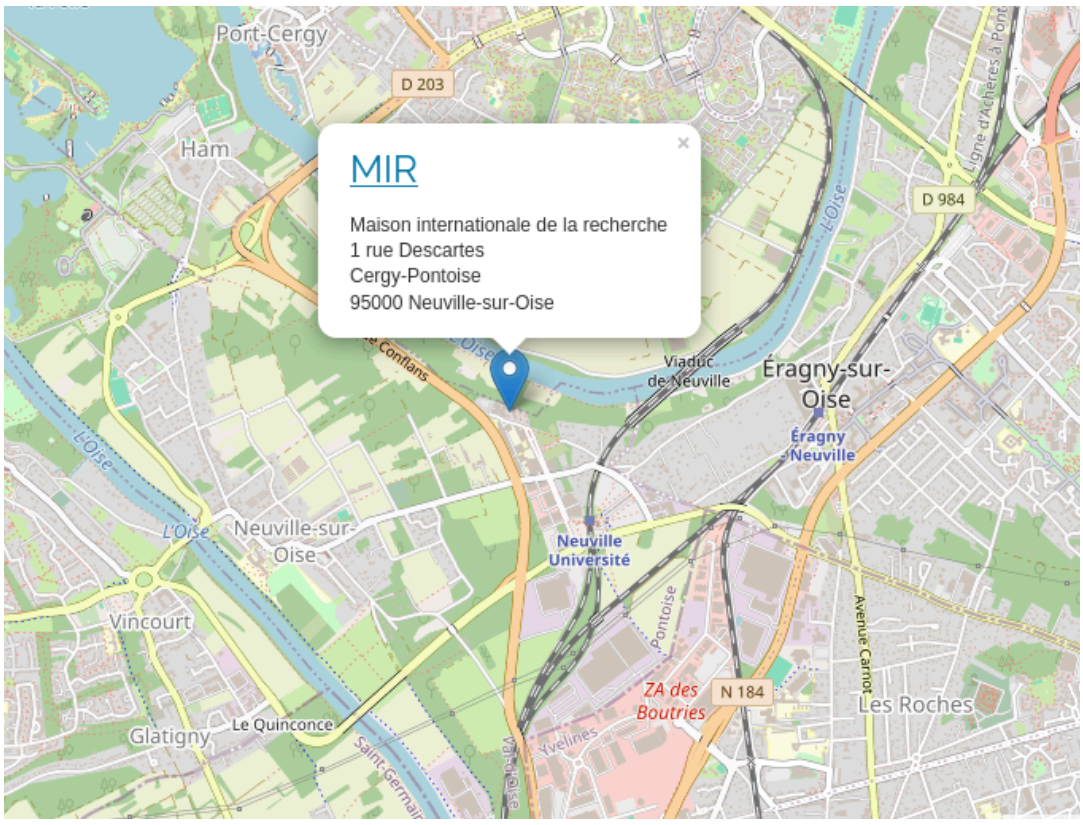
Access Details

1 Rue Descartes
95000 Neuville-Sur-Oise, France

Closest train station: Neuville–Université (served by **RERA** and **Transilien Line L**).

If you are arriving from Paris, exit the train and take the stairs up to the station concourse. Leave the station via the **left-hand exit**, then turn **right** onto **Mail Gay-Lussac**. Continue straight for approximately **400 m**. The road curves slightly to the left and becomes **Rue Descartes**. Walk a further **100 m**; the **MIR Building** will be on your right.

Enter through the main entrance. The conference room (**Auditorium**) is located immediately to your **left** upon entering the building.



Scientific Organising Committee

François Dulieu
Florian Gallier
Dimitrios Kotzinos
Michel Lorin
Sébastien Peralta
Guy Trambly de Laissardière
Llinersy Uranga Pina
W. M. C. Sameera

Invited Talks

Gunnar Nyman (University of Gothenburg, Sweden)
Rita Prosmiti (Institute of Fundamental Physics (IFF-CSIC), Madrid, Spain)
Alejandro Rivero (University of Lille, France)
Majdi Hochlaf (Gustave Eiffel University, France)
Marie-Pierre Gaigeot (Université Evry Val d'Essone, France)
Duncan Bossion (University of Rennes, France)
Bogdan Iorga (PSL University, Paris, France)
Liuba Mazzanti (PSL University, Paris, France)

Contributed Talks

Clarke Esmerian (Chalmers University of Technology, Sweden)
Maikel Ballester (Universidade Federal de Juiz de Fora, Brazil)
Salah-Eddine (CY Cergy Paris Université, France)
Aliezer Martinez (University of Havana, Cuba)
Hema Malani (Kyoto University, Japan)
Dimitris Kotzinos (CY Cergy Paris Université, France)
Michel Lorin (CY Cergy Paris Université, France)
François Dulieu (CY Cergy Paris Université, France)
W. M. C. Sameera (CY Cergy Paris Université, France)
Himasha Gunathilaka (University of Colombo, Sri Lanka)
Nishshanka M. Lakshan (The Ohio State University, Columbus, Ohio, USA)

Acknowledgements

Programme

Invited Talks: 45 minutes (including 5–10 minutes for questions and discussion)

Contributed Talks: 30 minutes (including 5–10 minutes for questions and discussion)

Speakers are kindly requested to keep their presentations within the allocated time to ensure a smooth running of the programme.

