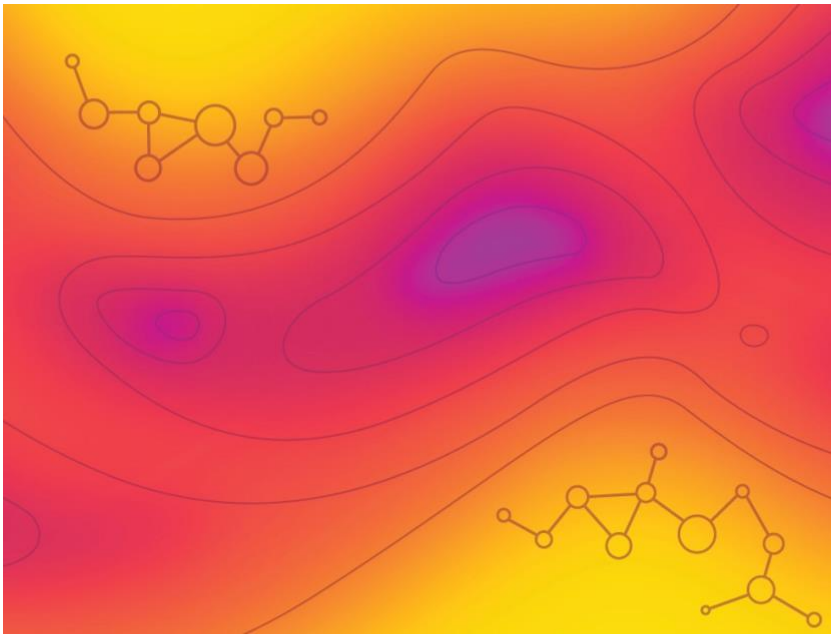
Advancing simulation, analysis and prediction of complex chemical systems using modern chemical graph theory and computational topology



July 16 - July 18, 2025
CECAM-HQ-EPFL, Lausanne, Switzerland

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1. Description

The simulation of complex chemical, materials and biophysical systems is increasingly reliant upon the transfer of information across length and timescales to both accelerate simulation time as well as interpret collective phenomena that derive from many body interactions beyond the scale of electrons. Ultimately, it is desirable to extend many-body theories beyond traditional domains of electronic structure theory and into complex condensed matter systems, where propagating system states in time must be able to self-consistently account for many-body effects (described by different granularities of information).This presents a unique grand challenge for the computational chemistry community and will require interdisciplinary collaboration with the mathematics and computer science communities – where multidimensional data analysis inspired by machine learning and AI is rapidly advancing the mathematical languages associated with the shape of data, specifically the mathematical languages of graph theory and computational topology.

The focus of this CECAM workshop will be to bring together computational chemists, materials scientists and biophysicists with leaders in the mathematics of graphs and computational topology. The workshop will educate these communities, foster collaboration and inspire development of both applied and fundamental computational methods in chemistry. We will focus upon each scale of information relevant to computational chemistry (from electrons to the mesoscale) and identify opportunities where graph theory and topology can help in method development and information transfer to accelerate interdisciplinary innovation.

For example, at the smallest scale of electrons, continued development is needed for reduced-complexity electronic structure methods (e.g., through effective Hamiltonians). There, fundamental questions remain about how to achieve the best parametrization, what optimization methods to employ, how electronic data is represented, and perhaps most importantly – how to maintain physical transparency through step-by-step coarse-graining that may use nonphysics neural network structures to represent the data from electronic structure calculations. As chemical complexity grows via molecular degrees of freedom, chemical composition, or diversity of intermolecular interactions, the breadth of configuration ensembles can increase significantly - reflecting an increasingly rugged underlying potential energy landscape. Thus, there is need to characterize and predict spatial heterogeneities, collective dynamics and the relation to energy landscape topology. This is important not only in sampling, but also for predictive models that seek to understand the relationships between physicochemical properties and the configurational phase space. Fundamentally, such chemical insight can be greatly accelerated through mathematical notions of distance (e.g., distances to compare the precise graph combinatorial structure). This may include summaries of the spectral structures of graph representations of the molecular system in combination with the energy landscape - such as the spectra of the graph Laplace operator or the diffusion operator associated with input graphs. Recent advancements in topological data analysis also provide new ways to compare graph representation of high-dimensional data via persistent homology, that have the potential to be adapted for chemical systems.

