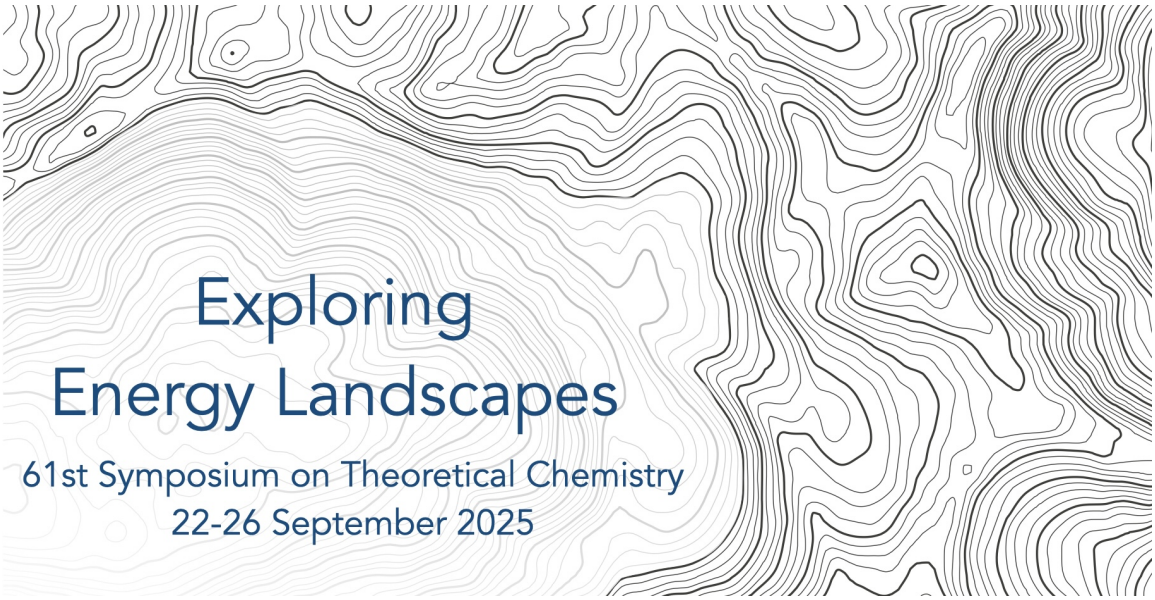
61st Symposium on Theoretical Chemistry

Exploring Energy Landscapes
22-26 September 2025
Freie Universität Berlin, Germany

Organizers:
Prof. Dr. Bettina Keller and Prof. Dr. Beate Paulus

Venue:
Freie Universität Berlin, Department of Biology, Chemistry, Pharmacy
Arnimallee 22, D-14195 Berlin



FREIE
UNIVERSITÄT
BERLIN

Berlin, September 2025

Dear colleagues and friends,

A very warm welcome to Berlin – and to the Institute of Chemistry and Biochemistry at Freie Universität Berlin.

For the *61st Symposium on Theoretical Chemistry* we've put together a program covering a wide range of topics in theoretical chemistry, with exciting connections to physics, mathematics, computer science, pharmacy, and biology. Our thanks go to all speakers and poster presenters for sharing their work and ideas with the community. One highlight will be the special session on Tuesday afternoon, celebrating the Hans G.A. Hellmann Award and the Sigrid Peyerimhoff Award 2025.

Three poster sessions (with food and drinks, of course) will give us plenty of time to exchange ideas and discuss the research of more than 300 poster contributions in a relaxed setting.

On Friday, together with Prof. Benjamin Pölloth, we will try out a new format on the theme "Using Computations to Teach Chemistry." The aim is to open a discussion on how computational methods and simulations can become part of the general chemistry curriculum, with plenty of room for exchange.

We hope you'll enjoy the science, take home fresh ideas, and reconnect with old friends - and perhaps make a few new ones, too.

Sincerely,
Bettina Keller, Beate Paulus and the whole organizational team

Time	Mon 22.9.	Tue 23.9.	Wed 24.9.	Thu 25.9.	Fri 26.9.
09:00 - 09:20		Annika Bande	Thomas D. Kühne	Karsten Reuter	Benjamin Pölloth
09:20 - 09:40					Charlotte Müller
09:40 - 10:00		Olga S. Bokareva	Clara Zens	Rico Friedrich	J. Brossette, M. Peterknecht
10:00 - 10:20		Rhiannon A. Zarotiadis	Maren Podewitz	Lukas Hasecke	Committee of experts
10:20 - 10:40		Werner Dobrautz		Maria Drosou	
10:40 - 11:10		*Coffee*	*Coffee*	*Coffee*	*Coffee*
11:10 - 11:30	Registration	Jean C. Tremblay	Jonny Proppe	Nicola Gaston	Parallel:
11:30 - 11:50					Workshop & Hands-On
11:50 - 12:10		Loïse Attal	Johannes Hoja	Frank Ortmann	
12:10 - 12:30		Jindra Dušek	Sophia Wesely	Jan Hermann	Poster Prizes
12:30 - 13:40		*Lunch*	*Lunch*	*Lunch*	Closing
13:40 - 14:00	Opening				
14:00 - 14:20	Lillian Chong	AGTC Meeting	Excursion	Michael Römelt	
14:20 - 14:40					
14:40 - 15:00	Johannes Dietschreit			Stella Stopkowicz	
15:00 - 15:20	Federico Lazzari			Yannick Franzke	
15:20 - 15:50	*Coffee*	*Coffee*		*Coffee*	
15:50 - 16:10	Johannes Kästner	Award Ceremony		Shirin Faraji	
16:10 - 16:30					
16:30 - 16:50	Laura Grazioli			Elke Fasshauer	
16:50 - 17:10	Chanbum Park			Markus Reiher	
17:10 - 17:30	George Trenins				
17:30 - 18:00	*Break*	*Break*	*Break*	*Break*	
18:00 - 21:00	Poster session 1	Dinner	Poster session 2	Poster session 3	

The conference dinner and the excursions are formally included as part of the official conference program.

Contents

Conference webpage

Scan the QR code to access

- up-to-date **online program**
- **practical information** on lunch options, excursions and conference dinner

`https://www.bcp.fu-berlin.de/en/stc2025`

Supporters

Lecture abstracts

1 Lectures on Monday (Sep. 22, 2025)

Instructions for Speakers

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Catching Rare Events in Action with Weighted Ensemble MD

Lillian Chong
University of Pittsburgh

Rare biological and chemical events often lie beyond the reach of conventional simulations. The weighted ensemble (WE) path sampling strategy overcomes this barrier, extending accessible timescales by orders of magnitude while maintaining rigorous kinetics. By directly simulating pathways and stepwise rates, WE reveals molecular mechanisms in unprecedented detail. In this talk, I will highlight recent advances in WE methodology and showcase applications to ligand unbinding and chemical reactions.

What the PMF Gets Wrong - and How to Fix It

Johannes Dietschreit
University of Vienna

Understanding chemical reactions at the molecular level often relies on projecting dynamics onto a few collective variables (CVs) that capture the key, slow degrees of freedom. A widely used construct in this context is the potential of mean force (PMF)—a free energy-like profile derived from the marginal Boltzmann distribution along a CV. While commonly interpreted as an analogue of the minimum energy path, the PMF depends on the chosen CV function and can potentially assign different values to identical configurations in Cartesian space, potentially making such interpretations inconsistent.
While neglecting this property can be a valid approximation for some reactions, it can lead to substantial errors in estimating reaction energetics. As an alternative, we derive exact expressions for the free energy, internal energy, and entropy profiles as functions of the CV that are gauge-invariant [1]. This leads to simple and consistent definitions of reaction [2] and activation [3] energies and entropies that, unlike the PMF, account for particle masses, which is crucial for the correct description of kinetics.
We illustrate how this framework enables the extraction of quantitative insights from entropy and energy profiles in realistic physicochemical processes, including intramolecular organic reactions.

References

[1] Dietschreit, J.C.B.; Diestler, D.J.; Gómez-Bombarelli, R. J. Chem. Theory Comput. 2023, 19(16), 5369-5379
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Efficient Discovery and Refinement of Low-Energy Conformers: From Modular Ring Fragments to Accurate Structures

Federico Lazzari
Scuola Superiore Meridionale

Accurate electronic energies for large molecules are now routine, yet underlying geometries are often unreliable downstream. Conformational workflows thus separate exhaustive exploration from costly high-level refinement, a split hard to reconcile.

We introduce a descriptor-guided pipeline in which the same molecular-perception features ("synthons"), first devised for Δ-ML geometry correction,[1,2] steer both steps.
Hard degrees of freedom are tackled with Pharma-LEGO: SMILES from the 300-structure LCB25 set[3] are fragmented into rings, recombined into chemically valid scaffolds, and ranked by synthon similarity before optimisation.
Soft degrees of freedom (torsions) are searched with a hydrogen-bond-aware island-model genetic algorithm.[4,5] A fitness penalty discourages poses that collapse into known minima, boosting diversity. When geometry and energy correlate strongly, an active Bayesian loop can replace the genetic stage, exchanging breadth for query efficiency.
Selected conformers enter exploitation and are re-optimised by two complementary schemes:

- BDPCS3[6]: revDSD double-hybrid plus a-posteriori core–valence correlation; bond-length errors $<$0.001 Å.
- BHPCS2[7]: a Δ-ML surrogate trained on B3LYP geometries; similar accuracy at far lower cost.

Because both methods share the synthon feature space, exploration and refinement remain internally consistent. The modular protocol reunites exploration and exploitation. Ring perception, torsional search, and high-level optimisation are decoupled yet seamless, enabling automated, chemically meaningful sampling of macrocycles and drug-like molecules, sidestepping transition-state barriers and providing tunable cost-accuracy trade-offs for high-resolution spectroscopy, conformational mapping, and reactive-intermediate studies

References

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Transferable and Uniformly Accurate Interatomic Potentials

Johannes Kästner
Universität Stuttgart

The development of machine-learned interatomic potentials requires generating sufficiently expressive atomistic data sets. Active learning algorithms select data points on which labels, i.e., energies and forces, are calculated for inclusion in the training set. However, for batch mode active learning, i.e., when multiple data points are selected at once, conventional active-learning algorithms can perform poorly. Therefore, we investigate algorithms specifically designed for this setting and show that they can outperform traditional algorithms. We investigate selection based on the resulting training set's informativeness, diversity, and representativeness. We propose using gradient features specific to atomistic neural networks to evaluate the informativeness of queried samples, including several approximations allowing for their efficient evaluation. To avoid selecting similar structures, we present several methods that enforce the diversity and representativeness of the selected batch. Furthermore, we use transfer learning to improve the quality of the resulting potential, use training data from cluster calculations to predict bulk properties, and present a scheme to learn tensorial quantities, like the magnetic anisotropy.

Excited States as Critical Points of the Potential Energy Surface

Laura Grazioli
École nationale des ponts et chaussées, INRIA Paris

In exact theory, excited states are defined as higher-energy solutions of the Schrödinger equation. From a mathematical point of view, we can interpret excited states as saddle points on the electronic energy functional of a molecular system. For a Morse function, saddle points can be classified on the basis of the number of negative eigenvalues of the Hessian matrix. The nth excited state can be seen as a saddle point with n negative eigenvalue (Morse-index n). However, when applying a nonlinear parameterization of the wave function to the linear Schrödinger equation, spurious critical points may appear. Therefore, a careful analysis of the saddle points is needed to identify, among the critical points, those having the physical interpretation of excited states. We will develop manifold constrained saddle-point search algorithms on the manifold of admissible electronic states to locate all index-1 saddle points. A first global exploration of the energy can be performed through stochastic algorithms, to identify the area in which the saddle points are located, extending ideas from [1] to Riemannian manifolds. In the identified area, local critical-point search algorithms can be applied to find the saddle point, using the Riemannian gradient of the energy functional and part of the information contained in the Riemannian Hessian. For both steps, it is key to carefully exploit the geometry of the manifold of admissible electronic states. We will start from Hartree-Fock theory, which can be identified as models on Grassmann manifolds, and then turn to MCSCF and CASSCF theory. This definition of the excited states will be compared to the one obtained through linear-response theory, for which a new derivation scheme, based on the structure of Kähler manifolds, has been developed [2].

References

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[2] Grazioli, L.; Hu, Y.; Cancès, E., arXiv:2506.16420.

Deciphering the Structural and Electronic Properties Across the Gold–Water Interface

Chanbum Park
Ruhr-Universität Bochum

Metal-water interfaces play a crucial role in electrochemical reaction mechanisms relevant to energy storage and conversion devices. However, since these interfaces are buried between solid and liquid phases, it remains challenging to experimentally resolve the intrinsic structural and electronic properties of such electrified interfaces, in particular those of the interfacial water molecules. As a result, their fundamental nature is still far from being fully understood up to being controversial. In this work, we quantify the structural and electronic interactions at the gold-water interface. Our findings reveal that the dipole moments and electronic properties of water molecules near the metal surface can vary significantly depending on their orientation and hydrogen-bonding states. By employing a novel efficient implementation for localizing molecular orbitals in hybrid systems such as water interacting with a metallic surface via partially occupied Wannier functions—which allows us to compute the contributions of individual water molecules to the total interfacial electronic dipole—we uncover that water molecules in close proximity to the gold surface exhibit significantly increased dipole moments. We disclose that this is due to distinct polarization of those electron lone pairs which point toward the metal surface, thus belonging to water molecules with their O-H bonds pointing toward the water layer.
Additionally, we present evidence of electronic polarization and charge transfer effects in vibrational spectra through peak broadening and frequency shifts of dangling O-H bonds near the metal surface, as observed in both sum-frequency generation (SFG) spectroscopy and fully atomistic ab initio molecular dynamics simulations. Overall, the strong electronic interactions between metal and water that we reveal give rise to orientation-dependent electronic heterogeneity. Our findings provide new insights into the fundamental properties of metal-aqueous interfaces with broad implications for electrochemistry, catalysis, and energy-related applications.

Memory Matters for Quantum Nuclear Motion on Metals

George Trenins
Max Planck Institute for the Structure and Dynamics of Matter

Electronically nonadiabatic interactions open a key energy dissipation channel for dynamics on conducting surfaces. An established perturbative formulation enables practical simulations of the resulting dissipative dynamics using ab initio "electronic friction" (EF), computed from electron-phonon coupling matrix elements. Currently, such simulations almost exclusively treat atomic nuclei classically. To account for nuclear zero-point energy (ZPE) and tunnelling, we combine EF with ring-polymer molecular dynamics (RPMD): an imaginary-time path integral method that captures these effects at the cost of a molecular dynamics simulation in an extended phase-space. Our formulation encompasses spatially-dependent friction and accounts for non-Markovian (memory) effects. Memory plays a major role in the surface diffusion of hydrogen on Cu(111), effectively masking the rate enhancement due to ZPE. Using RPMD+EF, we can explain the anomalous agreement of classical simulations with experiment and open the way to accurate modelling of nonadiabatic interfacial dynamics. [G. Trenins and M. Rossi, Phys. Rev. Lett. 134, 226201 (2025)]

2 Lectures on Tuesday (Sep. 23, 2025)

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21st Century Electron Dynamics Simulations

Annika Bande
Leibniz Hannover University, Helmholtz-Zentrum Berlin

The theory of electron dynamics solves the time-dependent Schrödinger equation and allows to predict the electronic motion in molecular structures [1,2]. It enables understanding of the fundamentals of chemical reactivity and of intricate ultrafast and light-driven and scattering processes, which shall be motivated by a didactically sound visualization of excitation processes [3] in addition to the basic explanation of the theory.
However, the most accurate wave function-based techniques reach their computational limits at an order of some ten electrons! At the same time, electron dynamics is challenged by complex and large-scale material-scientific problems relevant to modern society.
This presentation identifies strategies to address some of the major methodological and computational obstacles. For realistic calculations of (large) target structures in their true environment, description of energy and charge transfer processes among electrons and nuclei in the neighborhood are established [4]. Moreover, different ways of modeling nano-sized structures are considered [5,6]. Finally, modern computing strategies, machine learning from the field of data science [7], and quantum simulations from the field of quantum information technology [8], are explored for their use in electron dynamics computations.

References

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Excited-State Dynamics of Cyclometalated Cobalt(III) Complexes

Olga S. Bokareva
Leibniz Institute for Catalysis; University of Rostock

Transition-metal complexes exhibit rich photochemical and photophysical properties due to their ability to access long-lived electronically excited states. Replicating such behavior in first-row (3d) transition metals presents significant challenges that warrant further investigation. Recent progress in ligand-field photocatalysis, particularly with cobalt(III) cyclometalated complexes, has revealed novel excited-state reactivity. However, the photophysics and photochemistry of cobalt(III) complexes remain underexplored.
In this work, I present excited-state dynamical simulations using mixed quantum-classical non-adiabatic surface-hopping and quantum multi-layer MCTDH methods to unravel the excited-states dynamics of cobalt(III) photosensitizers. For polypyridyl cobalt(III) complexes, ground-state recovery occurs in the Marcus inverted region,[1] a notable deviation from typical first-row transition-metal behavior, such as that of isoelectronic iron(II) systems. This regime supports simultaneous enhancement of redox potential and excited-state lifetime,

enabling light-to-chemical energy conversion, including activation of oxidatively resistant substrates in photoredox catalysis. Initial triplet population timescales are captured through simulated population dynamics, while long-time recovery is recovered using transition state theory.
As a second example, I discuss how alkyl substituent functionalization affects the photodynamics of newly reported cobalt(III) complexes with imidazole-based NHC ligands.[2] The simulations reveal that ultrafast relaxation is driven by spin-orbit coupling, vibrational coherence, and structural dynamics, all influenced by the ligand environment. Overall, our findings highlight the necessity of integrating mixed quantum-classical and quantum dynamical approaches to accurately describe excited-state processes in transition-metal complexes.