Monday, June 8th 2026

13h30 Registration and welcome

13h45 Opening Remarks (W. M. C. Sameera, CY Cergy Paris Université)

Session 1 (Chair: Llinersy Uranga Pina, CY Cergy Paris Université)

14h00 **Invited Talk:** Rita Prosmiti (Institute of Fundamental Physics (IFF-CSIC), Madrid, Spain)
Data-Driven Computational Modeling of Ion Microsolvation

14h45 Clarke Esmerian (Chalmers University of Technology, Sweden)
Modelling Interstellar Dust Atom-by-Atom

15h15 Maikel Ballester (Universidade Federal de Juiz de Fora, Brazil)
On the third body effect in OH + SO collisions: a case study

15h45 Coffee Break

Session 2 (Chair: Llinersy Uranga Pina, CY Cergy Paris Université)

16h15 **Invited Talk:** Alejandro Rivero (University of Lille, France)
Theoretical Approaches to Gas–Surface Interactions: Combining AIMD with ML-Based Potential Energy Surfaces

17h00 Salah-Eddine (CY Cergy Paris Université, France)

17h30 Lab visit

18h00 End of the day

Tuesday, June 9th 2026

Session 3 (Chair: François Dulieu, CY Cergy Paris Université)

9h00 **Invited Talk:** Majdi Hochlaf (Gustave Eiffel University, France)
Structural and spectroscopic characterization of medium-sized molecules: from the isolated state to the adsorbed state, then in mixture

9h45 Aliezer Martinez (University of Havana, Cuba)
Non-adiabatic molecular dynamics simulations of spectroscopic properties and exciton dynamics in organic conjugated polymers

10h15 Hema Malani (Kyoto University, Japan)
The Mechanism of p-TsOH/H_2O_2 Catalyzed Wood Biomass Conversion: A Computational Investigation

10h45 Coffee Break

Session 4 (Chair: François Dulieu, CY Cergy Paris Université)

11h15 **Invited Talk:** Marie-Pierre Gaigeot (Université Evry Val d'Essone, France)
Topological Graphs, Machine-Learned Potentials, and Generative AI for Spectroscopy: Learning Complex Matter Across Representations

12h00 Dimitris Kotzinos (CY Cergy Paris Université, France)
Explainable Recommender Systems

12h30 Lunch

Session 5 (Chair: Emanuele Congiu, CY Cergy Paris Université)

14h00 **Invited Talk:** Duncan Bossion (University of Rennes, France)
Machine learning for astrochemistry: The multi-layer perceptron, presentation and applications

14h45 Michel Lorin (CY Cergy Paris Université, France)
The C(^{3}P3) + CH2(^{3}B1) reaction: accurate electronic structure calculations and kinetics for astrochemical modeling

15h15 François Dulieu (CY Cergy Paris Université, France)

15h45 Coffee Break

Session 6 (Chair: Saoud Baouche, CY Cergy Paris Université, France)

16h15 **Invited Talk:** Gunnar Nyman (University of Gothenburg, Sweden)
Quantum mechanical tunneling in astrochemistry

17h00 W. M. C. Sameera (CY Cergy Paris Université, France)
Beyond Radical Chemistry: The Emerging Role of Anions in Interstellar Ices

17h30 End of the day

Wednesday, June 10th 2026

Session 7 (Chair: W. M. C. Sameera, CY Cergy Paris Université, France)

9h00 **Invited Talk:** Bogdan Iorga (PSL University, Paris, France)
Computational strategies for investigating antibiotic resistance mechanisms

9h45 Himasha Gunathilaka (University of Colombo, Sri Lanka)
Targeting a Signaling-Deficient TNFα State: Molecular Dynamics Insights from Bambusa vulgaris Phytochemicals

10h15 Nishshanka M. Lakshan (The Ohio State University, Columbus, Ohio, USA)
Electronic Structure and Reactivity of Biomimetic Transition-Metal Clusters for Nitrogen Fixation

10h45 Coffee Break

Session 8 (Chair: W. M. C. Sameera, CY Cergy Paris Université, France)

11h15 **Invited Talk:** Liuba Mazzanti (PSL University, Paris, France)

12h00 Round-Table Discussion (Chair: François Dulieu, CY Cergy Paris Université, France)

12h30 Closing Remarks (François Dulieu, CY Cergy Paris Université, France)

Hands-on Practical Session I

Thursday, 11 June 2026

Practical Session: Computational Chemistry

The ORCA 6.1 electronic structure program will be used during the practical sessions. All participants must download and install ORCA 6.1 on their personal computers before the tutorials begin. For detailed installation instructions, please visit:
https://www.faccts.de/docs/orca/6.1/tutorials/first_steps/install.html

Additionally, please install Avogadro (https://two.avogadro.cc/install/index.html), which will be used as the graphical interface for building and visualising molecular structures.