Through an organizational structure that combines use-case scenarios, grand-challenge talks and methodological and software tutorials (alongside poster presentations and roundtable discussions), this CECAM workshop will set the stage for increased collaboration between the applied math and computational sciences.

Key References

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2. Program

Day 1 - Wednesday July 16th 2025

- 09:00 to 09:45 - Registration

Understanding Dynamic Systems Using Graphs and Topology

- 09:45 to 10:00 - Welcome & Introduction
- 10:00 to 10:45 - **Michele Ceriotti**
  Bringing insights from machine-learning potentials into collective variables
- 10:45 to 11:15 - **Ingrid Hotz**
  Topological descriptors for analysis and visualization of electronic structures
- 11:15 to 11:45 - **Mercedes Alfonso-Prieto**
  Quantum Mechanics/Molecular Mechanics simulations of proton transfer in biological systems
- 11:45 to 12:15 - Lightning Talks for Poster Sessions
- 12:15 to 12:45 - Discussion
- 12:45 to 14:00 - Lunch
- 14:00 to 15:25 - Poster session & aperitif

Energy Landscapes and Sampling Enabled by Graphs and Computational Topology

- 15:25 to 15:30 - Welcome & Introduction
- 15:30 to 16:15 - **David Wales**
  Energy landscapes: exploration and analysis
- 16:15 to 16:45 - **Henry Adams**
  Representations of energy landscapes by sublevelset persistent homology
- 16:45 to 17:15 - **Jessica Swanson**
  From dynamics to reactive flux: responsive kinetic network analysis of biomolecular mechanisms
- 17:15 to 17:45 - **Amber Mace**
  Computing transport properties in solid-state materials from the topology of potential energy surfaces
- 17:45 to 18:15 - Discussion

Day 2 - Thursday July 17th 2025

- 08:00 to 08:55 - Registration

Topology and Shape in Chemical Systems

- 08:55 to 09:00 - Welcome & Introduction

- 09:00 to 09:45 - **Herbert Edelsbrunner**
  Discrete geometry, topology, and algorithms for particle systems

- 09:45 to 10:15 - **Noel Jakse**
  Dynamic heterogeneities in undercooled metallic alloys: an unsupervised topological learning approach

- 10:15 to 10:45 - **Jun-Ho Choi**
  Graph theory and molecular aggregation and phase behavior in aqueous solutions

- 10:45 to 11:15 – **Minh Le**
  Homology of transient convection cycles over multiplex network flows

- 11:15 to 11:45 - Coffee break

- 11:45 to 12:15 - **Reidun Twarock**
  Protein nanoparticles under the mathematical microscope: from viral tiling theory to interaction networks

- 12:15 to 12:45 - **Senja Barthel**
  Studying crystalline materials through their underlying nets

- 12:45 to 13:15 – Discussion

- 13:15 to 14:15 - Lunch

Graph Theory and Computational Topology Software

- 14:15 to 15:30 - **Julien Tierny**
  An introduction to the Topology ToolKit with applications to quantum chemistry

- 15:30 to 16:45 - **Sana Bougueroua & Aurora Clark**
  Software overview for graph theory in chemistry