References

[1] A. Ghosh, J. T. Yarranton, J. K. McCusker. Nat. Chem. 2024, 16, 1665.
[2] A. Krishna, L. Fritsch, J. Steube, M. A. Arguello Cordero, R. Schoch, A. Neuba, S. Lochbrunner and M. Bauer, Inorg. Chem. 2025, 64, 1401.

Hybrid Light-Matter Landscapes - Lighting the Way to Photonic Qubits

Rhiannon A. Zarotiadis
Simons Center for Computational Physical Chemistry; New York University

It is well established that nuclei explore electronic potential energy landscapes, and that this exploration governs key phenomena in chemistry and materials science. Theoretical advances, ranging from ab-initio molecular dynamics to semiclassical and nonadiabatic methods such as ring-polymer dynamics and surface hopping, have enabled increasingly accurate modelling. In contrast, light remains an often neglected component in chemical theory. Commonly treated as a probe, it has rarely been considered an active, quantum-mechanical participant. As a result, it has not undergone the same rigorous development in chemical theory as electronic and nuclear dynamics.
Recent advances in strong light–matter interactions, which have applications in numerous fields from catalysis in chemistry to photovoltaic cells in material science and photonic qubits in quantum information science, however, require accurate theoretical methods to capture light-matter dynamics. In the strong light-matter coupling regime, light and matter form hybrid states that cannot be separated, giving rise to complex, coupled light–matter landscapes. Exploring these hybrid landscapes presents a high-dimensional computational and theoretical challenge that demands new theoretical approaches.
Here, we develop a photon sampling scheme based on cavity Multi-Trajectory Ehrenfest (cMTE) dynamics, which is inspired by existing approaches for nuclei. The cMTE method uses Wigner sampling to retain the quantum character of light while propagating its dynamics (semi)classically for favourable scaling. Coupled with real-time electronic structure calculations, this framework allows us to explore complex light–matter landscapes in realistic molecules, introducing a new paradigm of ab-initio quantum optics. We apply this method to study quantum effects in molecules coupled to waveguides, which is relevant to photonic qubit formation. This framework also naturally extends to include nuclear quantum dynamics, therefore offering a unified path towards simulating coupled electron–nuclear–photonic systems.

Transcorrelated Quantum Simulation: Toward Realistic Energy Landscapes on Near-Term Quantum Hardware

Werner Dobrautz
Helmholtz-Zentrum Dresden-Rossendorf; Center for Advanced Systems Understanding; Center for Scalable Data Analytics and Artificial Intelligence

Accurately exploring molecular energy landscapes remains a central challenge in computational quantum chemistry, particularly for systems exhibiting strong correlation. Quantum computers promise new capabilities in this regard, yet practical progress is hindered by noise, limited qubit counts, shallow circuit depths, and optimization difficulties in variational quantum algorithms (VQAs).

In this talk, I will present how transcorrelated quantum simulation—based on a similarity-transformed Hamiltonian incorporating electron–electron cusp information—reshapes the energy landscape to improve convergence toward chemically accurate solutions. This reformulation reduces basis set incompleteness errors[1] and enables more compact circuit representations[2], which are especially valuable on noisy, near-term quantum devices.
To fully leverage these benefits, we combine transcorrelation with adaptive ansätze[4], which iteratively construct compact quantum circuits tailored to the problem at hand. This combination significantly reduces both qubit requirements and gate counts.
To address the optimization challenges commonly encountered in flat or rugged variational landscapes, we developed qBang—a hybrid optimization scheme that interweaves geometric information from the Fubini–Study metric with adaptive momentum-based updates[4].
I will illustrate our method using benchmark studies on Hubbard models and small molecular systems, highlighting recent implementations of transcorrelated variational imaginary time evolution (TC-VarQITE). Results from both classical circuit simulations and runs on actual quantum hardware demonstrate that this approach enables more realistic and noise-resilient approximations to ground state energies—bringing us closer to chemically accurate energy landscapes using near-term quantum resources.

References

[1] W. Dobrautz et al., J. Chem. Theory Comput. 2024, 20, 10, 4146–4160
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Matrix Isolation Spectroscopy of Polyfluoride Anions: The Effect of Confinement

Jean Christophe Tremblay
Université de Lorraine

Matrix isolation spectroscopy has emerged as a powerful experimental tool to investigate polyfluoride anions and shed light on their peculiar bonding properties. The technique involves confining metastable species within a defective noble-gas crystal at low temperatures and characterizing their vibrational properties by IR spectroscopy. A central theoretical challenge is to explain why weakly bound polyfluoride anions show unexpected sensitivity to supposedly inert cryogenic matrices [1,2].
In this contribution, we present a theoretical framework for accurately investigating weakly interacting guest-host systems, enabling the subtle frequency shifts observed in different matrices to be rationalized in simple chemical terms [3-5]. Furthermore, it will be shown that confinement in a neon matrix leads to heavy-atom tunnelling in F5- [6], helping resolve a structure that had remained elusive for over a decade [2,7].

References

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A System-Bath Model to Investigate the Quantum Dynamics of Complex or Interacting Molecular Systems

Loïse Attal
Universität Potsdam; Université Paris-Saclay, CNRS

Addressing the dynamics of molecular systems coupled to an environment is a challenging task, especially when considering finite-size environments that can be affected by their interactions with the smaller system. In such cases, the usual open quantum system methods and approximations might fail as they assume the environment (or bath) to be infinite, always at thermodynamical equilibrium, and unperturbed by the system. In particular, they do not take into account the fact that finite environments can be heated by the excitation of the system and evolve out of equilibrium. Such situations may occur when studying, e.g., internal relaxation inside a large molecule, small molecules trapped in fullerenes or other finite clusters, or in contact with nano-scale devices.
In this context, we have developed a new theoretical model based on a system-bath approach where we consider a one-dimensional system (e.g. one vibrational mode) interacting with a large but finite harmonic bath ($\sim$100-1000 modes). The system and its coupling to individual bath modes are treated as rigorously as possible but the bath part of the Hamiltonian is simplified, with its modes being replaced by a single ladder of effective bath states that describe the energy stored inside the bath. This model allows us to treat large baths, to study the relaxation dynamics of the system at finite temperature and to analyze the response of the bath to the system's excitation.
We present this Effective Bath State (EBS) model and benchmark results obtained on a model system where an O-H stretching mode interacts with a bath of 40 to 600 harmonic oscillators. We also discuss infrared spectra obtained for the phenylacetylene molecule and compare our results with experiments. Finally, a recent extension of the model to a two-dimensional system, and its application to CO adsorbed on a NaCl(100) surface will be presented.

Perturbatively Corrected Ring-Polymer Instanton Rate Theory Rigorously Captures Anharmonicity and Deep Tunnelling

Jindra Dušek
ETH Zürich

Correctly describing quantum effects is necessary for determining the rate of many reactions, e. g. in atmospheric chemistry or catalysis. While transition state theory (TST) is widely used to calculate rate constants, it has limitations, as it fails to account for quantum tunneling and anharmonic effects. One efficient method that goes beyond TST is instanton theory [1]. It only requires information from the least-action tunnelling path (called the instanton) and in return it can describe quantum tunnelling. In this contribution, I will explain how to improve upon instanton theory by adding to it perturbative corrections which describe the anharmonicity perpendicular to the tunnelling pathway. With this, much greater accuracy is achieved while maintaining computational efficiency and physical insight already present in instanton theory.
Our perturbative corrections to instanton theory were derived using asymptotic theory similarly to our previous research on tunnelling splittings [2]. In addition to the instanton path and hessians along it (which are required for the leading-order theory), we now also require third and fourth derivatives along the instanton trajectory. Since the higher-order derivates are readily available by numerically differentiating the potential energy surface (PES), our method is efficient and scalable. As a result, both tunnelling and anharmonicity are included and our theory vastly exceeds the accuracy of TST for little effort.

References

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Sigrid Peyerimhoff Award:

Computational Investigation of Catalytic Reaction Mechanisms

Juliane Heitkämper
PhD: Universität Stuttgart, *now:* German Aerospace Center (DLR): Computational Investigation of Catalytic Reaction Mechanisms

Understanding catalytic reaction mechanisms is essential for the rational design of more efficient and selective catalysts. This requires detailed insights into fundamental reaction steps, energy barriers, and the kinetic factors that govern overall performance. This work presents a computational approach that integrates quantum chemical calculations, kinetic modeling, and experimental validation to unravel complex multi-step catalytic cycles. The methodology provides reliable information on elementary steps, activation barriers, and competing pathways, while emphasizing the crucial interplay between theoretical prediction and experimental evidence.

Sigrid Peyerimhoff Award:

Excitonic Renormalization: A Novel Fragmentation Scheme For Modular Ab Initio Electronic-Structure Calculations

Marco Bauer
PhD: Universität Heidelberg, *now:* KTH Stockholm

Excitonic renormalization (XR) [1-4] is a novel fragmentation scheme, in which the electronic structure of fully isolated fragments is calculated by a method of choice, which can differ between individual fragments. The interaction is then recovered by contracting the correlated monomer information in form of transition densities with computationally cheap integrals in an ab-initio manner. To account for the non-orthogonality of the orbitals between different fragments, a biorthogonal framework is used. This methodology is particularly useful for rather weakly bound fragments with several multi-reference centers, as e.g. encountered a lot in the field of small molecule activation. Here I will show how the Hamiltonian can be built efficiently, by expanding the overlap between non-orthogonal states in orders of orbital overlaps, leading to smooth and fast convergence and how to optimize the monomer information in a compact manner.

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3 Lectures on Wednesday (Sep. 24, 2025)

Instructions for Speakers

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Breaking the Exaflop Barrier with CP2K

Thomas D. Kühne
Center for Advanced Systems Understanding (CASUS); Helmholtz-Zentrum Dresden-Rossendorf (HZDR); Technische Universität Dresden

We push the boundaries of electronic structure-based ab-initio molecular dynamics(AIMD) beyond 100 million atoms. This scale is otherwise barely reachable with classical force-field methods or novel neural network and machine learning potentials. We achieve this breakthrough by combining innovations in linear-scaling AIMD, efficient and approximate sparse linear algebra, low and mixed-precision floating-point computation on GPUs, and a compensation scheme for the errors introduced by numerical approximations. The core of our work is the non-orthogonalized local submatrix method (NOLSM), which scales very favorably to massively parallel computing systems and translates large sparse matrix operations into highly parallel, dense matrix operations that are ideally suited to hardware accelerators. We demonstrate that the NOLSM method, which is at the center point of each AIMD step, is able to achieve a sustained performance of 1.1 EFLOP/s in FP16/FP32-mixed floating-point arithmetic when using 4400 NVIDIA A100 GPUs of the Perlmutter system.

Towards a Better Understanding of Charge Transfer Processes in Organic Radical Batteries – A Combined Molecular and Quantum Mechanical Approach

Clara Zens
Friedrich Schiller University Jena

Nowadays organic batteries are promising approaches in energy storage, e.g. due to their mechanical flexibility and sustainability.[1] Conjugated polymers were widely investigated in the scope of such batteries.[2] However, an unstable cell voltage over a broad capacity range prevents their application.[3] Alternatively, stable organic radicals show highly promising properties,[4] yet lacking the desired conductivity. Recently, in a joint-theoretical project, a new approach was realised by combining stable organic radicals with a conductive polymer-based backbone.[5,6] Thereby, the focus was set on the tetramethylpiperidinyl-N-oxyl radical (TEMPO) in combination with a polythiophene backbone.
Particular emphasis was set on the molecular and quantum mechanical modelling of intra- and intermolecular charge transfer (CT) processes of these materials.[5–7] First insights were gained by modelling the potential energy curves (PEC) of the intramolecular CT with multi-configurational methods. The CT was then assessed by Marcus theory. Key properties were explored and how they affect the PECs and thereby the CT.[5] Recent research endeavours focus on the influence of the surrounding environment on the inter- and intramolecular CT. Thereby, the environmental configurations are assessed via molecular mechanics, while quantum mechanical "snapshots" are taken with time-dependent density functional theory. Finally, PECs of intramolecular CT processes of other combinations of thiophene with organic radicals are explored. With these methods, in-depth insights are gained, that allow to tailor new organic radical batteries with optimal CT properties.

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Navigating Free Energy Landscapes from Static Mechanisms to Reaction Dynamics

Maren Podewitz
TU Wien

Computational chemistry has become an important tool for accelerating experimental discovery by exploring the reaction mechanisms of catalytic systems, guiding experimental design. However, achieving robust and transferable insights requires methodological advances in system representation and computational strategy. Reliable results depend on developing and selecting appropriate chemical and computational models, both of which are evolving continuously. In recent years, the field has moved beyond static, single-structure, implicit-environment studies towards ensemble-based, dynamic explorations with explicit solvation. This opens up new opportunities, but also raises challenges in terms of computational scalability, model reliability, and data analysis.
This talk will focus on methodological developments in modelling catalytic mechanisms across multiple levels of complexity. First, I will present advances in static modelling and highlight microsolvation strategies that identify strongly interacting solvent molecules, thereby improving the description of explicit environments [1, 2]. Then, I will discuss emerging tools for reaction dynamics and demonstrate how explainable machine learning (ML) approaches and time-resolved analyses provide mechanistic insights that are inaccessible to static models [3]. Together, these developments illustrate how new frameworks and computational tools can expand the accessible free energy landscape and enable a deeper, more predictive understanding of catalytic reactivity.

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Benchmarking Explainability of Molecular Machine Learning with WISP

Jonny Proppe
Technische Universität Braunschweig

Interpretable machine learning is crucial for building trust in predictive models, especially in chemistry and drug discovery. We present WISP (Workflow for Interpretability Scoring using Pairs), a framework implemented in Python and designed to systematically benchmark the explainability of machine-learning methods in the context of molecular property prediction. It combines scoring metrics with matched molecular pair (MMP) analysis, providing both quantitative and qualitative insights into how well model explanations align with known structure–property relationships. Alongside WISP, we introduce a descriptor- and model-agnostic atom attributor that generates robust atom-level explanations. Applied to diverse datasets—including Crippen logP, experimental logP, aqueous solubility, LCAP reaction yields, Factor Xa binding affinities, and AMES mutagenicity—WISP reveals how explanation quality depends on model performance and dataset complexity. For reaction yield prediction, WISP exposes functional group effects that would otherwise remain hidden, supporting rational molecular design and synthesis planning. Together, WISP and our atom attributor form a flexible toolkit to benchmark and improve explainability, enabling more reliable predictions and better informed decision-making.

Kinetics of Molecular Crystals: From Polymorphic Interconversion to Solid-State Reactivity

Johannes Hoja
University of Graz

Gaining quantitative insight into the dynamics and kinetics of molecular crystals is vital for drug development and for advancing solvent-free, sustainable synthesis methods that rely on solid-state reactions. However, this remains a difficult task as molecular crystals often exhibit multiple polymorphs that differ by only a few kJ/mol in their Gibbs free energies. Thus, a reliable description of these polymorphs requires very accurate calculations to correctly capture their relative stabilities [1]. Therefore, we have developed a multimer embedding approach [2], which approximates expensive periodic PBE0+MBD calculations by embedding multimers into lower-cost PBE+MBD calculations, thereby significantly reducing computational cost and memory requirements. This method reproduces lattice energies within 1 kJ/mol, unit cell volumes within 1 %, and harmonic vibrational free energies within 1 kJ/mol of the canonical periodic PBE0+MBD results and provided very accurate results in a recent crystal structure prediction blind test [3]. Building on this foundation, we utilize solid-state nudged elastic band (NEB) simulations to explore energy barriers and transition pathways of molecular crystal transformations, covering interconversions between polymorphs and a single-crystal Diels-Alder reaction. We showcase a novel interpolation method for automatically generating viable initial pathways that avoids atomic collisions, enabling NEB calculations for crystals containing larger and quite flexible molecules [4]. To accelerate these calculations, we further demonstrate the use and accuracy of machine-learned force fields trained on system-specific DFT data. Collectively, these advances bring us closer to a comprehensive, computationally efficient picture of polymorph transformation pathways and reaction mechanisms in molecular crystals.

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Exploring Excited-State Energy Landscapes with Machine Learning: The Example of Green Fluorescent Protein Chromophores

Sophia Wesely
Leipzig University

Understanding excited-state energy landscapes is central to designing photoreactive molecules for applications in bioimaging, optogenetics, or photopharmacology. The green fluorescent protein (GFP) chromophore, p-hydroxybenzylidene-2,3-dimethylimidazolinone anion ($HBDI^-$), is a model system for excited-state processes, but presents significant challenges for theory due to long-lived excited states, competing relaxation pathways, and the prohibitive cost of accurate quantum chemical simulations[1]. These factors have traditionally made systematic exploration of functional group modifications intractable. In this work, we overcome these limitations by combining our recently developed equivariant machine learning model for excited states, X-MACE [2], with nonadiabatic molecular dynamics. Trained on thousands of organic chromophores, X-MACE generates potential energy surfaces transferable across chemical space and electronic states with minimal additional data. This approach enables, for the first time, efficient screening of $HBDI^-$ derivatives to assess how structural changes modulate excited-state topologies and dynamics. Our results uncover design principles for tuning photophysical properties through targeted substitutions, demonstrating the potential of machine learning to unlock excited-state landscape exploration at scale.