Participants should ensure that both software applications are installed and ready to run calculations.

Schedule

9.00 - 9.20: Introduction to computational chemistry

9.20 - 09.40: Introduction to ORCA6.1 program

ORCA 6.1 Manual: https://www.faccts.de/docs/orca/6.1/manual/

ORCA 6.1 Tutorials: https://www.faccts.de/docs/orca/6.1/tutorials/

9.40 - 10.00: preparation for tutorials

10.00 - 10.15: Coffee break

10.15 – 11.00: Geometry optimisation, Vibrational frequencies

Geometry optimisation:
https://www.faccts.de/docs/orca/6.1/tutorials/prop/geoopt.html

Vibrational frequencies: https://www.faccts.de/docs/orca/6.1/tutorials/prop/freq.html

11.00 – 12.00: Finding Transition States

https://www.faccts.de/docs/orca/6.1/tutorials/react/nebts.html

12.00 – 13.00: Lunch

13.00 – 15.00: Thermodynamics

https://www.faccts.de/docs/orca/6.1/tutorials/prop/thermo.html

15.00 - 15.15: Coffee break

15.15 - 16.00: Kinetic Isotope Effects
https://www.faccts.de/docs/orca/6.1/tutorials/react/KIE.html

16.00 - 17.00: Multiscale models
https://www.faccts.de/docs/orca/6.1/tutorials/multi/basics.html

Hands-on Practical Session II

Friday, 12 June 2026

Applied AI for Chemical-Physics: From Lab to Code
Platform: Google Colaboratory (Python 3)

Overview

This tutorial is designed for experimentalists and theoreticians working on chemical / physics or related research areas. We will use **Google Colaboratory**, allowing us to run high-performance code and Neural Networks in the browser with zero local installation. We will focus on turning raw experimental data / artifitial data into predictive insights.

We will provide **pre-programmed Jupyter notebooks** to facilitate our hands-on tutorial. Although the session is designed to be **accessible without a programming background**, a foundational understanding is certainly an asset. We will guide you through interactng with the code to adjust variables and analyze outcomes.

Kindly note that the program may undergo slight adjustments leading up to the event.

Workshop Project Roadmap

Module 1 (Introduction): Target: Basic concepts of Machine Learning.

Module 2 (Denoising): Target: Spectral signals. *Tools:* SciPy Signal.

Module 3 (Mapping: Extraction of Main Features): Target: Spectra, Images. *Tools:* Scikitlearn PCA.

Module 4 (Morphometry): Target: Microscopy. *Tools:* Segment Anything (SAM).

Module 5 (Computer Vision): Target: Failure Detection / Main Features Detection in images. *Tools:* PyTorch CNNs.

Module 6 (Collaborative Group Projects): Target: Related Projects of General Interest (depending on the audience).

Module 1: Introduction to Machine Learning (09:00 – 10:15)

Tools: *Scikit-learn, NumPy, Matplotlib*

Supervised Learning: Understanding how models map inputs (*X*, like concentration) to outputs (*y*, like conductivity). We distinguish between **Regression** (continuous values) and **Classification** (discrete categories).

Unsupervised Learning: Discovering hidden structures in unlabeled data. Essential for exploratory research where you don't know the "answer" yet.

The ML Workflow: Learning the rigor of splitting data into *Training* and *Testing* sets to ensure our model generalizes to new experiments.

Loss Functions: A mathematical "ruler" (like Mean Squared Error) that tells the AI how far off its prediction is, guiding the optimization process.

Module 2: Data Foundations, Preprocessing & Denoising (10:30 – 12:00)

Tools: *Pandas, SciPy, Matplotlib*

Objective: Automate the transition from raw, noisy instrument output to "Publication-Ready" data.

Experimental Source: Cyclic Voltammetry (CV), TGA, high-frequency rheology, spectra.

Data Cleaning: Techniques to handle "human" errors in spreadsheets, such as missing values or inconsistent units, using Pandas dataframes.

Signal Denoising: Applying *Savitzky-Golay* filters to smooth noisy spectra (FTIR/Raman) or electrochemical signals while preserving peak intensity and position.

Hands-on Baseline Correction: Automating the removal of background drift in Cyclic Voltammetry (CV) or XRD patterns to isolate the true physical signal.

Module 3: Dimensionality Reduction for Spectroscopy (12:00 – 13:00)

Tools: *Scikit-learn (PCA, t-SNE)*

Objective: Visualize relationships between hundreds of chemical samples in a single 2D map.

Experimental Source: SEM/TEM micrographs, Optical microscopy, AFM height maps, spectra, etc.

PCA Concepts: Execute **Principal Component Analysis (PCA)** to identify the wavelengths (or another marker) responsible for 90% of variance, allowing for 2D visualization.

Eigenvectors & Variation: Understanding which specific wavelengths (or marker) contribute most to the differences between your samples.

Hands-on Clustering: Using *K-Means* to automatically group samples with similar (chemical or physical) signatures, identifying sub-phases or degradation states or synthesis success, etc.