- 16:45 to 18:15 - Poster session on software and algorithms

- 19:30 to 21:30 – Social dinner

Day 3 - Friday July 18th 2025

- 08:00 to 08:55 - Registration

Graph Structure and Pattern Identification in Chemistry

- 08:55 to 09:00 - Welcome & Introduction
- 09:00 to 09:45 - **Lee Cronin**
  Exploring chemical complexity with assembly theory and chemputation
- 09:45 to 10:15 - **Ernesto Estrada**
  The Euclidean geometry of the Huckel molecular orbital method
- 10:15 to 10:45 - **Julien Lam**
  Challenges in tracking crystal features in complex materials
- 10:45 to 11:15 - **Rawan Abouhaidar**
  Graph-theoretical analysis of interfacial hydrogen-bond networks induced by short-chain alcohols
- 11:15 to 11:45 - Coffee break
- 11:45 to 12:15 - **Ariel Francis Perez Mellor**
  Graph-theoretical approach unravels unimolecular dissociation and ion–molecule complex pathways of gas-phase protonated molecules
- 12:15 to 12:45 - **Victor Batista**
  Tackling subgraph isomorphism with multilayer Gaussian Boson Sampling
- 12:45 to 13:15 – Discussion
- 13:15 to 14:15 – Lunch
- 14:15 to 15:15 – Preparation for Perspective Article

3. Abstracts

An introduction to the topology toolkit with applications to quantum chemistry

Julien Tierny
CNRS - Sorbonne University, France

This talk gives a global overview of the Topology ToolKit (TTK), an open-source library for topological data analysis and visualization. After introducing the main concepts behind TTK's usage, I will demo how to use it with simple examples in ParaView and Python. Then, I will present TTK's capabilities, going from simple critical point extraction to more advanced features (persistence diagrams, Reeb graphs, Morse-Smale complexes, distances and barycenters of persistence diagrams, etc) as well as TTK's current capabilities for processing point cloud data. In the process, I will provide links to numerous online resources containing further tutorials, documentations, examples and exercises. Finally, I will present an application of TTK for a robust QTAIM-based analysis in molecular dynamics.

Bringing insights from machine-learning potentials into collective variables

Michele Ceriotti
EPFL, Switzerland

The problem of finding collective variables to describe a complex molecular rearrangement shares many similarities with that of finding the most concise, effective representation of a structure to machine-learn its properties. This suggests that the conceptual and software infrastructure that has been developed to build surrogate models of the interatomic potential, and other atomic-scale properties, could be used to identify motifs that can be used to define collective variables and accelerate phase-space sampling. In this talk I will give an overview of the theory and practice of representations used for symmetry-adapted and unconstrained ML models and present a modular software infrastructure that can be used to build, rationalize, and visualize order parameters to be used to accelerate sampling, and study rare events in molecular dynamics.

Challenges in tracking crystal features in complex materials

Julien Lam
CNRS, France

To accurately identify local structures in atomic-scale simulations of complex materials is crucial for the study of numerous physical phenomena including dynamic plasticity, crystal nucleation and glass formation. In this talk, we will begin by presenting the Steinhardt Gaussian Mixture Analysis which a supervised learning approach combining Steinhardt's bond orientational order parameters in with a classical Gaussian mixture model. Then, we will present few examples where the method was successfully employed including nanoparticle melting, defect identification and crystal nucleation.

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Computing transport properties in solid-state materials from the topology of potential energy surfaces

Amber Mace[1], Hannes Gustafsson[1], Fabian Schwarz[1], Senja Barthel[2]
[1]Uppsala University, Sweden
[2]Vrije Universiteit, Amsterdam, Netherlands

The structure and dynamics of a material are essentially determined by the complex combination of potential energy landscapes experienced by the individual atoms in the system. In turn, valuable information on the properties of the material is encoded in the shapes of the potential energy landscape. For example, configurations of particles within a solid are determined by the shapes and presence of energetic basins, and the self-diffusion of mobile particles is defined by the geometry of how these energetic basins are connected to form paths.

Understanding diffusion processes in solids at the atomistic scale is crucial for many important applications such as predicting Li-ion conduction through a solid-state battery cell or membranes for separation processes including carbon capture and water purification. While modeling can facilitate such understanding, there are still many challenges to overcome in terms of reaching relevant length and time scales that capture the complexity of the material.

I will present my work on the development of a multiscale modeling approach to predict and understand (self-)diffusion of ions and other small molecules within a crystalline framework. This approach is based on constructing and analyzing the topology and geometry of the potential energy landscape and constructs a statistical model by computing the hopping rates between energy minima using transition state theory and kinetic Monte Carlo. I will discuss the role of different entropic contributions and how they can be included to provide the effective free energy experienced by the mobile particle. I will further discuss how we are working to extend this approach towards non-periodic material systems, such as solid polymer electrolytes as well as composite materials consisting of multiple phases.