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4 Lectures on Thursday (Sep. 25, 2025)

Instructions for Speakers

You're welcome to either bring your own laptop or share your talk with us as a PDF (on a USB stick or by email to the set-up team). Our team will be around during the coffee breaks and happy to help you get everything ready. To keep things running smoothly, please use a coffee break before your talk to test your set-up.

Out of the Crystalline Comfort Zone: Tackling Working Interfaces with Machine Learning

Karsten Reuter
Fritz-Haber-Institut der Max-Planck-Gesellschaft

Machine learning (ML) promises a significant enhancement of multi-scale modeling capabilities in the context of energy conversion and storage (ECS). In particular, ML interatomic potentials (MLIPs) trained with first-principles data already offer orders of magnitude speed-ups in the computation of predictive-quality energies and forces in atomic-scale simulations. This new efficiency finally allows to heads-on tackle the highly dynamic evolution of working interfaces in ECS systems, where the targeted functionality like catalytic activity or ion mobility both inherently drives and results from ongoing substantial structural, compositional and morphological changes. Unable to fully capture such operando evolution, direct first-principles based multiscale modeling focused hitherto on model (single-)crystalline surfaces or interfaces, where the system dynamics was typically restricted to select reacting or diffusing species that were considered central for a targeted primary function. The MLIP-enabled enhanced sampling capabilities instead allow to assess the thermodynamic stability of complex, possibly amorphous configurations and thereby establish reliable structural models for the working interfaces. Automated process exploration in turn provides more systematic access to the elementary steps that drive the operando evolution, paving the way for microkinetic simulations that analyze the entanglement of this evolution with the primary function.

Accurate Thermochemistry of Ionic Materials from Coordination Corrected Enthalpies

Rico Friedrich
Technische Universität Dresden

The accurate description of enthalpies of ionic materials is a critical enabler for the discovery and design of novel compounds such as two-dimensional systems and high-entropy ceramics. While standard density functional theory (DFT) can quantitatively describe the thermochemistry of intermetallic compounds, they fail to produce accurate results for ionic materials such as oxides. Formation enthalpies thus typically exhibit mean errors of several hundred meV compared to high-level thermochemical reference data [1].
To address this critical problem, we have developed the method of coordination corrected enthalpies (CCE). The correction is based on the chemical intuition that the number of bonds in a material determines its thermodynamic stability [1]. As such it is developed as a topological correction taking into account the cation-anion connectivity. In addition, CCE takes into account the cation oxidation state. The method substantially improves formation enthalpy predictions reducing mean absolute errors down to 27 meV/atom for oxides, halides, and nitrides [1,2]. Moreover CCE is capable of correcting the relative stability of different polymorphs predicted with wrong energetic ordering from plain DFT – a distinct advantage compared to all earlier correction schemes. CCE has been implemented into the freely available AFLOW software suite for computational materials design offering automated structural analysis for coordination numbers, determination of oxidation states, and enthalpy correction based on only structural inputs [3]. It comes with command line functionality, a web interface, and a python environment. CCE is in particular an important enabler for the discovery of novel high-entropy ceramics which relies on accurate enthalpies between competing phases [4].

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Development and Application of Scalable Multicomponent Methods

Lukas Hasecke
Georg-August-Universität Göttingen

The simulation of nuclear quantum effects (NQE) like nuclear delocalization, zero-point vibration, and tunnelling is crucial to accurately describe systems and processes that involve light nuclei especially hydrogen atoms. The significance of these effects has been demonstrated in various fields from biochemistry to condensed matter. [1] In particular, many processes with complex energy landscapes such as proton-coupled electron transfer, hydrogen absorption on surfaces and dynamics at aqueous metal interfaces highlight the tremendous importance of NQEs for an accurate potential energy surface. [2,3]
Although electronic structure theory methods have become standard tools for quantum chemical investigations, addressing NQEs still lacks computationally accessible and straightforward approaches. To tackle this challenge, we combined the elegant and computationally efficient Nuclear-Electronic Orbital framework developed by Hammes-Schiffer and coworkers with local and canonical density fitting approximations. [4,5] This combination provides new low-order scaling methods, which for the first time allow to include NQEs of large systems within a few hours and for small to medium-sized systems in minutes.
We demonstrate the accuracy and transferability of our approach by benchmarking it to real use cases relevant to chemical, biological, and material science applications. Thereby, emphasizing the necessity of employing multicomponent energy surfaces to match with experimental conclusions. [5,6] Overall, our methods provide a compelling instrument to include NQEs within PESs with exceptional computational efficiency and marks a significant step towards an accurate ab-initio simulation with wide-ranging applications from material design to energy conversion.

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Towards a Multireference-Multiscale Description of Photosynthetic Pigment-Protein Complexes

Maria Drosou
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A first-principles description of the primary photochemical processes driving Photosynthesis is a grand scientific challenge. These processes involve diverse pigment assemblies embedded in membrane protein complexes. Popular quantum chemical (QM) approaches based on density functional theory face key limitations, including non-transferability, imbalanced description of charge-transfer transitions, and inherent inability of single-reference approaches to describe double excitations. Multireference wavefunction methods can offer the highest level of insight by explicitly describing the wavefunction for each individual state, but they require informed user input and are computationally more intensive than "black-box" TD-DFT.

Here, we present a solid, transparent, and transferable methodological framework for the multireference description of low-lying excited states of protein-embedded chlorin-based pigments relevant to photosynthetic reaction centers and apply this protocol to the description of the reaction center of Photosystem II.[1] For the QM description of the pigment excited states, we use the complete active space self-consistent field (CASSCF) method, incorporating dynamic correlation effects with n-electron valence state perturbation theory (NEVPT2) to obtain accurate excited-state energies. We then integrate this approach with molecular mechanics (MM) in a QM/MM framework to capture electrostatic effects from the protein matrix, which can uniquely diversify otherwise chemically identical pigments.[2] Our protocol extends to describe multichromophoric charge transfer states that define the primary charge separation events in the Reaction Center of Photosystem II. For CASSCF calculations on multichromophoric systems, we employ a dynamic-correlation-assisted approach, namely active space selection by 1st order perturbation theory (ASS1ST).[3] This optimized protocol is transferable to any photoactive embedded pigment system, marking the first step towards large-scale multireference studies of photosynthetic reaction centers and light-harvesting complexes.

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Why is Gallium Liquid at Room Temperature?

Nicola Gaston
University of Auckland

The use of low-temperature liquid metals, such as gallium, as media for the dilution of other metals has led to an increasing variety of examples of how temperature- and concentration-dependent interactions can be used to direct the self-assembly of nanostructure, with astonishing precision, resulting in novel pattern formation and structural control. However the underlying interactions driving such phenomena are still poorly understood. A question of fundamental importance remains to be answered: why does gallium have such a low melting temperature, of 29.8 degrees Celsius, to begin with?
Recent first-principles simulations have demonstrated that, in contrast to previous assumptions, covalent bonding becomes more important in the liquid at higher temperatures, meaning that covalency is not a significant feature of the liquid near the phase transition temperature. This explains the experimental observation of a decrease of resistivity of the metal upon melting, and its subsequent anomalously nonlinear increase with temperature. It also suggests that the change of enthalpy upon the change from solid to liquid phase is not anomalous, and that instead the entropy difference between the dimeric solid and monatomic liquid explains the room temperature (on a nice day) melting point [1].

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Insights from Quantum Dynamics Simulations: From Molecules to Organic-Material Interfaces

Frank Ortmann
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Understanding charge and exciton dynamics in molecular systems is critical for advancing organic semiconductor and optoelectronic technologies. We present insights from our work addressing distinct yet complementary aspects of these phenomena for organic electronic materials. First, we explore charge-transfer dynamics in

electron-phonon coupled model systems, identifying regimes such as transient localization and polaron transport, emphasizing their seamless transitions across vibrational modes and temperatures. Second, a comparative analysis of the Matrix Product State (MPS) and Multilayer Multiconfiguration Time-Dependent Hartree (MCTDH) methods demonstrates their efficacy in modeling non-adiabatic exciton dissociation, revealing specific sensitivities to electronic-vibrational entanglement in complex systems. Finally, a quantum mechanical assessment of ultrafast charge transfer at donor-acceptor interfaces benchmarks MPS against semi-classical hopping models, showcasing their convergence while highlighting the role of vibrational dynamics in optimizing photovoltaic performance. These works underline the importance of methodical and theoretical advances in capturing the interplay of electronic and vibrational degrees of freedom in molecular optoelectronics.

Skala: Accurate and Scalable Exchange-Correlation with Deep Learning

Jan Hermann
Microsoft Research AI for Science

Density Functional Theory (DFT) is the most widely used electronic structure method for predicting the properties of molecules and materials. Although DFT is, in principle, an exact reformulation of the Schrödinger equation, practical applications rely on approximations to the unknown exchange-correlation (XC) functional. Most existing XC functionals are constructed using a limited set of increasingly complex, hand-crafted features that improve accuracy at the expense of computational efficiency. Yet, no current approximation achieves the accuracy and generality for predictive modeling of laboratory experiments at chemical accuracy – typically defined as errors below 1 kcal/mol. In this work, we present Skala, a modern deep learning-based XC functional that bypasses expensive hand-designed features by learning representations directly from data. Skala achieves chemical accuracy for atomization energies of small molecules while retaining the computational efficiency typical of semi-local DFT. This performance is enabled by training on an unprecedented volume of high-accuracy reference data generated using computationally intensive wavefunction-based methods. Notably, Skala systematically improves with additional training data covering diverse chemistry. By incorporating a modest amount of additional high-accuracy data tailored to chemistry beyond atomization energies, Skala achieves accuracy competitive with the best-performing hybrid functionals across general main group chemistry, at the cost of semi-local DFT. As the training dataset continues to expand, Skala is poised to further enhance the predictive power of first-principles simulations.

Combining Heatbath-CI-SCF and N-electron Valence State Perturbation State Theory to Treat Molecules with Many Strongly Correlated Electrons

Michael Römelt
Humboldt-Universität zu Berlin

The exploration of energy landscapes becomes complicated when multiple electronic states are close in energy, as for example observed in transition metal complexes with multiple open shells. In such cases, multireference electronic structure methods provide a sound approach to deal with strong correlation effects.[1,2] Recently, we have reported a configuration-based variant of heatbath-CI (HCI) that allows for SCF calculations with large active spaces while retaining spin symmetry.[3] Our implementation utilizes the HCI logic[4], extensively exploits symmetry and introduces a novel parallelization scheme based on configuration prefixes to achieve high efficiency. In addition to energy calculations, state averaged nuclear gradients allow for the exploration of energy landscapes for the ground and excited states even in the presence of (near-) degeneracies.[5] Reliable results can, however, only be obtained when dynamic electron correlation effects are considered.[6] Therefore, we present two variants of second order N-electron valence state perturbation theory (NEVPT2) to capture these effects on top of our HCISCF method. A "canonical" variant incorporates the important residual terms[7] to avoid the appearance of false intruder states in the infamous Si and Sa perturber spaces. In contrast, a combination of Epstein-Nesbet PT2 and NEVPT2 avoids the critical terms altogether. Both variants make use of the heatbath-CI logic to dramatically reduce the associated computational cost and furthermore use prefix-based

parallelization to extend their applicability. Embedded in the open-source HUMboldt MultiReference (HUMMR) program[8] this allows for accurate calculations of chemically relevant systems with many strongly correlated electrons.

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Prediction and Assignment of Strongly Magnetized White Dwarf Spectra

Stella Stopkowicz
Universität des Saarlandes

The atmospheric composition of white dwarf stars is typically inferred through analysis of their observed spectra, obtained using both Earth-based and space-based telescopes. For example, the Hubble Space Telescope has provided high-resolution ultraviolet spectra critical to such investigations. Accurate interpretation and assignment of these spectra require advanced quantum-chemical calculations to identify the atomic and molecular species present. A significant fraction of white dwarfs exhibit strong magnetic fields, with field strengths reaching up to approximately 100 megagauss (MG), or 100,000 tesla. At lower field strengths, magnetic effects can often be treated as small perturbations. However, this perturbative approach breaks down in the regime of strong magnetic fields, where magnetic interactions lead to complex and non-intuitive alterations of spectral features, greatly complicating their assignment.
In these high-field cases, it becomes necessary to incorporate the magnetic field explicitly within finite-field quantum-chemical frameworks. Such methods allow for the prediction of field-induced shifts, splittings, and changes in transition intensities. This presentation will illustrate examples of these predictive approaches and discuss the specific challenges associated with spectral interpretation under strong magnetic fields. The impact of field-dependent pressure broadening on spectral line profiles will also be addressed.

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General and Transferable Local Hybrid Functional for Electronic Structure Theory and Many-Fermion Approaches

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The development of density functional approximations strongly focuses on the electronic structure. However, DFT is not only applicable to electrons but also to other fermions within the framework of multicomponent DFT. Ideally, a general density functional approximation applicable to electrons, protons, and other Fermions with similar accuracy should be constructed. This requires a tailored correlation term, which should be derived in a non-empirical way to ensure transferability. Utilizing the class of local hybrids (LHs), we construct exchange-correlation functionals from first principles and show that theoretical constraint satisfaction can be achieved with full exact exchange without sacrificing accuracy [1]. Here, LHs are especially advantageous for strongly localized fermions such as protons, as they allow to smoothly switch from 0% to 100% exact exchange and thus mitigate the self-interaction error.
The new functional shows excellent performance for thermochemical properties, excitation energies, NMR properties, and Mossbauer isomer shifts. The transferability to other Fermions is illustrated for electron-proton correlation energies and compared to results from the multicomponent random phase approximation [2].
Our implementation in TURBOMOLE uses an efficient seminumerical scheme [3] and is available in a relativistic two-component formalism to include spin-orbit interaction [4,5]. Therefore, it is applicable to a wide range of real-world systems, as demonstrated for the NMR shifts of organophosphorous molecules [6] and EPR properties of Bi or Tl compounds.

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Coupled Electron-Nuclear Dynamics in Complex Environments: An Efficient Simulation Strategy and Software Infrastructure

Shirin Faraji
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Light-driven processes such as the photovoltaic effect, charge migration, and proton-coupled electron transfer are fundamentally quantum in nature and central to technologies like optogenetics, photopharmacology, and photoresponsive materials. However, accurate modeling remains challenging due to (i) the need for high-level electronic structure methods, (ii) coupled electron-nuclear dynamics, and (iii) the effect of the complex environment.
Recent progress in direct dynamics approaches—such as semiclassical trajectory surface hopping and on-the-fly quantum dynamics—has significantly enhanced the ability to simulate such processes. Nevertheless, the computational burden remains substantial, particularly due to the large number of required electronic structure calculations. This challenge is addressed by a database-accelerated framework that combines interpolation techniques and adaptive sampling to drastically reduce computational effort. Moreover, integration with a quantum mechanics/molecular mechanics scheme enables the explicit treatment of complex environments.
The focus is on software infrastructure and efficient implementation, designed for rapid prototyping and development in data-science contexts. Representative test systems demonstrate the strengths and limitations of the framework, highlighting the trade-off between accuracy and efficiency. The presented computational framework paves the way for more routine simulations of complex light-driven processes in realistic environments.

Where do Fano Profiles Go?

Elke Fasshauer
University of Tübingen

Fano profiles are omnipresent in atomic spectra. They are caused by interference between two channels evolving to the same final state. and therefore carry intricate information about the underlying electronic rearrangements in time. For electronic decay processes in molecules, however, these signatures are washed out. Amongst others, the famous example of the combined autoionization and photo-dissociation spectra of the hydrogen molecule shows no Fano profiles, neither in experiment, nor in simulations including nuclear motion [1]. We discuss this phenomenon for different model potentials and experimental conditions, and thereby reveal under which conditions a peak structure can be observed [2].

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Automated Reaction Network Exploration

Markus Reiher
ETH Zürich

In this talk, I will discuss the latest developments of the Chemoton program [1] for automated reaction network explorations [2,3,4] from first principles. Chemoton is a versatile software for this purpose that we have been developing for almost a decade. It is freely available and open source as part of our SCINE package [5]. The capabilities of SCINE are broad and range from automated mechanism elucidation to rolling benchmarking with uncertainty quantification [6] and integrated microkinetic modeling [7,8,9]. Automated reaction network elucidation based on first-principles methods requires significant computational resources for the exploratory algorithms that crawl and search across Born-Oppenheimer potential energy surfaces. Accordingly, cheap quantum chemical methods such as density functional tight binding are often employed. However, they trade speed for accuracy with significant setbacks on the reliability of relative energies and even on network topology. Machine learning potentials (MLPs) promise to achieve comparatively high accuracy at the speed of force field evaluations. However, a significant initial training effort and the lack of MLP flexibility had hampered their application in an exploratory context. To address this problem, we developed lifelong-learning MLPs [10], which allow one to continually grow a knowledge base for quantum chemical reactivity studies. This new concept required significant methodological developments [11,12]. In view of the growing dominance of foundational models, which tend to become more and more important also for reaction exploration, lifelong data selection can be an important mechanism for fine-tuning such a general model to a specific reactivity study at hand.