Module 4: General Image Processing & Morphometry (14:00 – 15:15)

Tools: *OpenCV, Scikit-Image, Segment Anything (SAM)*

Objective: Quantify physical structures (pores, fibers, grains) without manual tracing.

Experimental Source: SEM/TEM micrographs, Optical microscopy, or AFM height maps, etc.

Beyond Simple Thresholding: Moving past “black and white” filters to AI-driven segmentation that can handle shadows and low-contrast micrographs (SEM/TEM).

Automated Feature Extraction: Using Python to count particles, measure grain surface areas, and calculate porosity distributions across hundreds of images in seconds.

Hands-on Morphometry: Extracting the “Aspect Ratio” and “Sphericity” of particles to correlate physical shape with macroscopic material performance.

Module 5: Convolutional Neural Networks (CNNs) (15:30 – 17:00)

Tools: *PyTorch or TensorFlow/Keras*

Objective: Moving beyond peak-fitting by training a Deep Learning model to “read” raw experimental waveforms / microscopy images.

The 1D Convolution: Understanding how a sliding “filter” (kernel) identifies local patterns in a spectrum, such as shoulders, asymmetric broadening, or specific oscillation frequencies.

Translation Invariance: Why CNNs are superior to standard regression for signals: they can recognize a chemical signature even if the peak shifts slightly due to calibration drift or temperature.

Hierarchical Learning: How the first layers detect “edges” (slopes) and deeper layers detect “motifs” (complex peak patterns or redox signatures).

Hands-on Categorizing: Categorize unknown samples into distinct physical states (e.g., *Cross-linked* vs. *Non-cross-linked* or *Degraded* vs. *Pristine*).

Module 6: Collaborative Group Projects (17:00 – 18:00)

The following are just examples of potential collaborative projects, but in practice, projects will be adapted to specific interests of participants.

High-Dimensional Data Mining

Focus: FTIR, UV-Vis-NIR, and Hyperspectral Imaging. Handling thousands of variables per sample.

Project 1: The Spectral Fingerprint

Goal: Extracting meaningful chemical trends from raw ”Big Data” spectra.

Techniques: FTIR/UV-Vis with Integrating Spheres.

AI Strategy: Dimensionality Reduction (PCA) and Manifold Learning (t-SNE).

Hands-on: Visualizing the ”Chemical Space” of a 100-sample aging study. Identifying outliers and ”hidden” degradation phases that aren’t visible in individual plots.

Project 2: Automated Surface & Image Analysis

Goal: Turning micrographs into quantitative physical tensors.

Techniques: SEM, Optical Microscopy, and Profilometry.

AI Strategy: Computer Vision (Zero-Shot Segmentation with SAM).

Hands-on: Automated quantification of surface roughness and pore-size distributions in IPN membranes. Transitioning from ”qualitative photos” to ”statistical data.”

Modeling Functional Signals

Focus: EIS, TGA, and Mechanical Testing. Modeling curves where ”shape” carries the physics.

Project 3: Smart Fitting of Complex Impedance

Goal: Replacing manual equivalent circuit ”guessing” with AI-driven parameter extraction.

Techniques: Electrochemical Impedance Spectroscopy (EIS).

AI Strategy: Functional Data Analysis and Genetic Algorithms for Optimization.

Hands-on: Using an AI agent to automatically fit Nyquist plots and extract charge-transfer resistance (R_{ct}) across a temperature series.

Project 4: 1D-CNNs for Signal Recognition

Goal: Training ”Expert Systems” to recognize physical states from raw waveforms.

Techniques: TGA/FTIR Coupling, Tensile Tests, and CV.

AI Strategy: 1D Convolutional Neural Networks (1D-CNN).

Hands-on: Training a model to ”read” a TGA-FTIR trace and instantly identify the chemical family of the evolved gas based on the 1D waveform shape.

Abstracts

Rita Prosmiti (Institute of Fundamental Physics (IFF-CSIC), Madrid, Spain)
Data-driven computational modeling of ion microsolvation

Abstract:

Computer simulations based on machine-learned potential energy surfaces (ML-PESs) are powerful tools for investigating the structure, energetics, spectroscopy, and dynamics of molecular systems, from finite aggregates to bulk environments. Here, we present computational studies of ion solvation in two media of very different nature: quantum helium and polar water nanoclusters.1-4

In He-solvated light cations, ML-PESs trained on high-level CCSD(T)/CBS electronic-structure data accurately describe the delicate balance between ion–He and He–He interactions. When combined with diffusion Monte Carlo (DMC), path-integral molecular dynamics (PIMD), Feynman–Hibbs, and classical molecular dynamics simulations, these models provide detailed insight into cluster growth mechanisms, magic numbers, and the role of nuclear quantum effects in determining the stability and structural evolution of charged He nanodroplets.1-2

In ion–water clusters, transferable bottom-up data-driven PESs capture the complex many-body hydrogen-bond network governing ion hydration. These models enable a realistic description of temperature-dependent structural rearrangements, the preference for surface-solvated halide anions, and the evolution from finite clusters toward bulk solvation energetics.3-4

Together, these studies demonstrate that, by bridging accurate electronic-structure calculations with advanced quantum simulations, ML-PESs provide a key framework for understanding microsolvation processes and quantum effects in both helium and aqueous environments.