*[1] F. Schwarz, S. Barthel, A. Mace, Chem. Mater., **36**, 11359-11376 (2024)*
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Discrete geometry, topology, and algorithms for particle systems

Herbert Edelsbrunner
IST Austria, Austria

Starting with the modeling of bio-molecules as unions of balls (solid spheres), we discuss a sequence of discrete data structures that analyze and manipulate particle systems and make relevant measures readily accessible. These data structures include dual alpha complexes defined as sublevel sets of the radius function on Delaunay mosaics, persistence modules and diagrams of Euclidean distance functions, six-packs of diagrams to distinguish between types of particles, and shadow monomials to quantify translational symmetry. We touch upon combinatorial and stochastic properties as well as supporting algorithms of these data structures.

Dynamic heterogeneities in undercooled metallic alloys: an unsupervised topological learning approach

Noel Jakse
Université Grenoble Alpes, France

Understanding evolutions of transport properties in undercooled liquids and their interplay with their structural features represents an important issue for solidification processes of metallic alloys, such as crystallization and formation of quasi-crystalline or amorphous phases [1–4]. In the present work, we focus on various classes of Aluminum alloys such as Al-Ni [5], Al-Cu [6], Al-Cr [7] and Al-Zn-Cr [8] that we investigated using ab initio molecular dynamics. We simulate the undercooling process of these alloys during which we monitor the structural and atomic transport properties. We find that diffusion, viscosity and structural relaxation time undergo a crossover between an Arrhenius and non-Arrhenius behavior at a temperature TX during the slowing down, which corresponds to an onset of developing dynamic heterogeneities (DHs). The structural features display characteristics compatible with the occurrence of the icosahedral short-range order (ISRO) as well as the development of a medium range order (MRO) upon cooling. The interplay between the ISRO and MRO in relation the dynamic heterogeneities is examined through large-scale molecular dynamics of homogeneous nucleation using an unsupervised topological learning [9,10].

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Energy landscapes: exploration and analysis

David Wales
Cambridge University, United Kingdom

The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science [1-10]. This talk will summarize recent developments for global optimization, quantum dynamics, enhanced sampling of thermodynamic properties, and rare event dynamics.
Representing the landscape in terms of a kinetic transition network produces a graph representation, where the nodes are local minima and the edges are connections mediated by transition states. This graph can be employed in analysis of structure, dynamics and emergent thermodynamic properties. Applications range from analysis of high-resolution spectra, design principles for self-assembly, machine learning, self-consistent fields, and quantum computing.

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Exploring chemical complexity with assembly theory and chemputation

Lee Cronin
University of Glasgow, United Kingdom

Recent advancements in automation and digitization of chemistry have opened new avenues for exploring chemical complexity. In this talk I will explain how Assembly Theory [1-2] and Chemputation [3-4] can be used to develop a new paradigm to understand and harness the principles of Assembly Theory in chemical synthesis. Assembly Theory provides a framework for quantifying molecular complexity and understanding the emergence of complex chemical systems. Chemputation, on the other hand, offers a standardized method for digitizing and automating chemical synthesis through modular robotic platforms and a chemical programming language (χDL). By combining these approaches, researchers can systematically explore vast chemical spaces, optimize reaction conditions, and potentially discover novel molecules and materials. The integration of these two methodologies enables a new approach to explore chemical space with autonomous experimentation and discovery. As these technologies continue to evolve, they promise to accelerate chemical research, improve reproducibility, provide new insights into the fundamental nature of chemical complexity, as well as an entirely new language.