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5 Lectures on Friday (Sep. 26, 2025)

Instructions for Speakers

You're welcome to either bring your own laptop or share your talk with us as a PDF (on a USB stick or by email to the set-up team). Our team will be around during the coffee breaks and happy to help you get everything ready. To keep things running smoothly, please use a coffee break before your talk to test your set-up.

Lab Bench to Laptop: Using Computations to Teach Chemistry. Computational chemistry can transform the way we teach chemistry. In this session, we will explore best practices for using simulations and quantum-chemical calculations to visualize concepts, replace or complement traditional lab experiments, and deepen student understanding. Join us to see how virtual experiments can help students navigate challenging chemical concepts.

From Trial-and-Error to Energy-Based Reasoning: Bringing Computational Chemistry into the Chemistry Classroom

Benjamin Pölloth
Freie Universität Berlin

Computational chemistry (CC) has become indispensable for exploring molecular energetics and reaction mechanisms. Yet, despite its central role in research, CC remains largely absent from high school curricula and from many areas of university teaching. CC could enable students to connect chemical structure and potential energy—a central relationship in chemistry that students are rarely able to make.[1] Furthermore, the implementation of CC could allow students to engage in authentic scientific inquiry via model-based simulations and to reflect on epistemic questions.[2]
Therefore, we developed the Comp-Chem-Lab (CCL), an intuitive browser-based learning environment that enables high school students to use ORCA for real-time energy calculations.[3] In a qualitative empirical study, upper-secondary students used the CCL to investigate bond dissociation energies and reaction energetics of simple reaction systems. The analysis of observation data reveals that most students began with trial-and-error, but their problem-solving strategies evolved over time. After some time, most students were able to use CC in scientific inquiry and to reason about the energetic aspects of chemical reactions.
Based on these findings, we discuss how CC can support scientific inquiry activities, such as enabling students to interpret and analyze data, while fostering conceptual change in the understanding of energy. On the one hand, the findings highlight existing challenges in integrating CC into chemistry education.[4] On the other hand, they also show how a thorough empirical analysis of students' learning difficulties, the tailored design of learning environments and structured feedback can help to overcome these obstacles. Embedding CC in chemistry education at different learning stages could bridge the gap between classroom practice and modern research and help students to better understand the core concept of energy.[5]

References

[1] Pölloth, Diekemper, Schwarzer, Chem. Educ. Res. Pract. 2023, 24, 1153.
[2] Seoane, Greca, Arriassecq, SIMULATION 2022, 98, 87.
[3] Pölloth, J. Chem. Educ. 2025, 102, 1367.
[4] Tuvi-Arad, Isr. J. Chem. 2022, 62.
[5] Pölloth, Sieve, Unterricht Chemie 2024, 35, 3-7.

Designing Simulation-Use in the Classroom: Lessons Learned

Charlotte Müller
ETH Zürich

Chemistry, and theoretical chemistry in particular, is unable to shake the reputation of being hard to learn [1]. But why is that? One reason is the imperceptibility and intangibility of many salient concepts in the discipline. Students always relate new information to prior experiences, and this becomes harder if there is no immediate connection to the world that they interact with every day [2]. However, teachers and lecturers can create these connections by offering bridging representations that bring the imperceptible concepts to the world of the students [3]. Here, we will present the case of a real-time quantum chemistry simulation that offered haptic feedback to bachelor students [4]. While we expected that, aligned with the reasoning above, the haptic feedback will allow the students to feel forces that normally are inaccessible to them, we found that the students who did not receive such feedback outperformed the ones who did [5, 6]. We will discuss the reasons for this result and offer some lessons that we learned in the process.

[1] A. H. Johnstone, J. Comput. Assist. Learn., 1991, 7(2), 75–83.

[2] K. Niebert, H. Gropengießer, Int. J. Sci. Educ., 2015, 37(5–6), 903–933.

[3] L. Pham, R. Tytler, Res. Sci. Educ., 2022, 52(3), 853–869.

[4] C. H. Müller, M. Steiner, J. P. Unsleber, T. Weymuth, M. Bensberg, K.-S. Csizi, M. Mörchen, P. L. Türtscher, M. Reiher, J. Phys. Chem. A, 2024, 128(41), 9028–9044.

[5] C. H. Müller, M. Reiher, M. Kapur, J. Comput. Assist. Learn., 2024, 40(2), 715–730.

[6] C. H. Müller, M. Reiher, M. Kapur, Proc. 18th Int. Conf. Learning Sciences (ICLS 2024), ISLS, 2024, 1043–1046.

High School Student Computer Lab at LMU München

Jan Brossette and Marina Peterknecht
LMU München

Despite the enormous success of computational chemistry in academic research, it has been underappreciated in the context of high school teaching, even though computational chemistry offers great opportunities for visualization and conceptual understanding of chemical questions. In our student lab for computational chemistry (SC^2-LAB), we offer high school students and their teachers the opportunity to get hands-on experience in different fields of computational chemistry, such as machine learning-based protein design, molecular protein and reaction dynamics and density functional theory for understanding chemical reactions. Here we want to illustrate the fundamental design of our SC^2-LAB and key strategies in the use of computational chemistry for high school students.

Computer experiments for Bachelor and Master in Chemistry

Bettina Keller
Freie Universität Berlin

I will give a brief introduction to the hands-on computer experiments. See below.

Committee of experts

Shirin Faraji (Heinrich-Heine Universität Düsseldorf), Alina Jansen (Freie Universität Berlin), Beate Paulus (Freie Universität Berlin), Markus Reiher (ETH Zürich), Peter Saalfrank (Universität Potsdam)

Moderation: Benjamin Pölloth (Freie Universität Berlin)

Workshop: Sharing Perspectives on the Role of TC in Teaching

At this STC, we want to put a specific focus on the question of how the potential of theoretical chemistry (TC) and computational chemistry (CC) for transforming the way chemistry is taught can be fostered. During the conference, you will be invited to participate in a survey about the current and future role of TC in teaching.

The workshop will provide an open forum to discuss the survey results and exchange perspectives on the visibility of TC, the black-box use of CC, and the role of mathematics in teaching. Together, we will explore how TC and CC could complement traditional approaches, deepen student understanding, and inspire innovative teaching methods. We will also reflect on current challenges that still need to be solved and consider how they might be addressed in the future. This workshop could serve as a starting point for a broader expert study or as a platform to map diverse viewpoints within the community. You are invited to share your expertise and perspective on these important questions for chemistry education.

Hands-On: Computer experiments for Bachelor and Master in Chemistry

In this session, you can try out two interactive computer experiments developed during a series of hackathons. The first experiment helps students develop an intuition for linear expansions of functions and the variational principle. The second experiment illustrates a key concept from first-year physical chemistry in an accessible, hands-on way.

Poster session

6 Poster session on Monday (Sep. 22, 2025)

Instructions for Poster Presenters

Your poster number is given in the conference program. The format is "Day Number" (e.g. "Mon 22"). On the poster wall, only the number is shown (the day is not included). Mount your poster on the poster wall labeled with your number. Pins are provided at the poster wall.

- Posters can be put up starting **Monday, 22 September 2025, at 12:30 pm**.
- Please remove your poster again by **Tuesday, 23 September 2025, at 11:00 am** (end of the coffee break).

Enjoy the poster session!

In lieu of an abstract

Instead of submitting an abstract, we asked poster presenters to assign their contribution to the following topics:

- Biochemical Systems
- Electronic Structure Theory
- Machine Learning in Chemistry
- Materials and Solid-State Theory
- Method Development
- Molecular Dynamics and Simulation
- Spectroscopy and Properties
- Reaction Mechanisms and Catalysis

In the program, each poster contribution is listed together with its assigned topic.

Posters

Mon 1 **Periodic DFT Investigation of the Distant Binuclear Vanadium V(II) Cationic Sites in Zeolites. Splitting Dioxygen - Reactivity of Low-Valency Vanadium Species Stabilized in Zeolite Matrices**
Sklenak, Stepan
J. Heyrovsky Institute of Physical Chemistry of the Czech Academy of Sciences, Czech Republic
Reaction Mechanisms and Catalysis

Mon 2 **Quantum Chemical Study of the Reactivity of Platina(II)Pnictinidenes with Maleic Anhydride**
Wegerich, Nils[1]; Neben, Marc C.[2]; Schneider, Sven[2]; Holthausen, Max C.[1]
1: Goethe University Frankfurt; 2: Georg August University Göttingen
Reaction Mechanisms and Catalysis

Mon 3 **Accurate Correlation Potentials from the Self-Consistent Random Phase Approximation**
Fauser, Steffen; Görling, Andreas
Lehrstuhl für Theoretische Chemie, FAU Erlangen-Nürnberg, Germany
Electron Structure Theory - Method Development

Mon 4 **Simulating (Time-Resolved) Resonant Inelastic X-Ray Scattering in the Time Domain**
Freibert, Antonia[1]; Mendive-Tapia, David[2]; Vendrell, Oriol[2]; Huse, Nils[1]
1: University of Hamburg, Germany; 2: Heidelberg University, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 5 **DFT and TDDFT Studies of Copper Oxide Clusters with Vanadium Substitution Used in Photochemical Applications**
Bensiradj, Nour El Houda[1,2]; Nassar, Meriem.[2]; Ouamerali, Ourida[2]
1: Ecole Normale Supérieure ENS Kouba Algiers Algeria, Algeria; 2: Université de Sciences et de Technologie Houari Boumedienne USTHB Algiers Algeria
Electron Structure Theory

Mon 6 **First-Principles Characterization of Noncovalent Interactions in the Enantioselective Oxetane Ring Opening via SPHENOL-Based Chiral Phosphoric Acid Catalyst**

Khera, Mayank[1]; Kaur, Navjot[2]; Goel, Neetu[3]

1: Chandigarh Group of Colleges, Jhanjeri, Mohali, India; 2: Faculty of Science, SGT University, Gurugram; 3: Department of Chemistry, Panjab University, Chandigarh

Reaction Mechanisms and Catalysis

Mon 7 **Machine Learning-Driven Discovery of Novel Photosensitizers via Large-Scale Excited-State Modeling**

Giugliano, Giulia[1]; Barrett, Rhyan[2]; Mattioli, Edoardo Jun[1]; Westermayr, Julia[2,3]; Calvaresi, Matteo[1]; Zerbetto, Francesco[1]

1: Alma Mater Studiorum-University of Bologna, Italy; 2: Leipzig University, Wilhelm Ostwald Institute for Physical and Theoretical Chemistry, Linnéstraße 2, 04103 Leipzig, Germany; 3: Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig, Humboldtstraße 25, 04105 Leipzig, Germany

Electron Structure Theory - Machine Learning in Chemistry - Spectroscopy and Properties

Mon 8 **Coupled Resonances to Explain Asymmetric Lineshapes in Photoelectron Spectra**

Dutoi, Anthony D.[1]; Guzman-Bucio, Dulce Maria[2]; Cabrera-German, Dagoberto[3]; Carmona-Carmona, Abraham[4]; Herrera-Gomez, Alberto[2]

1: University of the Pacific, USA; 2: CINVESTAV-Unidad Queretaro, Mexico; 3: Universidad de Sonora, Mexico; 4: Benemérita Universidad Autónoma de Puebla, Mexico

Spectroscopy and Properties - Materials and Solid-State Theory

Mon 9 **Fully Analytic Nuclear Gradients for the GW Method and the Bethe–Salpeter Equation**

Tölle, Johannes

Universität Hamburg, Germany

Electron Structure Theory - Spectroscopy and Properties - Method Development

Mon 10 **Flux in Frustration: Capturing the Dynamic Evolution of Frustration between Frustrated Lewis Pairs**

Faizan, Mohmmad; Pawar, Ravinder

National Institute of Technology Warangal, India

Molecular Dynamics and Simulation - Machine Learning in Chemistry - Reaction Mechanisms and Catalysis

Mon 11 **Pyrolysis of Cyclic Peptides: From Quantum Chemistry to Reactor-Scale Simulation**

Schnieder, Bastian[1]; Debiagi, Paulo[2]; Pelucchi, Matteo[3]; Schmid, Rochus[1]; Hättig, Christof[1]

1: Ruhr-Universität Bochum, Bochum, Germany; 2: Nottingham Ningbo China Beacons of Excellence Research and Innovation Institute, Ningbo, China; 3: Politecnico di Milano, Milan, Italy

Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Mon 12 **Comparison of Experimental and Computational pKa Assists in Structure Determination**

Syed, Tahir Ali

Federal Urdu University of Arts, Science and Technology Karachi Pakistan, Pakistan

Method Development

Mon 13 **Shaping Energy Landscapes with Vibrational Strong Light-Matter Coupling: Insights from Coupled Cluster Theory**

Fischer, Eric

Humboldt-Universität zu Berlin, Germany

Electron Structure Theory - Method Development

Mon 14 **Electron Transfer Mediated Decay Process for the Auger Final State of Ne+(1S-1) (H2O)N (N=1,4) Cluster**

Rana, Meenakshi

Ashoka University, India

Electron Structure Theory

Mon 15 **Structure and Transport Mechanisms in Naphthalene-Diimide Organic Mixed Ionic-Electronic Conductors: An Atomistic Perspective**

Severi, Marco[1]; Garattoni, Filippo Tommaso[1]; Yu, Simiao[2]; Nielsen, Christian[2]; Fazzi, Daniele[1]

1: Department of Chemistry G. Ciamician, University of Bologna, via Piero Gobetti 85, 40129 Bologna, Italy; 2: Department of Chemistry, Queen Mary University of London, Room 1.08, Joseph Priestley Building, Mile End Road, London E1 4NS

Molecular Dynamics and Simulation - Materials and Solid-State Theory

Mon 16 **Rationalizing NMR Chemical Shifts of Transition Metal Compounds**

Auer, Alexander

Max Planck Institut für Kohlenforschung, Germany

Electron Structure Theory - Spectroscopy and Properties

Mon 17 **Conformation-Dependent Excited State Properties in Extended Conjugated Systems: Static and Dynamics Studies**
Mandal, Palak; Panda, Aditya N.
Indian Institute of Technology (IIT) Guwahati, India
Electron Structure Theory - Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 18 **Resonance Raman Spectra of a Bodipy Monomer and an Excitonic Dimer via a Time-Dependent Approach**
Ortlepp, Jan Christoph
Heinrich-Heine-Universität Düsseldorf, Germany
Electron Structure Theory - Spectroscopy and Properties

Mon 19 **Development of an Extensive and Diverse Solvation Benchmark Set with Experimental References**
Selzer, Christian Erik; Wittmann, Lukas; Grimme, Stefan
Bonn University, Germany
Electron Structure Theory

Mon 20 **Configurations Out of Chaos: A Hierarchical Sampling Approach to Amorphous Solids**
Hückmann, Lukas; Cottom, Jonathon; Meyer, Jörg
Leiden Institute of Chemistry, Leiden University, The Netherlands
Materials and Solid-State Theory

Mon 21 **Shaking up ICEC: Exploring Nuclear Dynamics in Interparticle Coulombic Electron Capture**
Jahr, Elena Marie[1]; Senk, Jan[2,3]; Drennhaus, Jan P.[4]; Kolorenc, Premysl[3]; Sisourat, Nicolas[2]; Fasshauer, Elke[1]
1: University of Tübingen, Germany; 2: Sorbonne Université, France; 3: Charles University, Czech Republic; 4: KU Leuven, Belgium
Molecular Dynamics and Simulation - Spectroscopy and Properties - Method Development - Reaction Mechanisms and Catalysis

Mon 22 **Using Molecular Grids for Sampling-Free Dynamics**
Zupan, Hana; Keller, Bettina
Freie Universität Berlin, Germany
Molecular Dynamics and Simulation - Method Development

Mon 23 **Nuclear Quantum Effects in Liquid Water and Its Isotopologues: Path Integral Simulations with CCSD(T) Accuracy**
Stolte, Nore[1]; Malik, Ravi[2]; Daru, János[3]; Forbert, Harald[1]; Chandra, Amalendu[2]; Behler, Jörg[1]; Marx, Dominik[1]
1: Ruhr-Universität Bochum, Germany; 2: Indian Institute of Technology Kanpur; 3: Eötvös Loránd University
Molecular Dynamics and Simulation

Mon 24 **DFT- and ML-Supported Catalyst Design for the Ring-Opening Polymerization of Lactide**
Schäfer, Martin Alexander[1,2]; Bannwarth, Christoph[1]; Herres-Pawlis, Sonja[2]
1: Institute of Physical Chemistry, RWTH Aachen University, Germany; 2: Institute of Inorganic Chemistry, RWTH Aachen University, Germany
Electron Structure Theory - Machine Learning in Chemistry - Reaction Mechanisms and Catalysis

Mon 25 **New Ways to Tackle Photosynthesis Research with QM and QM/MM Calculations**
Götze, Jan
Freie Universität Berlin, Institut für Chemie und Biochemie, Arnimallee 22, 14195 Berlin, Germany
Electron Structure Theory - Molecular Dynamics and Simulation - Machine Learning in Chemistry - Spectroscopy and Properties - Biochemical Systems