References:

1. Yanes-Rodríguez, R.; Villarreal, P.; Prosmiti, R. *Phys. Chem. Chem. Phys.* 2025, 27, 8259.

2. Sarsa, A.; Montes de Oca-Estévez, M.J.; Villarreal, P.; Hernández-Rojas, J.; Prosmiti, R. *Phys. Chem. Chem. Phys.* 2026, 28, 5369.

3. Rodríguez-Segundo, R.; Arismendi-Arrieta, D. J.; Prosmiti, R. *Molecules*, 2022, 27, 1654.

4. Rodríguez-Segundo, R.; Gijón-Gijón, A.; Prosmiti, R. *Phys. Chem. Chem. Phys.* 2022, 24, 14964.

Clarke Esmerian (Chalmers University of Technology, Sweden)
Modelling Interstellar Dust Atom-by-Atom

Abstract:

Interstellar dust is a fundamentally important component of the ISM and cosmic galaxy population, both observationally and dynamically. Yet many basic questions about the origin, evolution, and properties of this dust remain unanswered, in large part because of the complexities of dust physics. I will present work I have been leading to advance our understanding of cosmic grain microphysics using the methods of modern computational chemistry, specifically by conducting a large program of molecular dynamics simulations of individual dust grains in which every atom is accounted for. This has enabled updated calculations of fundamental grain quantities and processes such as binding energies1, grain collision outcomes2, and gas-phase accretion rates3. Some of these results significantly change our understanding of grain microphysics, and I will discuss their implications for the properties and evolution of dust grain populations in the ISM. I will also look ahead to how we can use these updated first-principles calculations to more realistically model interstellar dust throughout the universe and across cosmic time.

References:

1. Hansson, K.; Sameera, W. M. C.; Esmerian, C. J.; et al. *Astronomy & Astrophysics*, 2026, 707, A54.

2. Esmerian, C. J.; Hashemi S. R.; Sameera, W. M. C.; et al. arXiv:2605.22225

3. Esmerian, C. J.; Bossion, D.; Dulieu, F.; et al. in prep.

Maikel Ballester (Universidade Federal de Juiz de Fora, Brazil)
On the third body effect in OH + SO collisions: a case study

Abstract:

The reaction between sulfur monoxide and the hydroxyl radical has been the subject of several studies due to its relevance in atmospheric, combustion, and astrochemical events [1, 2, 3]. The collision evolves through the formation of an HOSO structure with a well depth of more than 70 kcal mol−1 [4]. In this talk, the possibility of stabilizing this complex in the presence of a third body is explored. For such a task, a global potential energy surface (PES) for Ar − HSO2 was developed using a previously PES for HSO2 (2 A) [4] and Ar − X diatomic interactions. Subsequently, the quasi- classical trajectory method is employed in dynamic calculations. The formation of HOSO now appears as a competing output channel to the H + SO2 production.

Acknowledgments: CNPq, PPGF-UFJF, UFJF, FAPEMIG.

References

1. A. Fuente et al. In: *Astronomy & astrophysics* 624 (Apr. 2019). ISSN: 1432-0746. DOI:10.1051/0004-6361/201834654.

2. J. M. Colom-Diaz et al. In: *Proceedings of the combustion institute* 37.1 (2019), pp. 727–734. ISSN: 1540-7489. DOI: 10.1016/j.proci.2018.05.005.

3. Juan de Dios Garrido et al. In: *Molecular physics* 118.17 (Sept. 2020). ISSN: 0026- 8976.DOI : 10.1080/00268976.2020.1751321.

4. MY Ballester et al. In: *Physical Chemistry Chemical Physics* 7.11 (2005), pp. 2305– 2317. ISSN : 1463-9076. DOI : 10.1039/b500990a.

Alejandro Rivero (University of Lille, France)

Theoretical Approaches to Gas–Surface Interactions: Combining AIMD with ML-Based Potential Energy Surface

Abstract:

Gas–surface interactions are central to many phenomena in atmospheric and astrophysical environments. Here, we illustrate how the combination of Ab Initio Molecular Dynamics (AIMD) with Machine Learning Interatomic Potentials (MLIPs) advances our understanding of these processes. Two representative situations are analyzed: the oxidation of NO on oxygen-functionalized graphite, and the photodesorption of CO from molecular ices.

For NO on epoxy-functionalized highly oriented pyrolytic graphite (O–HOPG), we will present results from our recent AIMD study1 published in J. Phys. Chem. C together with new developments included in a work currently in preparation. AIMD trajectories identified accessible reaction channels and the role of surface oxygen groups. A dedicated MLIP was then constructed to describe the breaking and formation of chemical bonds. This framework enabled extended simulations that revealed the microscopic mechanisms driving NO_2 production and emphasized the cata-lytic function of oxygenated sites at the surface.