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From dynamics to reactive flux: responsive kinetic network analysis of biomolecular mechanisms

Jessica Swanson
University of Utah, United States

Although it is well understood that biomolecular mechanisms proceed through a network of intermediates connected by rare-event transitions, it remains an outstanding challenge to properly quantifying the flux through such networks for the range of conditions that are biologically relevant. In this talk, I'll describe our efforts to develop multiscale responsive kinetic modeling (MsRKM), an experimentally driven theoretical framework that combines data from simulations and experiments to describe reaction networks. Focusing on ion channels and transporters, MsRKM defines condition-responsive rates to quantify the flux through intermediates under a range of electrochemical driving forces. This quantitative bridge is then used to identify solutions that are consistent with both simulations and non-equilibrium assays. Our results demonstrate the fundamental and practical differences between electrically and chemically driven ion flux and explain how properties such as ion binding site locations and bulk ion concentrations result in channel properties such as I-V trends and rectification (directional flux). I will also highlight key challenges where graph theory and topology may enable new advances, including solution refinement and quantitative reaction path analysis.

Graph theory and molecular aggregation and phase behavior in aqueous solutions

Jun-Ho Choi, Ravi Singh, Jiwon Seo
GIST, Republic of Korea

Graph theory has widely been utilized to examine physical properties in various aqueous solution systems such as salt solubility, miscibility, liquid-liquid phase separation behavior. Under concentrated solutions, molecules tend to aggregate and exhibit a spatial inhomogeneous distribuiton in mixture system. Recently, a hypothesis on molecular aggregation in aqueous solution systems was proposed [1]. That is, some molecules or ions form self-associate aggregates by avoiding interaction with water, while others tend to form spatially extended network to significantly interact with water. Combination study of graph theory and molecular dynamics (MD) simulation and measure of spatial inhomogeneity [2] revealed that this bifurcating aggregation pattern affects water H-bond structure and dynamics [3], and ultimately solubility in salt solutions [1], miscibility and phase behavior in binary liquid systems [4]. Graph theoretical analyses in various solution systems such as degree distribution, eigenvalue spectrum are presented to examine network properties of solutes and their effect on solution properties.

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Graph-theoretical analysis of interfacial hydrogen-bond networks induced by short-chain alcohols

Rawan Abouhaidar[1], Sana Bougueroua[1], Denis Duflot[2], Marie-Pierre Gaigeot[1], Barbara Wyslouzil[3], Celine Toubin[2]
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[2]Université de Lille, France
[3]Ohio State University, United States

Ice clouds in the upper troposphere are crucial for regulating Earth's climate by affecting stratospheric humidity and the global radiative balance. A key aspect of cloud formation is heterogeneous ice nucleation, influenced by the surface properties of aerosol particles, particularly those with chemical groups capable of hydrogen bonding with water, such as short-chain alcohols. In this study, we focus on 1-pentanol and 3-hexanol to investigate how such alcohols affect the structural organization of interfacial water, a key factor in the onset of freezing processes.

Interfacial water is known to form a highly collective, two-dimensional hydrogen-bonded (2D-HB) network parallel to the air–water interface, with a thickness of approximately 5–10 Å [1,2]. We hence investigate the possible disruption/strengthening caused by alcohol films within this 2D-HB water network at the surface and how this can be correlated with freezing. Using classical molecular dynamics simulations combined with graph theory (GT) analysis, we transform the three-dimensional molecular structures sampled over time into a series of non-isomorphic topological graphs [3,4]. These graphs encode intra- and inter-molecular hydrogen bonding patterns, allowing us to track the structural evolution and statistical features of the interfacial water network.

Our results reveal that alcohol molecules insert themselves into the 2D-HB water network, influencing its topological organization. Notably, 1-pentanol enhances the formation of six-membered hydrogen-bonded rings, a structural motif associated with ice nucleation, more effectively than 3-hexanol, particularly at lower temperatures [5]. This enhanced structuring suggests a greater propensity for ice-like cluster formation at the interface in the presence of 1-pentanol. These findings highlight the utility of graph-theoretical approaches in elucidating interfacial phenomena relevant to atmospheric science and climate dynamics.