Mon 26 **Hydroxyl Radical Initiated Reaction of Nerol: A Pathway to Secondary Pollutants in Indoor Environment**
Angappan, Mano Priya; EL DIB, Gisèle
Universite de Rennes, France
Reaction Mechanisms and Catalysis

Mon 27 **Quantification of Reaction Barriers under Diffusion Controlled Conditions**
Mähr, Martin; Podewtiz, Maren; Talmazan, Radu A.
TU Wien, Austria
Method Development - Reaction Mechanisms and Catalysis

Mon 28 **Analyzing Microsolvation Shell Buildup of Helium Around the Zundel Cation Using Highly Accurate Path Integral Simulations Based on Machine Learning Potentials**
Gil Olaria, Eduard[1]; Schran, Christoph[2]; Forbert, Harald[3]; Marx, Dominik[1]
1: Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany; 2: Cavendish Laboratory, University of Cambridge, CB3 0HE Cambridge, United Kingdom; 3: Center for Solvation Science ZEMOS, Ruhr-Universität Bochum, 44780 Bochum, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry

Mon 29 **The Fate of the Hesitating Proton: Chemically Accurate Free Energies for the Adsorption of Ethanol in H-ZSM-5**
Kumar, Dipanshu; Galimberti, Daria Ruth
Radboud University, The Netherlands
Electron Structure Theory - Molecular Dynamics and Simulation - Spectroscopy and Properties - Materials and Solid-State Theory

Mon 30 **Revealing the Unique Role of Water in the Formation of Benzothiazoles**
Kumar, Dipanshu; Neumann, Kevin; Galimberti, Daria Ruth
Radboud University, The Netherlands
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Mon 31 **Development of Parallel Crystal Algorithm Towards Reaction Discovery in Molecular Photoswitches**
Pandey, Ankit[1]; Poirier, Bill[2]; Liang, Ruibin[1]
1: Texas Tech University, United States of America; 2: University of Vermont, United States of America
Method Development - Reaction Mechanisms and Catalysis - Biochemical Systems

Mon 32 **Rates and Optimal Pathways of Phase Transitions in Active and Reactive Nonequilibrium Systems**
Heller, Eric; Limmer, David
University of California, Berkeley, United States of America
Molecular Dynamics and Simulation - Method Development - Reaction Mechanisms and Catalysis

Mon 33 **ChemLab Platform: Automating Quantum Chemical Research and Managing Computational Data**
Mikhailin, Aleksandr
Chemlab, Austria
Molecular Dynamics and Simulation

Mon 34 **ChemLab Platform: Automating Quantum Chemical Research and Managing Computational Data**
Mikhailin, Aleksandr
ChemLab, Austria
Molecular Dynamics and Simulation

Mon 35 **Combining Theory and Experiment – Integrating Microkinetic Modelling with Quantum Chemical Methods for Reaction Mechanism Elucidation**
Beck, Alexander; Kaestner, Johannes
University of Stuttgart, Germany
Method Development - Reaction Mechanisms and Catalysis

Mon 36 **What Makes an Efficient Long Wavelength Photoinitiator with Tin and Germanium?**
Kelterer, Anne-Marie[1]; Haslinger, Carola[2]; Liska, Robert[2]
1: Graz University of Technology, Austria; 2: Vienna University of Technology, Austria
Spectroscopy and Properties

Mon 37 **Halogen Bonds in the Ligand-Protein Systems: Quantum-Chemical Study of Methionine and Aminopyrimidine Derivatives**
Wojtkowiak, Kamil; Panek, Jarosław; Jezierska, Aneta
University of Wroclaw, Poland
Molecular Dynamics and Simulation - Biochemical Systems

Mon 38 **Quantum Dynamics Simulation of Exciton-Polariton Transport**
Krupp, Niclas
Heidelberg University, Germany
Molecular Dynamics and Simulation - Materials and Solid-State Theory

Mon 39 **Neural ODE-Based Diabatization via Parallel Transport of Electronic States**
Hütter, Michael; Ončák, Milan
Institut für Ionenphysik und Angewandte Physik der Universität Innsbruck, Austria
Machine Learning in Chemistry - Method Development

Mon 40 **Fundamental Insights into the Nitrogen Oxidation Reaction over Pd-Based Electrodes**
Ontaneda, Jorge; Exner, Kai S.
University of Duisburg-Essen, Germany
Reaction Mechanisms and Catalysis

Mon 41 **Quantifying Trust in Interpretable Machine Learning for Materials Science**
S. Nair, Akhil[1,2]; Yao, Yi[3]; Foppa, Lucas[2]; Scheffler, Matthias[2,3]; Paulus, Beate[1]
1: Institute of Chemistry and Biochemistry, Freie University Berlin, Arnimallee 22, 14195 Berlin, Germany; 2: The NOMAD Laboratory at the Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany; 3: Molecular Simulations from First Principles E.V, D-14195 Berlin, Germany
Machine Learning in Chemistry - Materials and Solid-State Theory

Mon 42 **Orbital-Driven Insights into Enantioselective Hydrofunctionalization of Alkenes Catalyzed by Co-Salen Complexes: Study on Singlet and Triplet States**

Gupta, Shivangi; Rawal, Parveen; Gupta, Dr. Puneet

IIT Roorkee, India

Electron Structure Theory

Mon 43 **First-Principles Approaches to Model Metal-Chiral Molecule Interfaces to Understand CISS Effect**

Naskar, Sumit[1,2]; Mujica, Vladimiro[3]; Alonso-Gomez, Jose Lorenzo[4]; Herrmann, Carmen[1]

1: Friedrich-Schiller-Universität Jena, Germany; 2: University of Hamburg, Hamburg, Germany; 3: Arizona State University, TEMPE, Arizona, United States; 4: University of Vigo, Vigo, Spain

Electron Structure Theory - Method Development - Materials and Solid-State Theory

Mon 44 **Predicting Lipophilicity through Graph Neural Networks: A Step Toward Intelligent Molecular Property Prediction**

KUMAR, Sandeep[1]; Bande, Annika[1,2]

1: Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, DE 10409, Germany; 2: Leibniz University Hannover, Institute of Inorganic Chemistry, Hannover, DE 30167, Germany

Machine Learning in Chemistry

Mon 45 **Bringing Error Bars into Density Functional Theory**

Laqua, Henryk; Head-Gordon, Martin

UC Berkeley, United States of America

Electron Structure Theory - Method Development

Mon 46 **Decomposition of Magnetic Coupling in M-Oxo-Bridged Metal Complexes**

Krampe, Justin; Krewald, Vera

TU Darmstadt, Germany

Electron Structure Theory

Mon 47 **Ultrafast Excited-State Proton Transfer Dynamics of a Super-Photoacid in Non-Aqueous Solution**

Sülzner, Niklas[1,2]; Mattos, Rafael Souza[2]; Barbatti, Mario[2,3]

1: Ruhr-Universität Bochum, Bochum 44801, Germany; 2: Aix Marseille University, CNRS, ICR, Marseille 13397, France; 3: Institut Universitaire de France, Paris 75231, France

Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 48 **Ligand Non-Innocence in a Cobalt CO2RR Catalyst: MR Insights**

Gerndt, Leon; Roemelt, Michael

Humboldt Universität zu Berlin, Germany

Electron Structure Theory - Reaction Mechanisms and Catalysis

Mon 49 **Calculation of State-Averaged Nuclear Gradients for Large Active Spaces with Implicit Solvation and Screened Potentials**

Woite, Philipp; Roemelt, Michael

Humboldt Universität zu Berlin, Germany

Method Development

Mon 50 **Extending the Tool Set for Excited States in Solids — From Static Excited-State Properties to Non-Adiabatic Molecular Dynamics**

Hehn, Anna

Christian-Albrechts-Universität Kiel, Germany

Electron Structure Theory - Molecular Dynamics and Simulation - Spectroscopy and Properties - Method Development - Materials and Solid-State Theory

Mon 51 **Machine-Learned Intrinsic Coordinates for Vibrational Calculations**

Yachmenev, Andrey[1,3]; Saleh, Yahya[2,3]; Fernández Corral, Álvaro[3]; Vogt, Emil[3]; Iske, Armin[2]; Küpper, Jochen[3]

1: University of Stuttgart, Institute for Theoretical Chemistry, Germany; 2: Department of Mathematics, Universität Hamburg, Germany; 3: Center for Free-Electron Laser Science, DESY, Hamburg, Germany

Machine Learning in Chemistry - Spectroscopy and Properties - Method Development

Mon 52 **Shaping Ground- and Excited-State Energy Landscapes through Solvation and Pressure**

Pausch, Ansgar

Vrije Universiteit Amsterdam, The Netherlands

Electron Structure Theory - Spectroscopy and Properties - Method Development

Mon 53 **When Water Drives Self-Assembly: Thermodynamic Insights from Small Molecules**

Froböse, Nikolas; Keller, Bettina

Freie Universität Berlin, Germany

Molecular Dynamics and Simulation - Method Development

Mon 54 **Automated and Efficient Exploration of Intermolecular Interactions: The Docker and Solvator Tools**
Plett, Christoph; de Souza, Bernardo; Neugebauer, Hagen; Bursch, Markus
FACCTs GmbH, Germany
Method Development - Reaction Mechanisms and Catalysis - Biochemical Systems

Mon 55 **Going Beyond the Global Minimum Approach: Modelling Molecular Kinetics with Thousands of Isomers**
Schöpfer, Gabriel[1]; Salzburger, Magdalena[1]; O'Neill, Olivia[2]; van der Linde, Christian[1]; Beyer, Martin K.[1]; Ončák, Milan[1]
1: Institute for Ion Physics and Applied Physics, University of Innsbruck, Austria; 2: Department of Chemistry, University of Oxford, United Kingdom
Method Development

Mon 56 **A General and Minimally Empirical Implicit Solvation Model from First Principles**
Wittmann, Lukas; Grimme, Stefan
Mulliken Center for Theoretical Chemistry, University of Bonn, Beringstraße 4, 53115 Bonn, Germany
Method Development

Mon 57 **Unpolarized Cavities for QED-Coupled-Cluster Calculations**
Monzel, Laurenz[1]; Stopkowicz, Stella[1,2]
1: Saarland University, Germany; 2: Hylleraas Centre for Quantum Molecular Sciences, Norway
Electron Structure Theory - Method Development

Mon 58 **Long-Range Intermolecular Interactions Involving Excited States of Benzene**
Leson, Judith M.; Jansen, Georg
University of Duisburg-Essen, Germany
Electron Structure Theory - Spectroscopy and Properties

Mon 59 **The Electronic Ground State Term of the Group 14 Monofluoride Molecules: A Spin-Orbit Coupling Study**
Pantescu-Lucazeau, Julien[1,2]; Andrae, Dirk[2]
1: École Normale Supérieure de Lyon, Lyon, France; 2: Freie Universität Berlin, Institut für Chemie und Biochemie, Germany
Electron Structure Theory - Spectroscopy and Properties

Mon 60 **Dissociative Photoionization of 2-Thiouracil and 4-Thiouracil: A Molecular Dynamics Study**
Roy, Bonasree[1]; Titov, Evgenii[1]; Robinson, Matthew S.[2]; Gühr, Markus[3,4]; Saalfrank, Peter[1]
1: Theoretical Chemistry, Institute of Chemistry, University of Potsdam, Germany; 2: European XFEL, Holzkoppel 4, 22869 Schenefeld, Germany; 3: Deutsches Elektronen-Synchrotron (DESY), Notkestraße 85, 22607 Hamburg, Germany; 4: Institute of Physical Chemistry, University of Hamburg, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties - Biochemical Systems

Mon 61 **Field-Dependent NMR Shifts in Paramagnetic Molecules: Theory and Interpretation**
Lang, Lucas
Institut für Chemie, Technische Universität Berlin, Straße des 17. Juni 135, 10623 Berlin, Germany
Spectroscopy and Properties

Mon 62 **Simulating Deep Eutectic Electrolytes Using Machine-Learned Interatomic Potentials**
Shayestehpour, Omid
Paderborn University, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Materials and Solid-State Theory

Mon 63 **Simulations of Liquid Metal Catalyst Interfaces with Machine-Learned Interatomic Potentials**
Steffen, Julien; Mölkner, Andreas; Bechtel, Maximilian; Görling, Andreas
Friedrich-Alexander-Universtität Erlangen-Nürnberg, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Materials and Solid-State Theory

Mon 64 **Overcoming DFT'S Limitations: New Developments in N- and H-Representability for Accurate Strong Correlation in RDMFT**
Erhard, Jannis
Mc Master University, Canada
Electron Structure Theory - Method Development

Mon 65 **Beyond AIMD: Exploring Multiscale Ion Transport with Traditional and Machine-Learned Models**
Dreßler, Christian
Theoretical Solid State Physics, TU Ilmenau, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Mon 66 **Modelling Exciton Dynamics in Multiphotochromic Systems**
Titov, Evgenii
Universität Potsdam, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 67 **Exploring Chemistry and Catalysis by Biasing Skewed Distributions via Deep Learning**
Zhang, Zhikun[1]; Leonard, Kai[1]; Piccini, GiovanniMaria[2]
1: RWTH Aachen University, Germany; 2: University of Modena and Reggio Emilia, Italy
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Mon 68 **Effective Electron-Vibration Coupling by Ab Initio Methods**
Dorfner, Maximilian F.X.; Ortmann, Frank
TUM School of Natural Sciences, Atomistic Modeling Center, Munich Data Science Institute, Technische Universität München, Germany
Electron Structure Theory

Mon 69 **DFT Based Support for the Design of Organic Radical Polymer-Based Batteries**
Achazi, Andreas J.[1]; Mollenhauer, Doreen[1,2,3]
1: HIPOLE Jena (Helmholtz Institute for Polymers in Energy Applications Jena), Lessingstrasse 12-14, 07743 Jena, Germany; 2: Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), 14109 Berlin, Germany; 3: Institute for Technical and Environmental Chemistry, Friedrich Schiller University Jena, 07743 Jena, Germany
Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Mon 70 **Linear-Scaling DLPNO-MP2 for Periodic Systems**
Nejad, Arman; Zhu, Andrew; Sorathia, Kesha; Tew, David
University of Oxford, United Kingdom
Electron Structure Theory - Method Development - Materials and Solid-State Theory

Mon 71 **Spin-Flip Time-Dependent Density Functional Theory Within the Sternheimer Formalism**
Hernandez Segura, Luis Ignacio; Luber, Sandra
University of Zurich, Switzerland
Electron Structure Theory - Spectroscopy and Properties - Method Development

Mon 72 **A Novel Constraint-Based Orbital-Optimized Excited State Method**
Kussmann, Jörg; Lemke, Yannick; Ochsenfeld, Christian
University of Munich (LMU), Germany
Electron Structure Theory - Spectroscopy and Properties - Method Development

Mon 73 **ESPECDAS: A Database of Electronic Transitions from Automated Multireference Calculations for Identifying Potential Carriers of Diffuse Interstellar Bands**
Gatt, Michael; Reimann, Marc; Schöpfer, Gabriel; Ončák, Milan
Universität Innsbruck, Austria
Spectroscopy and Properties

Mon 74 **Reducing the Cost of Excited State MD: Extrapolation for Excited States in a Linear Response TD-DFT Formalism.**
Nottoli, Michele; Stamm, Benjamin
Universität Stuttgart, Germany
Electron Structure Theory - Molecular Dynamics and Simulation - Method Development

Mon 75 **Ultrafast Dynamics of Multi-Mode Multi-State Molecular Quantum Systems Coupled to a Dissipative Environment**
Picconi, David
Heinrich-Heine-Universität Düsseldorf, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties - Method Development

Mon 76 **Community-Driven and Systematic Benchmarks to Advance and Democratize Nonadiabatic Molecular Dynamics**
Ibele, Lea
CNRS/Aix Marseille University, France
Molecular Dynamics and Simulation

Mon 77 **Towards Ab Initio Simulation of in Situ/Operando Raman Spectroscopy: Application to Sulfur/Carbon Copolymer Cathodes for Li-S Batteries**
Kiani, Rana[1]; Sheng, Huiying[2]; Held, Timo[1]; Löhmann, Oliver[2]; Risse, Sebastian[2]; Sebastiani, Daniel[1]; Partovi-Azar, Pouya[1]
1: Institut für Chemie, Martin-Luther-Universität Halle-Wittenberg, Germany; 2: Department for Electrochemical Energy Storage, Helmholtz-Zentrum Berlin für Materialien und Energie
Molecular Dynamics and Simulation - Spectroscopy and Properties - Method Development

Mon 78 **The Free Energy Landscape of Flexible Molecules – Interaction Tensor Driven MD Simulations Break the Former Computational Limitations**
Sternberg, Ulrich[1,2]
1: COSMOS Software GbR Jena, Germany; 2: Research Partner of Karlsruhe Institute of Technology (INT)
Molecular Dynamics and Simulation - Spectroscopy and Properties - Method Development - Biochemical Systems

Mon 79 **Benchmarking Electrical Properties of Transition Metal Oxides Using Various Functionals**
Öztürk, Aykut; Kraus, Peter
TU-Berlin/Institute of Materials Science and Technology, Germany
Electron Structure Theory - Materials and Solid-State Theory