In the case of CO photodesorption, we will build on results from our earlier contribution in Phys. Rev. Lett.2 and from a recent study published in *J. Chem. Phys*.3. AIMD provided reference data for the relaxation of CO vibrationally excited molecules in CO ices environment. These results served to build a deep-learning PES capable of representing the vibrational relaxation of an excited CO molecule within a condensed CO environment across a wide range of excitation levels. The resulting model not only reproduces experimental CO desorption yields, but also uncovers how vibrational energy is redistributed into translational and rotational motions.

References:

1. Alou Angulo et al. *J. Phys. Chem. C.* 2024, 128, 42, 17894–17904.

2. Del Fré et al. *Phys. Rev. Lett.* 2023, 131, 238001.

3. Infuso et al. *J. Chem. Phys.* 2025, 163, 084303.

Majdi Hochlaf (Gustave Eiffel University, France)

Structural and spectroscopic characterization of medium-sized molecules: from the isolated state to the adsorbed state, then in mixture

Abstract:

I will present a comparative study, using first principles methodologies, of the structures and vibrational spectroscopic characteristics of medium sized molecules isolated, interacting with metallic surfaces, or in mixture. As applications, I will treat the conformers of biofuels precursors. First, I will consider furfural-acetone-furfural (FAF) i either isolated or adsorbed on a Ru(0001) metal surface ii. The choice of FAF is motivated by the ease of its synthesis via the aldol condensation of furfural with acetone, followed by hydrogenation and hydrodeoxygenation, producing high-value C_8–C_{13} hydrocarbons, iii,iv which are components of diesel fuels v. Our work shows that FAF conformers undergo significant energetic and structural deformations upon adsorption compared to their structures in the gas phase. Various topological descriptors are used for explanation. Second, I will treat the case of a-carotenes, another biofuel precursors, for which a large conformational landscape exists. vi We use artificial intelligence based-tools to reduce such large number of conformers to clusters. The reduced number of representatives is then investigated using advanced DFT to compute RAMAN spectra useful to their identification in mixtures. Our strategy is viewed to be cost effective and can be generalized to other medium-sized compounds of organic, inorganic and energy relevance.

We would like to thank the COST Action CA21101 “COSY – Confined Molecular Systems: From a New Generation of Materials to Stars.”

References:

1. Benmoussa et al., *J. Comput. Chem.* 2026, 47, e70297.

2. Kamalakannan et al. (2026). To be submitted.

3. Parejas et al. *Catalysts*, 2019, 9, 203.

4. Faba et al. *Catal. Today*, 2016, 269, 132.

5. Lange et al. *Angew. Chem., Int. Ed.* 2010, 49, 4479–4483.

6. de Boer et al. (2026). Submitted

Aliezer Martinez (University of Havana, Cuba)

Non-adiabatic molecular dynamics simulations of spectroscopic properties and exciton dynamics in organic conjugated polymers

Abstract:

Emulating the efficient light-harvesting and subsequent electronic energy transfer of natural photosynthetic systems through multi-chromophoric ensembles has attracted growing interest for next-generation applications in organic photovoltaics, light-emitting diodes, catalysis, and optoelectronics. Despite rapid progress in synthesis and experimental characterization, establishing precise structure-property-dynamics relationships within these architectures remains a significant challenge. This is primarily due to the complex cascade of coupled electronic and vibrational phenomena, including nonadiabatic internal conversion, transient exciton self-trapping, and vibrational energy redistribution. Furthermore, directly validating theoretical models against experimental observables requires robust computational techniques capable of simulating real-time spectroscopic signals within large molecular frameworks.

To address these challenges, we perform on-the-fly nonadiabatic molecular dynamics simulations via the NEXMD software package. This computational framework is applied across a diverse set of systems: perylene-based donor-acceptor antennas1, branched pyrene-cored dendrimers2, size-varied carbon nanocages3, and paraphenylene-derived rings and chains4,5.

Herein, we summarize recent simulation results that elucidate branch-to-core funneling and transient absorption pump-probe spectra in light-harvesting architectures; tunable photoinduced dynamics in carbon nanorings and alkyl-tethered para-phenylene chains; and exciton self- trapping alongside size-dependent spectral shifts in carbon nanocages. These results highlight the capability of on-the-fly nonadiabatic molecular dynamics and simulated transient spectroscopy in decoding sub-picosecond photophysical phenomena and establishing precise structure-property-dynamics relationships across varied dimensions. Ultimately, these findings offer predictive guidelines for tailoring spectroscopic properties and exciton migration to optimize solar energy conversion and molecular optoelectronic applications.