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Graph-theoretical approach unravels unimolecular dissociation and ion–molecule complex pathways of gas-phase protonated molecules

Ariel Francis Perez Mellor[1], Thomas Bürgi[1], Riccardo Spezia[2]
[1]University of Geneva, Switzerland
[2]Sorbonne Universite and CNRS, France

We present an automated pipeline that converts on-the-fly chemical-dynamics trajectories into a compact reaction network. The workflow combines permutation-invariant canonical labelling, depth-first fragmentation search, and centre-of-mass clustering [1,2]. Applied to the protonated cyclo-diglycine isomers CYC00, LIN00, and OXA00, it recovers every primary fragmentation pathway and its kinetics. We analyze the ensemble of trajectories based on a three-state model and fit it with RRK theory. The fit tracks how the system moves among the three states over time, letting us read off the "effective" rate constants and energy thresholds.

OXA00 shows a unique landscape: early, long-lived ion–molecule complexes confine phase-space sampling and open roaming routes that lower both the isomerisation barrier and the overall fragmentation threshold relative to the most stable isomer, CYC00—consistent with Collision-Induced Dissociation experiments [3].

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Homology of transient convection cycles over multiplex network flows

Minh Le
Ho Chi Minh City Open University, Vietnam

Markov chains (MCs) are widely used to construct models in the social, physical and biological sciences and engineer technologies for computing and communications. In recent work, we utilized tools from topological data analysis and persistent homology to automate the detection and summary of convection cycles that can arise for irreversible MCs. In the present work, we extend these methods to study convection cycles arising for multiplex Markov chains (MMCs) that are constructed by coupling together sets of MCs. MMCs are closely related to multilayer networks and multiplex networks, whereby network "layers" are interconnected. In the context of MMCs, convection cycles can arise within and/or across MC "layers" and that the strength \$\omega\$ of coupling between MCs acts as a homological "regularizer" for these cyclic flows. Motivated by applications in neuro-AI, we utilize this mathematical framework to develop homological characterizations for fMRI-recorded human brain activity and reinforcement learning.

Protein nanoparticles under the mathematical microscope: from viral tiling theory to interaction networks

Reidun Twarock
University of York, United Kingdom

The geometric principles underpinning virus structure provide a key to understanding viral infections. Most viruses have protein shells that surround, and thus protect, their genetic material. Similar protein architectures occur more widely in nature, as well as in de novo designed protein particles for specific applications in nanotechnology. Mathematical techniques from tiling theory, and related interaction networks, enable classification of their architectures in terms of surface lattices that encode the positions of individual protein units and the interactions between them. By combining these geometric, and related topological, descriptors of protein container architecture with stochastic simulations, I will demonstrate how container geometry provides insights into particle assembly and disassembly, paving the way to innovation in antiviral therapy and virus nanotechnology.

Quantum Mechanics/Molecular Mechanics simulations of proton transfer in biological systems

Mercedes Alfonso-Prieto[1], Irene Cuxart[2], Carme Rovira[2], Gabrielle Potocki-Véronèse[3], Isabelle André[3], Gabriella Chiariello[1], Emiliano Ippoliti[1], Natalia Dmitrieva[1], Samira Gholami[1], Christoph Fahlke[1], Paolo Carloni[1], Claudia Alleva[1]
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Proton transfer (PT) is an essential chemical reaction for a wide variety of biological processes, from enzymatic reactions to transport across membranes. In many enzymes, hydrogen bonds between active site residues and the substrate can help facilitate PT. However, in proton-coupled transporters, multiple co-existing PT pathways can be possible, which might involve Grotthuss-like proton shuttling through hydrogen-bonded chains of water molecules. Quantum Mechanics/Molecular Mechanics (QM/MM), combined with enhanced sampling, is one of the molecular dynamics (MD)-based simulation methods to study proton transfer in biological systems. However, selection of starting configurations suitable for studying PT has proved difficult, due to the reorganization of hydrogen bonded networks upon changes in residue protonation state and transient formation of water wires in the presence of an excess proton. Here I will show some QM/MM applications to study PT in an enzyme [1] and two proton-coupled membrane transporters [2-3], pointing out the aforementioned limitations.