Mon 80 **Robust Estimation of Position-Dependent Diffusivities from Biased Molecular Simulations**
von Domaros, Michael[1]; Thomas, Rinto[1]; Prabhakar, Praveen Ranganath[2]
1: Philipps-Universität Marburg, Germany; 2: University of California, Irvine, USA
Molecular Dynamics and Simulation - Method Development - Biochemical Systems

Mon 81 **Simulating the Human TFF1 Protein under Reducing Conditions**
Elmaci, Dilsah Nur[1]; Hopping, Gene[2]; Hoffmann, Werner[3]; Muttenthaler, Markus[2]; Stein, Matthias[1]
1: Max Planck Institute for Dynamics of Complex Technical Systems, Germany; 2: The University of Queensland, Australia; 3: Medical Faculty, Otto von Guericke University Magdeburg, Germany
Biochemical Systems

Mon 82 **Data-Driven Discovery of Metal-Organic Framework Catalysts for Small Molecule Conversions**
Das, Shubhajit[1]; Corminboeuf, Clemence[2]; Heine, Thomas[1]
1: TU Dresden, Germany; 2: Ecole Polytechnique Fedéralé de Lausanne (EPFL), Switzerland
Machine Learning in Chemistry - Reaction Mechanisms and Catalysis

Mon 83 **Pisa Composite Scheme Meets Generalized Internal Coordinates and Effective Gradients for Accurate Equilibrium Structures of Large Molecules at Reduced Cost**
Crisci, Luigi
Scuola Superiore Meridionale, Italy
Electron Structure Theory - Spectroscopy and Properties - Method Development

Mon 84 **Advancing the Exploration of Potential Energy Surfaces: Integrating on-the-Fly Machine Learning of Ab Initio Energies in MD Simulations and Evolutionary Global Optimization**
Dononelli, Wilke
Universität Bremen, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Mon 85 **Efficient Fitting of Multi-Dimensional Potential Energy Surfaces Using Bayesian Optimization**
Viswanathan, Narasimhan[1]; Thiele, Lennart[2]; Leonhard, Kai[3]
1: Institute of Technical Thermodynamics, RWTH Aachen, Germany; 2: Institute of Technical Thermodynamics, RWTH Aachen, Germany; 3: Institute of Technical Thermodynamics, RWTH Aachen, Germany
Machine Learning in Chemistry - Method Development

Mon 86 **Biasing the Mutational Landscape in Enzymes by Simulation of the Catalysed Reaction Mechanism**
Platero-Rochart, Daniel; Mandl, Spela; Sánchez Murcia, Pedro A
Laboratory of Computer-Aided Molecular Design, Division of Medicinal Chemistry, Otto-Loewi Research Center, Medical University of Graz, Austria
Reaction Mechanisms and Catalysis - Biochemical Systems

Mon 87 **Investigating Mechanism of Action of Microvionin by Computational Approaches.**
Unmesh, Krithika; Strätker, Melissa; Mainz, Andi; Mroginski, Maria Andrea; Süssmuth, Roderich
Technical University of Berlin, Germany
Molecular Dynamics and Simulation

Mon 88 **Intrinsic Dimensionality of Molecular Properties**
Banjafar, Ali; von Rudorff, Guido
University of Kassel, Germany
Machine Learning in Chemistry - Method Development

Mon 89 **Enhanced and Selective Unidirectional Proton Transport via Covalent Benzenesulfonic Functionalized Graphene and Nafion/Graphene Interface**
Calvani, Dario[1,2]; Caisachana, Maria-Judith[2]; Eren, Ismail[2]; Buda, Francesco[4]; Schneider, Grégory F.[4]; Heine, Thomas[1,2,3]; Kuc, Agnieszka[1,2]
1: Center for Advanced Systems Understanding (CASUS), Germany; 2: Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany; 3: TU Dresden, Germany; 4: Leiden University, The Netherlands
Molecular Dynamics and Simulation - Materials and Solid-State Theory

Mon 90 **Representative Random Sampling of Chemical Space**
Monterrubio Chanca, Diego Javier; von Rudorff, Guido
University of Kassel, Germany
Machine Learning in Chemistry - Method Development

Mon 91 **Spin-Isomers of Molecular Hydrogen in Weakly Bound Complexes**
Hartwig, Beppo; Hasselhorn, Jannes; Obenchain, Daniel
Georg-August-Universität Göttingen, Germany
Spectroscopy and Properties

Mon 92 **Quantum and Semiclassical Rate Constants of Cl + CH4 and Isotopes**
Hoppe, Hannes[1,2]; Richardson, Jeremy O.[1]; Manthe, Uwe[2]
1: ETH Zürich, Switzerland; 2: Bielefeld University, Germany
Molecular Dynamics and Simulation - Method Development - Reaction Mechanisms and Catalysis

Mon 93 **G-xTB: General-Purpose Accuracy for Ground and Excited States with Extended Tight-Binding**
Froitzheim, Thomas; Müller, Marcel; Hansen, Andreas; Grimme, Stefan
University of Bonn, Germany
Electron Structure Theory - Method Development

Mon 94 **Understanding the Carbyne Formation from Acetylene Complexes**
Hartmann, Peter E.; Corovic, Miljan Z.; Ehweiner, Madeleine A.; Sbüll, Felix; Belaj, Ferdinand; Boese, A. Daniel; Mösch-Zanetti, Nadia C.
Universität Graz, Austria
Reaction Mechanisms and Catalysis

Mon 95 **Graph Diffusion Models for Back Mapping in Chemical Compound Space**
Vazquez-Salazar, Luis Itza; Bereau, Tristan
Institute for Theoretical Physics, Heidelberg University, Germany
Machine Learning in Chemistry - Method Development

Mon 96 **Theory of Radical Chain Reactions Applied to Hofmann–Löffler–Freytag Reaction**
Zubčić, Gabrijel; Vrček, Valerije; Šakić, Davor
Faculty of Pharmacy and Biochemistry, University of Zagreb, Zagreb, Croatia
Reaction Mechanisms and Catalysis

Mon 97 **Using Ab-Initio Simulations and Experimental 31P NMR Chemical Shifts for the Development of Improved Nucleic Acid – Metal Ion Force Fields**
Christanell, Leo; König, Karl-Jakob; Mavromatis, Petros; Zhao, Hongqing; Holzinger, Julian; Schütz, Anne; Fingerhut, Benjamin P.
Ludwig-Maximilians-Universität München, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties - Biochemical Systems

Mon 98 **Assignment of the Intramolecular Charge Transfer State in Carotenoids**
Jaschke, Constantin; Fingerhut, Benjamin P.
LMU Munich, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 99 **Two-Dimensional Carbon-Based Catalysts: Hydrogen Evolution at Covalent Organic Frameworks**
Penschke, Christopher
University of Potsdam, Germany
Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Mon 100 **Probing the Temporal Response of Liquid Water to a THz Pump Pulse Using Machine Learning Accelerated Non-Equilibrium Molecular Dynamics**
Schienbein, Philipp
Ruhr-Universität Bochum, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Spectroscopy and Properties

Mon 101 **Real-Time Simulations of Photoinduced Interfacial Electron Transfer**
Menzel, Jan Paul[1,2]; Batista, Victor[1,2]
1: Department of Chemistry, Yale University, New Haven, USA; 2: Yale Energy Sciences Institute, West Haven, USA
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Mon 102 **Noncollinear Density Functional Theory Made Simple**
Gaul, Konstantin
Helmholtz Institut, Johannes Gutenberg-Universität Mainz, Germany
Electron Structure Theory - Method Development

Mon 103 **Chemical Reaction Discovery with Periodic Boundary Conditions**
Meisner, Jan
Heinrich-Heine-Universität Düsseldorf, Germany
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Mon 104 **Computing the pKw of Water at Ambient and Extreme Conditions via Ab Initio Simulations**
Muñoz-Santiburcio, Daniel
Spanish Research Council (CSIC), Spain
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Mon 105 **Accurate and Mode-Resolved Modeling of Non-Radiative Decay in Donor-Functionalized Radical-Emitters**
Toews, Robert; Koehn, Andreas
Institut für Theoretische Chemie, Universität Stuttgart, Germany
Spectroscopy and Properties

Mon 106 **Combining Genetic Algorithms with Omits in Kinematical Refinements of cRED Data: Pathways Towards Higher Accuracy**
Feige, Alexander[1]; Hager, Paul[2]; Cho, Jungyoun[2]; Pacoste, Laura[2]; Zou, Xiaodong[2]; Westermayr, Julia[1,3]
1: Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, Leipzig University, Germany; 2: Department of Chemistry, Stockholm University, Sweden; 3: ScaDS.AI Leipzig, Germany
Machine Learning in Chemistry

Mon 107 **Treatments of Solvent Effects Including State-Specific Corrections in Photochemical Processes**
Schank, Lukas[1]; Stopkowicz, Stella[1,2]
1: Physikalische und Theoretische Chemie, Universität des Saarlandes, 66123 Saarbrücken, Germany; 2: Hylleraas Centre for Quantum Molecular Science, University of Oslo, 0315 Oslo, Norway
Spectroscopy and Properties - Method Development

Mon 108 **ReaxMD: Tracking Atoms in Reactive Molecular Dynamics**
Alvarez, Luis[1]; Büchel, Ralf[1]; Vogiatzis, Konstantinos[2]; Frank, Irmgard[1]
1: Leibniz Universität Hannover, Germany; 2: The University of Tennessee, USA
Molecular Dynamics and Simulation

Mon 109 **Enhancing Hydrogen Diffusion Simulations between MOS_2Layers via Machine-Learning-Accelerated Path-Integral Methods**
Eren, Ismail[1]; Erbil, Ege Yigit[2]; Caisachana-Lozada, Maria Judith[3]; Mir Hosseini, Seyed Hossein[1]; Kühne, Thomas D.[1]; Kuc, Agnieszka B.[1]
1: Helmholtz-Zentrum Dresden-Rossendorf, Center for Advanced Systems Understanding (CASUS), Conrad-Schiedt-Straße 20, 02826 Görlitz, Germany; 2: Koç University, Rumelifeneri Yolu 34450 Sarıyer, İstanbul, Türkiye; 3: Helmholtz-Zentrum Dresden-Rossendorf, Institute of Resource Ecology, Department of Reactive Transport, Permoserstraße 15, 04318 Leipzig, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Materials and Solid-State Theory

Mon 110 **Development of SC-NEVPT2 Methods with SCI Wave Functions**
Ugandi, Mihkel
HU Berlin, Germany
Electron Structure Theory

Mon 111 **Exciton-Type Analysis of Metal/Molecule Hybrids from First Principles**
Jahn, Nicolas; Titov, Evgenii
University of Potsdam, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 112 **Analytic G0W0 Gradients: An IP/EA-EOM-Λ-rCCD Reformulation**
Kitsaras, Marios-Petros[1]; Tölle, Johannes[2]; Loos, Pierre-François[1]
1: Laboratoire de Chimie et Physique Quantiques (UMR 5626), Universite de Toulouse, CNRS, Toulouse, France; 2: Department of Chemistry, University of Hamburg, 22761 Hamburg, Germany; The Hamburg Centre for Ultrafast Imaging (CUI), Hamburg 22761, Germany
Electron Structure Theory - Spectroscopy and Properties - Method Development

Mon 113 **GPU Acceleration in Quantum Chemistry Software Made Simple through a Modular C++ Linear Algebra Library**
Heezen, Mark; Steinbach, Pit; Bannwarth, Christoph
Institute of Physical Chemistry, RWTH Aachen University, Melatener Str. 20, Aachen 52074, Germany
Method Development

Mon 114 **When Bonds Resist Rotation: Automated Classification and Representation of Atropisomers in the MolBar Identifier**
van Staalduinen, Nils; Bannwarth, Christoph
RWTH Aachen, Germany
Machine Learning in Chemistry

7 Poster session on Wednesday (Sep. 24, 2025)

Instructions for Poster Presenters

Your poster number is given in the conference program. The format is "Day Number" (e.g. "Wed 22"). On the poster wall, only the number is shown (the day is not included). Mount your poster on the poster wall labeled with your number. Pins are provided at the poster wall.

- Posters can be put up starting **Wednesday, 24 September 2025, at 12:30 pm**.
- Please remove your poster again by **Thursday, 25 September 2025, at 11:00 am** (end of the coffee break).

Enjoy the poster session!

In lieu of an abstract

Instead of submitting an abstract, we asked poster presenters to assign their contribution to the following topics:

- Biochemical Systems
- Electronic Structure Theory
- Machine Learning in Chemistry
- Materials and Solid-State Theory
- Method Development
- Molecular Dynamics and Simulation
- Spectroscopy and Properties
- Reaction Mechanisms and Catalysis

In the program, each poster contribution is listed together with its assigned topic.

Posters

Wed 1 **Q-ADC(2): the Second-Order Algebraic Diagrammatic Construction Method for Electronic Excitations by Quadrature**
Papapostolou, Antonia; Dreuw, Andreas
Interdisciplinary Center for Scientific Computing, Heidelberg University, Germany
Electron Structure Theory - Method Development

Wed 2 **First Principle Investigation of Light Driven Hydrogen Evolution Reaction on Photochemical Molecular Devices**
Putra, Miftahussurur Hamidi[1]; Groß, Axel[1,2]
1: Institute for Theoretical Chemistry Ulm University, Germany; 2: Helmholtz Institute Ulm (HIU), Electrochemical Energy Storage, 89069 Ulm, Germany
Reaction Mechanisms and Catalysis

Wed 3 **Charge Transfer Dynamics for Model CO2 Reduction Reaction**
Koreš, Jan; Jíra, Tomáš; Slavíček, Petr
UCT Prague, Czech Republic
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Wed 4 **Computational Investigation of Gas Pollutants Adsorption on Copper Squarate**
Belasri, Abdessamad[1,2]; Dalbouha, Samira[2]; Bahmann, Hilke[1]
1: Department of Physical and Theoretical Chemistry, University of Wuppertal, Wuppertal, Germany; 2: Department of Chemistry, Faculty of Sciences Agadir, Ibn Zohr University, Agadir, Morocco
Materials and Solid-State Theory

Wed 5 **Jellyfish: Ab Initio Electron Dynamics by Traditional and Quantum Algorithms**
Krause, Pascal[1]; Piñeiro, Carlos A.[1]; Lee, Ka Hei[1,2]; Bande, Annika[1,2]
1: Institute of Inorganic Chemistry, Leibniz Universität Hannover, Germany; 2: Theory of Electron Dynamics and Spectroscopy, Helmholtz Zentrum Berlin, Germany
Molecular Dynamics and Simulation - Method Development

Wed 6 **Charge Parameterization of the Highly Phosphorylated Small Biomolecule IP6**
Laux, Johann Arthur; Keller, Bettina
Freie Universität Berlin, Germany
Molecular Dynamics and Simulation - Method Development - Biochemical Systems

Wed 7 **Calculation of EPR and pNMR Quantities with DFT and X2C**
Bruder, Florian; Franzke, Yannick; Weigend, Florian
Karlsruhe Institute of Technology, Germany
Electron Structure Theory - Spectroscopy and Properties - Method Development

Wed 8 **Multi-Kernel Learning for Data-Efficient Kernel Models**
Qureshi, Sana; Von Rudorff, Guido Falk
Universität Kassel, Germany
Machine Learning in Chemistry

Wed 9 **Modeling Hydroxide Ion Dynamics in Aqueous and Membrane Systems: Comparative Analysis of Classical and Machine-Learned Multiscale Methods**
Hänseroth, Jonas
Technische Universität Ilmenau, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Wed 10 **How to Navigate the Potential Energy Surface with Confidence?**
Alizadeh, Vahideh
Max Planck Institute for the Structure and Dynamics of Matter, Germany
Molecular Dynamics and Simulation - Method Development

Wed 11 **Modeling and Descriptor Based Analysis of High-Entropy Ceramics**
Er, Chen Chen[1,2]; Friedrich, Rico[1,2]
1: Technische Universität Dresden, Germany; 2: Institute of Ion Beams Physics and Materials Research, Helmholtz-Zentrum Dresden-Rossendorf, Germany
Materials and Solid-State Theory

Wed 12 **Computational Investigation of Photochemistry and Reactivity in Macrocyclic Diarylethene Photoswitches**
Schwarz, Denise[1]; Bösking, Tom[2]; Pauls, Mike[1]; Kolarski, Dusan[3]; Hecht, Stefan[2,4]; Bannwarth, Christoph[1]
1: RWTH Aachen University, Germany; 2: DWI - Leibniz Institute for Interactive Materials, Germany; 3: Max Planck Institute for Multidisciplinary Sciences, Germany; 4: Humboldt University of Berlin, Germany
Reaction Mechanisms and Catalysis

Wed 13 **SymbolicCI: An Ab Initio Framework for Modeling Biexcitons in Molecular Aggregates**
Adelsperger, Johannes E.[1]; de Graaf, Coen[2]; Röhr, Merle I. S.[1]
1: Uni Würzburg, Germany; 2: Universitat Rovira I Virgili, Spain
Electron Structure Theory - Method Development

Wed 14 **Towards a Dyson-Density Description of Charge-Transfer Excitons**
Staschick, Patrick[1]; Kaiser, Andy[1]; Kühn, Oliver[1]; Bokarev, Sergey[2]
1: University of Rostock, Institute of Physics, Germany; 2: Technical University of Munich, Chemistry Department, Germany
Electron Structure Theory