References:

1. Perez-Castillo, R.; et al. *Chem. Sci.*, 2025, 16, 13520.

2. Perez-Castillo, R.; et al. *Chem. Sci.*, 2024, 15, 13250.

3. Rodriguez-Hernandez, B.; et al. *J. Phys. Chem. Lett.*, 2021, 12, 224.

4. Rodriguez-Hernandez, B.; et al. *Phys. Chem. Chem. Phys.*, 2020, 22, 15321.

5. Rodriguez-Hernandez, B.; et al. *J. Phys. Chem. C*, 2018, 122, 16639.

Hema Malani (Kyoto University, Japan)

The Mechanism of p-TsOH/H_2O_2 Catalyzed Wood Biomass Conversion: A Computational Investigation

Abstract:

The efficient utilization of lignocellulosic biomass is essential for the development of sustainable biorefineries and renewable chemical production1. Among emerging biomass fractionation technologies, acid hydrotropes such as p-toluene sulfonic acid (p-TsOH) based systems have attracted considerable attention due to their effectiveness in lignin removal under mild conditions1. Recent experimental studies conducted in the Nakamura Lab have demonstrated that the addition of hydrogen peroxide (H_2O_2) significantly enhances delignification performance, leading to improved biomass conversion. Despite these promising results, the molecular mechanisms responsible for the enhanced reactivity of the p-TsOH/H_2O_2 catalytic system remain largely unexplored.

In this work, density functional theory (DFT) calculations were employed to investigate the fundamental reaction pathways involved in p-TsOH/H_2O_2-mediated lignin conversion using lignin G-G dimer model. In particular, attention was devoted to exploring β-O-4 linkage cleavage and aromatic ring opening. Our results indicate that p-TsOH can react with H_2O_2 to generate a reactive peroxy acid species through a kinetically accessible pathway. The resulting oxidant promotes the transformation of lignin model compounds through energetically favorable oxidation processes. The calculations reveal efficient cleavage of β-O-4 linkages and activation of aromatic lignin units for subsequent ring-opening reactions, facilitating the lignin to break down into small compounds.

References:

1. Singhvi, M.; Kim, B. S. *Energies*, 2020, 13, 5300.

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Duncan Bossion (University of Rennes, France)

Machine learning for astrochemistry: The multi-layer perceptron, presentation and applications

Abstract:

Machine learning algorithms and in particular artificial neural networks are widely used tools in all fields of science. In this talk I will present one type of artificial neural network (ANN), the multi-layer perceptron (MLP), that is a common neural network used in supervised learning. After a general description of MLP and how they are trained, I will focus on two applications of machine learning to predict data of interest in astrochemistry.

The modeling of astrophysical media requires an accurate knowledge of the microphysical data of the environment. In particular, the rate constant of reaction is necessary to estimate the abundance of molecules and interpret observed spectra. The first application of MLP concerns the prediction of rate constants of reactions occuring in gas phase astrophysical environments.[1] The second application focuses on the sticking of gas phase atoms and molecules onto dust grains. This sticking process has a strong influence on dust growth, and on the depletion of particules of the gas phase. An ANN is used to predict the sticking coefficients of the incoming atoms for a wide range of temperatures.[2]

The ability to obtain in a fast and efficient manner large amount of data to complete astrophysical database using in particular ANN will have a strong impact on the astrophysical modeling. This in turn will improve the interpretation of observations and will lead to a better knowledge of the chemistry of various astrophysical environments.

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Michel Lorin (CY Cergy Paris Université, France)

The $C(^3P) + CH2(^3B1)$ reaction: accurate electronic structure calculations and kinetics for astrochemical modeling

Abstract:

In this work, we present a theoretical study of the C + CH2 - H + CCH reaction, which is expected to play a key role in the formation of carbon-chain species in molecular clouds. We employ high-level ab initio electronic structure methods, including the HEAT-345Q composite scheme and multi-reference configuration interaction, to characterize the potential energy surface. Reaction kinetics are investigated through both conventional transition state theory for tight transition states and variational reaction coordinate transition state theory (VRC- TST) for barrierless pathways. The master equation technique is used to account for competing complex formation, isomerization, and dissociation processes, particularly under collisionless conditions relevant to astrochemistry. Rate constants for product formation are calculated over a wide temperature range (10–300 K), and fitted to extended Arrhenius expressions. The results reveal that both singlet and triplet pathways contribute significantly to the overall reaction rate, with the triplet surface dominating under typical ISM conditions.

Gunnar Nyman (University of Gothenburg, Sweden)
Quantum mechanical tunneling in astrochemistry

Abstract:

I will discuss some aspects of quantum mechanical tunneling, particularly in an astrochemical setting with a focus on hydrogen atom diffusion on water ice. Simple theoretical calculations[2, 3, 5] will be used to illustrate and illuminate experimentally[1,4] observed tunneling. Methods used will involve transition state theory with quantum considerations, some analytic expression for tunneling estimates and molecular beam experiments. Kinetic isotope effects will be discussed and time permitting it will also be discussed in the context of tunneling associated with radiative association where resonances due to tunneling can be very prevalent[6]. We find that kinetic isotope effects can be very large as an effect of tunneling.

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W. M. C. Sameera (CY Cergy Paris Université, France)

Beyond Radical Chemistry: The Emerging Role of Anions in Interstellar Ices

Abstract:

The chemistry of the interstellar medium (ISM) is traditionally described by radical-driven reaction networks, whereas the role of anions in interstellar ice chemistry remains largely unexplored.[1] Recent experimental and theoretical studies suggest that hydroxide anions (OH^-) can form on interstellar ices and migrate through hydrogen-bonded networks via proton-hole transfer, thereby encountering and reacting with molecules trapped within the ice mantle.[2] Quantum chemical methods are essential for investigating such processes because atomic-scale reaction mechanisms and quantum effects cannot be determined directly from experiments.