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Representations of energy landscapes by sublevelset persistent homology

Henry Adams
University of Florida, United States

Encoding the complex features of an energy landscape is a challenging task, and often chemists pursue the most salient features (minima and barriers) along a highly reduced space, i.e. 2- or 3-dimensions. Even though disconnectivity graphs or merge trees summarize the connectivity of the local minima of an energy landscape via the lowest-barrier pathways, there is more information to be gained by also considering the topology of each connected component at different energy thresholds (or sublevelsets). We propose sublevelset persistent homology as an appropriate tool for this purpose. Our computations on the configuration phase space of n-alkanes from butane to octane allow us to conjecture, and then prove, a complete characterization of the sublevelset persistent homology of the alkane C_mH_{2m+2} potential energy landscapes, for all m, and in all homological dimensions. We further compare both the analytical configurational potential energy landscapes and sampled data from molecular dynamics simulation, using the united and all-atom descriptions of the intramolecular interactions. Joint work with Joshua Mirth, Yanqin Zhai, Johnathan Bush, Enrique Alvarado, Howie Jordan, Mark Heim, Bala Krishnamoorthy, Markus Pflaum, Aurora Clark, Yang Zang.

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Studying crystalline materials through their underlying nets

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Over the past century, the use of chemical graphs of molecules — particularly topological indices (i.e., graph invariants)— has become a fundamental approach to understanding the relationship between molecular structure and properties. In contrast, crystalline materials have traditionally been studied more from a group theoretical viewpoint, with an emphasis on symmetry. However, with the rise of reticular chemistry, increased attention has been given to the bond networks of crystalline materials and their meaningful simplifications. Descriptors derived from these nets (i.e., infinite periodic graphs) serve as powerful tools for characterizing crystalline materials, enabling structure–property correlations, guiding materials discovery, and informing machine learning models for property prediction.

In this short talk, we will see how to construct the underlying net(s) of a crystalline structure, discuss how to distinguish between different types of nets, introduce the concept of quotient graphs, and demonstrate how to derive net-based descriptors suitable for studying structure–property relationships, illustrated through recent projects.

Tackling subgraph isomorphism with multilayer Gaussian Boson Sampling

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We introduce a multilayer Gaussian boson sampling methodology to tackle the induced subgraph isomorphism problem common to a wide range of applications, including molecular search, molecular docking, and retrosynthesis. The proposed methodology is implementable on bosonic quantum devices using O(n) photonic modes, where n is the number of nodes in the graph. Sampling can be performed with high-fidelity photon-number-resolving detectors, or cost-effective threshold detectors that work at room temperature, offering both practicality and efficiency.

The Euclidean geometry of the Huckel molecular orbital method

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We consider a tight-binding (Huckel molecular orbital) Hamiltonian to a describe a conjugated molecule or solid. We define the probability that a pi-electron is at the jth molecular orbital on the basis of its energy and the canonical partition function. We then several probabilities of intersections between events like finding an electron at a molecular orbital with a given energy and the one of being at a given atom. These probabilities generalize the Coulson bond order and the charge density. We then define the difference of the probabilities of finding an electron at the atoms v or w and the probability of finding it hopping between the two atoms. We prove analytically that this quantity is a Euclidean distance between the corresponding atoms. We then define several geometric measures like the angle between the position vectors of two atoms in the Euclidean space, the Forman-Ricci curvature of a bond and the efficiency of electron delocalization in a molecule/solid. We then find analytical results for linear and circular polyenes and presented a few potential applications related to the geometric structure of polycyclic molecules and their reactivity.

Topological descriptors for analysis and visualization of electronic structures

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In this talk, I will present our work on the visual analysis of electronic transitions in molecules, describing interactions between light and matter. These processes can be effectively represented as bivariate scalar fields, such as hole and particle natural transition orbitals (NTOs). We explore various abstractions of these bivariate fields, including geometric and topological segmentations, as well as continuous scatterplots (CSPs). A key guiding principle in our approach is to ensure that these abstractions are not only visually interpretable but also suitable for downstream tasks such as clustering, comparison, and tracking of dynamic fields. All methods are integrated into interactive analysis pipelines that facilitate the comparative study and exploration of molecular ensembles.

4. Participant list

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