Wed 15 **Introducing Position Dependence of Exchange and Correlation Mixing into Double Hybrid Functionals: Local Double Hybrids and Doubly Local Double Hybrids**
Kovacs, Nora[1]; Śmiga, Szymon[2]; Kaupp, Martin[1]; Wodyński, Artur[1]
1: Technische Universität Berlin, Germany; 2: Nicolaus Copernicus University in Toruń
Electron Structure Theory - Machine Learning in Chemistry - Method Development

Wed 16 **Revealing Hidden Reaction Pathways in Electrochemical Interfaces Using Ab Initio Molecular Dynamics**
Zwarg, Tom-Luka; Meisner, Jan
Heinrich-Heine-Universität Düsseldorf, Germany
Molecular Dynamics and Simulation

Wed 17 **TurtleMap: Atom Mapping for Minimum Energy Path Search**
Lampe, Lukas; Mück-Lichtenfeld, Christian; Neugebauer, Johannes
University of Münster, Germany
Reaction Mechanisms and Catalysis

Wed 18 **From Methane to Methanol: Surface Design Strategies on WO3 Catalysts**
Carroll, Lenard Leslie; Paulus, Beate
Freie Universität Berlin, Germany
Reaction Mechanisms and Catalysis

Wed 19 **Characterization of Polymorphic Landscapes in Molecular Crystals**
Goncharova, Natalia; List, Alexander; Hoja, Johannes; Boese, A. Daniel
Department of Chemistry, University of Graz, 8010 Graz, Austria
Electron Structure Theory - Materials and Solid-State Theory

Wed 20 **Vibrational Spectroscopy of Water Confined Within C1N1 Bilayers**
Ojha, Deepak; Kühne, Thomas
CASUS Gorlitz, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 21 **Nonadiabatic Reaction Rates from Uniform Instanton Theory**
Krug, Simon León
ETH Zürich, Switzerland
Method Development - Reaction Mechanisms and Catalysis

Wed 22 **Engineering Π-Systems with BN Units: Excited-State Control Across BN-Doped PAHs and Photoswitches**
Bühler, Michael; Röhr, Merle I. S.
University Würzburg, Germany
Electron Structure Theory - Molecular Dynamics and Simulation

Wed 23 **Understanding Silicon and Silicon-Based Anodes for Lithium-Ion Batteries Using Molecular Dynamics Simulations.**
TIWARI, VISHWAS; Elgabarty, Hossam; Brehm, Martin
University of Paderborn, Germany
Molecular Dynamics and Simulation - Materials and Solid-State Theory

Wed 24 **Analytical Derivatives for Subsystem TDDFT**
Rikus, Anton; Neugebauer, Johannes
University of Münster, Organisch-Chemisches Institut and Center for Multiscale Theory and Computation (CMTC), Corrensstraße 36, 48149 Münster
Electron Structure Theory - Spectroscopy and Properties - Method Development

Wed 25 **Embedding Strategies and Self-Consistency in CASSCF-in-DFT Embedding**
Fischer, Leon; Neugebauer, Johannes
University of Münster, Organisch-Chemisches Institut and Center for Multiscale Theory and Computation (CMTC), Corrensstraße 36, 48149 Münster, Germany
Electron Structure Theory - Method Development

Wed 26 **Enhanced Conformer Ensemble Processing for Improved NMR Spectrum Prediction**
Hodecker, Manuel; Covito, Fabio; Shirazi, Reza G.; Pinski, Peter
HQS Quantum Simulations, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 27 **A 100,000-Fold Increase in C-H Bond Acidity Gives Palladium a Key Advantage in C(SP3)-H Activation Compared to Nickel**
Schramm, Tim Karl[1]; Lin, Lirong[2]; Kucheryavy, Pavel[2]; Lalancette, Roger A.[2]; Hansen, Andreas[1]; Prokopchuk, Demyan E.[2]
1: Mulliken Center for Theoretical Chemistry, University of Bonn, Germany; 2: Department of Chemistry, Rutgers University-Newark, United States
Electron Structure Theory - Reaction Mechanisms and Catalysis

Wed 28 **Distinguishing between Cavity and Non-Cavity Solvation Structures of the Hydrated Electron Using Ab Initio Molecular Dynamics Simulations with a Hybrid Meta-Density Functional**
Ho, Sy Dat; Fingerhut, Benjamin P.
Ludwig-Maximilians-Universität München
Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 29 **Implementation of Girsanov Reweighting in CP2K**
Jähnigen, Sascha; Keller, Bettina
Freie Universität Berlin, Germany
Molecular Dynamics and Simulation

Wed 30 **Accelerating JEDI: Real-Time Strain Energy Mapping for Interactive Exploration of Molecular Strain**
Weiß, Rahel[1]; Plump, Annelene[1]; Neudecker, Tim[1,2,3]
1: Institute for Physical and Theoretical Chemistry, University of Bremen; 2: Bremen Center for Computational Materials Science, University of Bremen; 3: MAPEX Center for Materials and Processes, University of Bremen
Method Development

Wed 31 **Cracking Allostery with Free Energy Landscapes**
Finn, Lauren
Freie Universität Berlin, Germany
Molecular Dynamics and Simulation - Biochemical Systems

Wed 32 **(Non-)Linear Optical Properties of Unsubstituted Adamantane**
Nizovtsev, Anton[1,2,3]; Mollenhauer, Doreen[1,2,3]
1: HIPOLE Jena, Germany; 2: Institute of Physical Chemistry, Justus-Liebig University Giessen, Germany; 3: Center for Materials Research (LaMa), Justus-Liebig University Giessen, Germany
Spectroscopy and Properties

Wed 33 **A Benchmark Study of the Theoretical Parameters Governing Hyperfine Coupling Constant Calculations**
Hendrix, Jenna; Klüner, Thorsten
Carl von Ossietzky Universität Oldenburg, Germany
Electron Structure Theory - Spectroscopy and Properties

Wed 34 **Assessing the Role of Accurate Potential Energy Surfaces in Conformational Sampling: A Benchmark Study**
Zurek, Christopher; Bannwarth, Christoph
RWTH Aachen University, Germany
Molecular Dynamics and Simulation - Method Development

Wed 35 **Atomistic Insights into Hybrid Nanosystems**
Schaefer, Karen[1,2]; Liu, Chih-Yin[1]; Bhattacharjee, Yudhajit[3]; Schlicke, Hendrik[3]; Vossmeyer, Tobias[1]; Herrmann, Carmen[1,2]
1: University of Hamburg, Germany; 2: The Hamburg Centre for Ultrafast Imaging (CUI), Germany; 3: Leibniz Institute of Polymer Research Dresden
Molecular Dynamics and Simulation

Wed 36 **Intermolecular Interactions of Propeller-Twisted Watson-Crick Base Pairs**
Buchwald, Andrea; Fink, Reinhold F.
University Tuebingen, Germany
Biochemical Systems

Wed 37 **Why Active Space Matters: Conical Intersections in DNA/RNA**
Cuéllar-Zuquin, Juliana; Segarra-Martí, Javier
Instituto de Ciencia Molecular, Universitat de València
Electron Structure Theory

Wed 38 **An Ontology for Theoretical Chemistry**
Wolter, Mario; Jacob, Christoph R.
Technische Universität Braunschweig, Institute of Physical and Theoretical Chemistry, Germany
Machine Learning in Chemistry - Method Development

Wed 39 **Photocatalytic Activity of Ion-Exchanged in Poly(Heptazine Imide) Materials by GW Method**
Hajiahmadi, Zahra; D. Kühne, Thomas
HZDR-CASUS, Germany
Electron Structure Theory - Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Wed 40 **Benchmarking Locally Range Separation Functionals for Excited State Properties**
Esquivel Curichimba, Jeyson; Bahmann, Hilke
Bergische Universität Wuppertal, Germany
Spectroscopy and Properties - Method Development

Wed 41 **Ultrafast Electron Chirality Flips in the Triatomic Molecule NSF**
Haase, Dietrich[1]; Manz, Jörn[1]; Paulus, Beate[1]; Scherlitzki, Jonathan[1]; Tremblay, Jean-Christophe[2]
1: Freie Universität Berlin, Germany; 2: CNRS-Université de Lorraine, France
Electron Structure Theory - Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 42 **Exploring the Energy Landscapes of Adaptable and Knotted Metal-Organic Cages**
Teeuwen, Paula[1]; Xu, Houyang[1]; Yang, Yuchong[1]; Pracht, Philipp[1]; Zucchelli, Simone[2]; Posocco, Paola[2]; Wales, David[1]; Nitschke, Jonathan[1]
1: Yusuf Hamied Department of Chemistry, University of Cambridge, Cambridge, United Kingdom; 2: Department of Architecture and Engineering, University of Trieste, Trieste, Italy
Reaction Mechanisms and Catalysis

Wed 43 **pH Dependent Reaction Networks from Ab Initio Nanoreactor Simulations**
Werner, Ben A.[1]; Kopp, Wassja A.[1]; Welz, Oliver[2]; Gorges, Maike[2]; Deglmann, Peter[2]; Meisner, Jan[1]
1: Heinrich-Heine-Universität Düsseldorf, Germany; 2: BASF SE, Ludwigshafen, Germany
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Wed 44 **Developing Orbital-Dependent Corrections for the Non-Additive Kinetic Energy in Subsystem Density Functional Theory**

Eitelhuber, Larissa S.; Artiukhin, Denis G.

Freie Universität Berlin, Germany

Method Development

Wed 45 **Modeling Pressure-Induced Changes in the Raman Spectra of Water Clusters Using X-HCFF**

Kißing, Nico[1]; Neudecker, Tim[1,2,3]

1: University of Bremen, Institute for Physical and Theoretical Chemistry, Leobener Straße 6, D-28359 Bremen, Germany; 2: Bremen Center for Computational Materials Science, University of Bremen, am Fallturm 1, D-28359 Bremen, Germany; 3: MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, D-28359 Bremen, Germany

Molecular Dynamics and Simulation - Spectroscopy and Properties - Method Development

Wed 46 **Nuclear-Electronic Orbital Frozen-Density Embedding**

Artiukhin, Denis

Freie Universität Berlin, Germany

Electron Structure Theory - Method Development

Wed 47 **Multiscale Computational Analysis of Fluorinated 2D Materials for PFAS Detection**

Camargo Diaz, Javier; Paulus, Beate

FU Berlin, Germany

Electron Structure Theory - Materials and Solid-State Theory

Wed 48 **Reaction Discovery in Porous Materials Using Periodic Nanoreactor Molecular Dynamics**

Deißenbeck, Daniel[1]; Meier, Patrick[1]; Kopp, Wassja A.[1]; Debellis, Anthony D.[2]; Meisner, Jan[1]

1: Institute for Physical Chemistry, Heinrich-Heine-Universität Düsseldorf, Germany; 2: BASF Corporation, 540 White Plains Road, Tarrytown, New York 10591, United States

Molecular Dynamics and Simulation - Method Development - Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Wed 49 **Modal Backflow Neural Quantum State for Anharmonic Vibrational Calculations**

Ding, Lexin; Reiher, Markus

ETH Zurich, Switzerland

Machine Learning in Chemistry - Spectroscopy and Properties - Method Development

Wed 50 **A Memory-Efficient Reformulation of ADC(4)**

Müller, Adrian J.; Rehn, Dirk R.; Dreuw, Andreas

Interdisciplinary Center for Scientific Computing, Heidelberg University, Germany

Electron Structure Theory - Method Development

Wed 51 **Determination of the Ka and Kc Quantum Numbers in Rovibrational Spectroscopy for Different Orientations of the Molecule**

Das, Subhasish; Rauhut, Guntram

Universität Stuttgart, Germany

Spectroscopy and Properties

Wed 52 **Low-Rank Representation of Two-Electron Integrals: Applications in Molecular Systems**

Paulicks, Niklas[1]; Tölle, Johannes[1,2]

1: Department of Chemistry, University of Hamburg, 22761 Hamburg, Germany; 2: The Hamburg Centre for Ultrafast Imaging (CUI), Hamburg 22761, Germany

Electron Structure Theory

Wed 53 **The Merits and Pitfalls of Molecule-Specific Semiempirical Parametrization by Machine Learning**

Baltruschat, Philipp; Herrmann, Carmen; Deffner, Michael

University of Hamburg, Germany

Machine Learning in Chemistry

Wed 54 **Molecular Excitons and Plasmons in Acenes and Their Radical Cations**

Weidlich, Anna Marleen; Dreuw, Andreas

Interdisciplinary Center for Scientific Computing Heidelberg, Germany

Spectroscopy and Properties

Wed 55 **Investigations into Radical MOST Systems**

Pauly, Sebastian

Universität Heidelberg, Germany

Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 56 **Efficient Implementation of Analytical Raman Intensities in ORCA**
Pikulová, Petra; Neese, Frank
MPI für Kohlenforschung, Germany
Spectroscopy and Properties - Method Development

Wed 57 **Probing Chiral Spin Dynamics with Time-Resolved Photoelectron Circular Dichroism: A First-Principles Approach**
Pototschnig, Ulrich; Herrmann, Carmen
University of Hamburg, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 58 **Electron Spin Decoherence of Molecular Spin Qubits in Nuclear Spin Baths**
Suchaneck, Sarah; Tesi, Lorenzo; Köhn, Andreas
University of Stuttgart
Molecular Dynamics and Simulation

Wed 59 **Investigating the Electronic Structure of Lanthanoid Trifluorides Using X-Ray Spectroscopy and First Principle Methods**
Goeritz, Fabian
FU Berlin, Germany
Materials and Solid-State Theory

Wed 60 **Quantum Chemical Study of Possible Reaction Pathways between IO and CH3OO**
Kalinicenko, Michelle; Eisfeld, Wolfgang
University Bielefeld, Germany
Electron Structure Theory - Reaction Mechanisms and Catalysis

Wed 61 **Computing Bulk Phase IR Spectra from Finite Cluster Data via Equivariant Neural Networks**
Jindal, Aman; Schienbein, Philipp; Das, Banshi; Marx, Dominik
Ruhr University Bochum, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry

Wed 62 **Ab Initio 2D IR Spectroscopy for Histidine-Containing Cu(II)-Peptide Complexes**
Chekmeneva, Maria; van Bodegraven, Anna Maria; Jacob, Christoph R.
TU Braunschweig, Germany
Spectroscopy and Properties - Method Development

Wed 63 **Gradients in Polaritonic and Field-Dependent Coupled Cluster Theory**
Harrer, Christoph[1]; Monzel, Laurenz[1]; Stopkowicz, Stella[1,2]
1: Department of Chemistry, Saarland University, Campus B2.2, D-66123 Saarbrücken, Germany; 2: Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo, P.O. Box 1033, Blindern N-0315, Oslo, Norway
Electron Structure Theory - Method Development

Wed 64 **On the Structural and Electronic Properties of N-Heterotriangulene Derivatives on Metal Surfaces**
Popko, Christoph; Amirjalayer, Saeed
IWR Heidelberg University, Germany
Materials and Solid-State Theory

Wed 65 **Molecular Properties Employing ADC(2/1+)**
Schneider, Friederike; Rehn, Dirk R.; Dreuw, Andreas
Interdisciplinary Center for Scientific Computing, Universität Heidelberg, im Neuenheimer Feld 205, 69120 Heidelberg, Germany
Spectroscopy and Properties - Method Development

Wed 66 **Automatic Code and Equation Generation with ADCGen**
Leitner, Jonas; Dittmer, Linus B.; Dempwolff, Adrian L.; Dreuw, Andreas
Interdisciplinary Center for Scientifiy Computing, Ruprecht-Karls Universiy, Germany
Method Development

Wed 67 **Modeling Electronic Processes in Open-Shell Molecules Using ADC**
Dempwolff, Adrian L.[1]; Alexandru, Marcus[1]; Trofimov, Alexander B.[2,3]; Dreuw, Andreas[1]
1: Interdisciplinary Center for Scientific Computing, Heidelberg University, Germany; 2: Laboratory of Quantum Chemistry, Irkutsk State University, Karl Marx Street 1, 664003 Irkutsk, Russia; 3: A. E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences, 1 Favorsky Street, 664033 Irkutsk, Russia
Electron Structure Theory - Spectroscopy and Properties - Method Development

Wed 68 **Uncertainty-Aware Prediction of Experimental Free Solvation Energies**
Meßler, Alexander; Bahmann, Hilke
University of Wuppertal, Germany
Machine Learning in Chemistry

Wed 69 **A Many-Electron Perspective on Aromaticity: Investigating Delocalization Using Probability Density Analysis**
Schulz, Hannah L.; Heinz, Michel V.; Lüchow, Arne
RWTH Aachen University, Germany
Electron Structure Theory

Wed 70 **Enabling OF-DFT with Machine Learning**
Kaczun, Tobias; Remme, Roman; Ebert, Tim; Gehrig, Christof A.; Geng, Dominik; Gerhartz, Gerrit; Ickler, Marc K.; Klockow, Manuel V.; Lippmann, Peter; Schmidt, Johannes S.; Wagner, Simon; Hamprecht, Fred A.; Dreuw, Andreas
IWR, Heidelberg University, Germany
Electron Structure Theory - Machine Learning in Chemistry - Method Development