Ab initio computations, employing density functional theory and an unbiased search for reaction mechanisms,[3,4] reveal that the reactivity of OH^- is highly molecule-dependent. The reaction between CO_2 and OH^- has an activation barrier and becomes effective at interstellar temperatures (~10 K) mainly via quantum tunnelling, resulting in the formation of HCO_3^-. In contrast, the analogous CO_2 + OH radical reaction is effectively inactive under the same conditions. Not all OH^- reactions need quantum tunnelling to occur: the OH^- + SO_2 reaction is barrierless, while analogous reactions with CS_2 and OCS have significant barriers and are less reactive.[6] These results show that anion-driven chemistry offers new pathways for molecular evolution in interstellar ices and should be incorporated alongside conventional radical chemistry in astrochemical models.

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Himasha Gunathilaka (University of Colombo, Sri Lanka)

Targeting a Signaling-Deficient TNFα State: Molecular Dynamics Insights from Bambusa vulgaris Phytochemicals

Abstract:

Severe dengue is frequently associated with a cytokine storm characterized by excessive production of pro-inflammatory cytokines, leading to vascular leakage. Tumor necrosis factor alpha (TNFα) is a key mediator of this pathological inflammatory response and has therefore emerged as an attractive therapeutic target. The symmetric trimeric conformation of TNFα is signaling-competent and binds three TNF receptor 1 molecules, whereas the asymmetric trimeric conformation exhibits attenuated inflammatory signaling. Stabilization of this signaling-deficient state represent a novel strategy for controlling cytokine storm in severe dengue. Although juvenile shoots of Bambusa vulgaris have traditionally been used in dengue management their potential to stabilize the signaling-deficient conformation of TNFα remains unexplored. To investigate this possibility, phytochemicals reported from juvenile shoots of Bambusa vulgaris were screened against the asymmetric TNFα structure (PDB ID: 6OP0) using molecular docking. TNFα inhibitor SAR441566 was used as the positive control. Sterols emerged as the most promising class of phytochemicals, with ergosterol exhibiting the strongest binding affinity (-11.9 kcal mol^{-1}), while β-sitosterol, stigmasterol, campesterol, and stigmastanol displayed docking scores of -12.4 kcal mol^{-1}. To evaluate the stability of these interactions, 1000 ns molecular dynamics simulations were performed in triplicate for the apo protein and the ligand- TNFα complexes. The simulations demonstrated that all sterols remained stably bound within the asymmetric TNFα binding pocket throughout simulations and exhibited greater structural stability. These findings highlight the potential of molecular dynamics simulations to identify ligands that modulate protein conformational landscapes and stabilize signaling-deficient TNFα states.

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Nishshanka M. Lakshan (The Ohio State University, Columbus, Ohio)

Electronic Structure and Reactivity of Biomimetic Transition-Metal Clusters for Nitrogen Fixation

Abstract:

Transition-metal clusters are known for their ability to activate and transform otherwise inert small molecules under relatively mild conditions. Among these transformations, the reduction of dinitrogen (N_2) has attracted particular interest because of its central role in biological nitrogen fixation. As a result, significant efforts have been directed towards elucidating biomimetic nitrogen-reduction mechanisms that enable the conversion of N_2 into valuable chemical products, such as tris(trimethylsilyl)amine.[1-2] However, the electronic structures of these systems are often complex, and many key bonding interactions and reaction intermediates are difficult to characterise experimentally.

To address these questions, density functional theory (DFT) calculations were performed on several Fe-, Co-, Ni-, and Mo-containing transition-metal clusters. The calculations were used to examine their electronic structures, bonding properties, and reactivity. Particular attention was given to identifying ground-state electronic configurations, clarifying the nature of chemical bonding, and investigating the underlying reaction mechanisms.[1-3]

These studies provide molecular-level insight into the relationship between electronic structure and catalytic activity. These findings provide molecular-level insight into nitrogen fixation by biomimetic transition-metal clusters and guide the design of next-generation catalysts capable of activating small molecules under mild conditions.[1-3]

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Liuba Mazzanti (PSL University, France)

Modeling biomolecules and their complexes in silico: from single structures to ensembles

Abstract:

Highly dynamic and flexible systems departing from the “one sequence, one structure, one function” paradigm for protein folding play an essential role in biological processes. On the one hand, such systems, including intrinsically disordered proteins, protein-protein interactions, and RNAs, represent a challenge for biophysical modeling. On the other hand, they are a class of largely underexplored yet promising biological targets. As novel targets are needed to develop new therapeutical strategies that overcome the limitations of existing therapies, deciphering the conformational ensembles, dynamics, and mechanisms, of these systems is a key issue in health sciences. This talk will illustrate a variety of applications ranging from RNA structural modeling and peptide translocation across lipid membranes to disordered protein-protein interactions and protein-RNA interactions, where methods including coarse-graining, integration of experimental data, AI-based models, have been specifically employed and combined.

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