Wed 71 **Speeding up Convergence with Subspace Diagonalization: A Novel Approach for Dense-Sparse Quantum Monte Carlo for Second Order Algebraic Diagrammatic Construction**
Kulahlioglu, Adem Halil; Dreuw, Andreas
Heidelberg University, IWR, Germany
Electron Structure Theory - Method Development

Wed 72 **Breaking down Charge Transport: A New DFTB Pseudoatom-Based Fragmentation Strategy**
Mächtel, Kevin
KIT, Germany
Molecular Dynamics and Simulation - Method Development

Wed 73 **Uncertainty Sampling as an Enhanced Molecular Sampling Technique**
Schmidt, Pascal
Karlsruhe Institute of Technology, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Wed 74 **Quantifying Hydrogen Isotope Effects in Chemical Bonding**
kehelwalathenne, Siyara; Tonner-Zech, Ralf
University of Leipzig, Germany
Electron Structure Theory

Wed 75 **JediAtoms: A Quantum Chemical Analysis Tool for the Investigation of Atomic Strain in Systems under Deformation**
Breier, Marvin[1]; Dononelli, Wilke[1,2,3]; Neudecker, Tim[1,2,3]
1: Institute for Physical and Theoretical Chemistry, University of Bremen; 2: Bremen Center for Computational Materials Science, University of Bremen; 3: MAPEX Center for Materials and Processes, University of Bremen
Method Development

Wed 76 **Exchange-Repulsion Forces in Dimers of Substituted Benzene**
Rahmouni, A.[1]; Fink, R. F.[2]; Sekkal-Rahal, M.[3]; Thelen, M.[2]; Henrichsineyer, J.[2]; Buchwald, A.[2]; Berriah, F. Z.[1]; Dellas, F. Z.[1]; Doumi, C.[1]; Hamidat, M.[1]
1: University of Saida, Algeria; 2: University of Tübingen; 3: University of Sidi Bel Abbes, Algeria
Electron Structure Theory - Spectroscopy and Properties

Wed 77 **Molecules in Quantum Solids: Protonated Methane in Para-Hydrogen Matrices**
Arandhara, Mrinal; Forbert, Harald; Marx, Dominik
Ruhr-University Bochum, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 78 **A High-Throughput Generative Workflow for Data-Driven Reaction Environment Optimization**
Curth, Robin[1,2]; Barrett, Rhyan[1]; Westermayr, Julia[1,2]
1: Wilhelm Ostwald Institute for Physical and Theoretical Chemistry, Leipzig University, Linnéstraße 2, 04103 Leipzig; 2: Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI) Dresden/Leipzig, Humboldtstraße 25, 04105 Leipzig
Machine Learning in Chemistry - Reaction Mechanisms and Catalysis

Wed 79 **Dispersion-Controlled Excited-State Dynamics of Azobenzenes**
Oberhof, Nils[1]; Saßmannshausen, Torben[2]; Strauss, Marcel A.[3]; Slavov, Chavdar[4]; Wegner, Hermann A.[3]; Wachtveitl, Josef[2]; Dreuw, Andreas[1]
1: Heidelberg University /IWR, Germany; 2: Goethe University Frankfurt /IPTC, Germany; 3: Justus Liebig University Giessen /Institute of Organic Chemistry & LaMa/ZfM, Germany; 4: University of South Florida / Department of Chemistry, USA
Molecular Dynamics and Simulation - Spectroscopy and Properties

Wed 80 **Enhancing the XAS-3DTM Dataset with TDDFT for XAS Prediction with Graph Neural Networks**
Karimi Nejad, Sara; Bande, Annika
Leibniz University Hannover, Germany
Machine Learning in Chemistry

Wed 81 **Quantum-Chemical Investigation of Dual Light- and pH-Responsive Molecular Systems by Coupled Stimuli**

Käfer, Sabine[1,2]; Baumert, Sebastian[1]; Dünnebacke, Torsten[1]; Hochstädt, Sebastian[3]; Linke, Walter Robert[3]; Hansen, Michael Ryan[3]; Fernández, Gustavo[1]; Neugebauer, Johannes[1,2]

1: University of Münster, Institute of Organic Chemistry, Corrensstraße 36, 48149 Münster, Germany; 2: University of Münster, Center for Multiscale Theory and Computation (CMTC), Corrensstraße 40, 48149 Münster, Germany; 3: University of Münster, Institute of Physical Chemistry, Corrensstraße 28/30, 48149 Münster, Germany

Electron Structure Theory - Reaction Mechanisms and Catalysis

Wed 82 **From Cyclohexane to PMMA: Environment-Dependent TADF Properties**

Kremper, Jennifer[1,2]; Weingart, Oliver[2,3]; Meisner, Jan[1]

1: Institute for Physical Chemistry, Heinrich-Heine-Universität Düsseldorf, Germany; 2: Institute for Theoretical and Computational Chemistry, Heinrich-Heine-Universität Düsseldorf, Germany; 3: Center for Information and Media Technology, Heinrich-Heine-Universität Düsseldorf, Germany

Spectroscopy and Properties - Method Development - Materials and Solid-State Theory

Wed 83 **Projection-Based Embedding Theory for CO2 Reduction Intermediates on Cu(111)-Clusters**

Kolodzeiski, Elena; Stein, Christopher J.

TU Munich, Germany

Electron Structure Theory - Method Development - Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Wed 84 **How Good Can Tight-Binding Approaches Be for Simple Electrolyte Solutions?**

Nikolaeva, Tatiana[1]; Kulik, Heather[2]; Stein, Christopher[1]

1: Technical University of Munich, School of Natural Sciences, Lichtenbergstr. 4, D-85748 Garching, Germany; 2: Massachusetts Institute of Technology, Department of Chemical Engineering and Department of Chemistry, Cambridge, Massachusetts 02139, United States

Electron Structure Theory - Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Wed 85 **Towards a Knowledge Graph for Mathematical Models and Algorithms: Application to Surface Hopping Trajectories**

Schmidt, Burkhard; Shehu, Aurela; Tabelow, Karsten; Koprucki, Thomas

Weierstraß-Institut, Berlin, Germany

Machine Learning in Chemistry

Wed 86 **Insights into Enantioselective, Energy-Transfer-Enabled Photocatalytic Reactions - A Case Study**

Wiegmann, Thorben[1,2]; Mück-Lichtenfeld, Christian[1,2]; Neugebauer, Johannes[1,2]

1: Institute for Organic Chemistry, University of Münster, Corrensstraße 36, 48149 Münster, Germany; 2: Center for Multiscale Theory and Computation (CMTC), University of Münster, Corrensstraße 36, 48149 Münster, Germany

Electron Structure Theory - Reaction Mechanisms and Catalysis

Wed 87 **Benchmarking Static Hyperpolarizabilities of Molecular Chains and the Response of Their Exchange–Correlation Potentials to Electric Fields**

Mandalia, Raviraj[1]; Trushin, Egor[1,2]; Fauser, Steffen[1]; Görling, Andreas[1,2]

1: Chair of Theoretical Chemistry FAU, Germany; 2: Erlangen National High Performance Computing Center (NHR@FAU), Germany

Electron Structure Theory - Method Development

Wed 88 **Excited-State Dynamics of Transition Metal Complexes**

Rezk, Hamada[1]; Bokareva, Olga S.[2]; Kühn, Oliver[3]

1: Institute of Physics, University of Rostock and Leibniz Institute for Catalysis, Rostock, Germany; 2: Institute of Chemistry, University of Rostock and Leibniz Institute for Catalysis, Rostock, Germany; 3: Institute of Physics, University of Rostock, Rostock, Germany

Spectroscopy and Properties

Wed 89 **An Automated Intermolecular Reaction Discovery Approach Relying on Heuristic Atom-Partitioned Frontier Orbital Features**

Chen, Ying; Bannwarth, Christoph

RWTH Aachen, Germany

Electron Structure Theory

Wed 90 **Designing Polyesters with Fluorine-Specific Non-Covalent Interactions and Hyperconjugation**

Steiner, Luca[1]; Steiner, Josefine[1]; Fornacon-Wood, Christoph[2]; Plajer, Alex[2]; Paulus, Beate[1]

1: Freie Universität Berlin, Germany; 2: Universität Bayreuth, Germany

Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Wed 91 **Nodal Structure of Π-Orbitals Is Mapped in the Intermolecular PES**

Henrichsmeyer, Johannes; Thelen, Michael; Buchwald, Andrea; Kraut, Keno; Leyrer, Benedikt; Jerbi, Jihene; Fink, Reinhold

University Tuebingen, Germany

Electron Structure Theory - Method Development

Wed 92 **Functionalization-Driven Modulation of Electronic and Optical Properties in Two-Dimensional Materials**
Dai, Jiajun
FUB, Germany
Materials and Solid-State Theory

Wed 93 **Study of GNR Formation and Translation on Au(111) Surface**
Eifler, Jonathan; Klamroth, Tillmann
University of Potsdam, Germany
Machine Learning in Chemistry - Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Wed 94 **Application of Machine-Learning Potentials for Condensed Phase Simulations**
Töpfer, Kai
Freie Universität Berlin, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Spectroscopy and Properties

Wed 95 **FALCON: Fast Active Learning for Machine Learning Potentials in Atomistic and Ab Initio Molecular Dynamics Simulations**
Felis, Noah[1]; Dononelli, Wilke[1,2,3]
1: Institute for Physical and Theoretical Chemistry, University of Bremen; 2: Bremen Center for Computational Materials Science, University of Bremen; 3: MAPEX Center for Materials and Processes, University of Bremen
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Method Development

Wed 96 **From Prediction to Performance: Enhancing Solvent Selection with Transformer Models**
Jansen, Alina[1,2]; Schaudt, Oliver[1]; Führer, Florian[1]
1: Bayer AG; 2: FU Berlin, Germany
Machine Learning in Chemistry

Wed 97 **Interaction of Sodium Ions in Hard Carbon Based Sytems**
Luehrs, Jonas; Partovi-Azar, Pouya
Martin-Luther-Universitaet Halle Wittenberg, Germany
Materials and Solid-State Theory

Wed 98 **Unraveling Intermode Couplings in Water under Vibrational Strong Coupling via IR Spectroscopic Signatures: A Full-Dimensional Quantum Dynamics Approach**
Sinha, Shreya[1]; Fischer, Eric W.[2]; Saalfrank, Peter[3]
1: Universität Potsdam, Germany; 2: Humbolt-Universität Berlin, Germany; 3: Universität Potsdam, Germany
Spectroscopy and Properties

Wed 99 **How Solvation Shapes Spectra: A Monte Carlo Study on Vibrational Probes**
Tsvetaev, Erik; Jacob, Christoph R.
Technische Universität Braunschweig, Germany
Spectroscopy and Properties

Wed 100 **Platinum-Catalyzed Hydrofluorination of Alkynes at Room Temperature Promoted by a Fluoride Shuttle**
Jameel, Froze[1]; He, Ouchan[2]; Flammang, Hannah[2]; S. Babu, Smrithi[1]; Braun, Thomas[2]; Kaupp, Martin[1]
1: Technische Universität Berlin, Germany; 2: Humboldt-Universität zu Berlin, Germany
Reaction Mechanisms and Catalysis

Wed 101 **Kinetics of Photocatalytic Water Splitting Reaction on Au(111) Pyramid and TIO2(101) Surfaces**
Khatua, Rudranarayan; Maria Merajoddin, Maria; Martínez, Jesús G.; Besteiro, Lucas V.
CINBIO, Universidade de Vigo, Spain
Reaction Mechanisms and Catalysis

Wed 102 **Noble Gas Atoms as Ligands to Fe+: Theory Meets Experiment**
Reimann, Marc; Jank, Dominik; Oncak, Milan; Beyer, Martin
Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria
Electron Structure Theory - Spectroscopy and Properties

Wed 103 **From Delocalization to Multiplicity - Decoding C2 with Probability Density Analysis**
Maser, Nicole; Heinz, Michel V.; Lüchow, Arne
RWTH Aachen University, Germany
Electron Structure Theory

Wed 104 **Critical Assessment of Curvature-Driven Surface Hopping Algorithms**
Jíra, Tomáš; Slavíček, Petr
University of Chemistry and Technology, Prague, Czech Republic
Molecular Dynamics and Simulation - Method Development

Wed 105 **Relativistic Two-Photon Absorptions from the Two-Component Bethe-Salpeter Equation**
Rauwolf, Nina
Karlsruhe Institute of Technology, Germany
Method Development

Wed 106 **Quantum-Chemical Methods for Spin Hamiltonians**
Ghassemi Tabrizi, Shadan
Helmholtz-Zentrum Dresden-Rossendorf, TU Dresden
Electron Structure Theory

Wed 107 **A Many-Electron Study of [1.1.1]Propellane with Probability Density Analysis**
Heinz, Michel V.; Lüchow, Arne
RWTH Aachen University, Germany
Electron Structure Theory - Method Development

Wed 108 **Understanding Optical Molecular Spectra in Optical Quantum Cavities Using Coupled Cluster Approaches**
Góger, Szabolcs[1]; Monzel, Laurenz[1]; Stopkowicz, Stella[1,2]
1: Physical and Theoretical Chemistry Group, Department of Chemistry, Universität des Saarlandes, Saarbrücken, Germany; 2: Hylleraas Centre for Quantum Molecular Science, University of Oslo, Oslo, Norway
Electron Structure Theory - Spectroscopy and Properties - Method Development

Wed 109 **Nonadiabatic Dynamics Simulations in Periodic Condensed Phase Systems in CP2K**
de Jong, Tjeerd
University of Zurich, Switzerland
Electron Structure Theory - Molecular Dynamics and Simulation - Method Development

Wed 110 **A Benchmark Dataset for Multicomponent Energies and Densities**
Schiebel, Laura; Schröder, Benjamin; Gimferrer, Martí; Mata, Ricardo A.
Georg-August-Universität Göttingen, Germany
Electron Structure Theory - Spectroscopy and Properties - Method Development

Wed 111 **COSE2 as an Advanced Anode Material for Sodium-Ion Batteries Using Machine Learning**
Rappoun, Hamza; Brehm, Martin; Elgabarty, Hossam
Universität Paderborn, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry - Materials and Solid-State Theory

Wed 112 **Phospha-Michael Additions in Organocatalysis: A Quantum-Chemical Analysis**
Brossette, Jan; Zipse, Hendrk; Ofial, Armin R.
Ludwig-Maximilians-Universität München, Germany
Reaction Mechanisms and Catalysis

Wed 113 **Selected Configuration Interaction in Presence of a Jastrow Factor with Quantum Monte Carlo**
Broecker, Felix; Heinz, Michel V.; Lüchow, Arne
RWTH Aachen University, Germany
Electron Structure Theory - Method Development

Wed 114 **DFT-Guided Self-Assembly of 2D Pyridyl-Linked Metal–Organic Frameworks on Au(111)**
Bisht, Neeta; Görling, Andreas
Friedrich Alexander University, Germany
Materials and Solid-State Theory

Wed 115 **Accurate Diabatic Potential Energy Model for NO3 Including Spin-Orbit Coupling**
Fritsch, Fabian; Eisfeld, Wolfgang
Universität Bielefeld, Germany
Spectroscopy and Properties - Method Development

Wed 116 **Analytical Gradients and Non-Adiabatic Couplings Within Algebraic Diagrammatic Construction Scheme**
Kim, Mira; Rehn, Dirk; Faraji, Shirin
Heinrich-Heine-Universität Düsseldorf, Germany
Electron Structure Theory - Method Development

8 Poster session on Thursday (Sep. 25, 2025)

Instructions for Poster Presenters

Your poster number is given in the conference program. The format is "Day Number" (e.g. "Thu 22"). On the poster wall, only the number is shown (the day is not included). Mount your poster on the poster wall labeled with your number. Pins are provided at the poster wall.

- Posters can be put up starting **Thurday, 25 September 2025, at 12:30 pm**.
- Please remove your poster again by **Friday, 26 September 2025, at 11:00 am** (end of the coffee break).

Enjoy the poster session!

In lieu of an abstract

Instead of submitting an abstract, we asked poster presenters to assign their contribution to the following topics:

- Biochemical Systems
- Electronic Structure Theory
- Machine Learning in Chemistry
- Materials and Solid-State Theory
- Method Development
- Molecular Dynamics and Simulation
- Spectroscopy and Properties
- Reaction Mechanisms and Catalysis

In the program, each poster contribution is listed together with its assigned topic.

Posters

Thu 1 **Vibronic Coupling Potential Energy Surface Generator**
Doedens, Kors; Faraji, Shirin
Heinrich-Heine-Universität Düsseldorf, Germany
Method Development

Thu 2 **Statistically Relevant Adsorption Dynamics of ECCO on Si(001) Using a Fine-Tuned Foundational Machine-Learning Model**
Weiske, Hendrik; Barett, Rhyan; Tonner-Zech, Ralf; Melix, Patrick; Westermayr, Julia
Univeristät Leipzig, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry

Thu 3 **Comparison of the Solvation Models COSMO and EC-RISM for the Prediction of Photoacidity in Aqueous Solution**
Tiska, Ömer[1]; Sülzner, Niklas[1]; Haberhauer, Julia[1]; Kibies, Patrick[2]; Kast, Stefan M.[2]; Hättig, Christof[1]
1: Ruhr-Universität Bochum, Germany; 2: Technische Universität Dortmund, Germany
Electron Structure Theory - Spectroscopy and Properties

Thu 4 **Fast and Generalizable Generation of Transition State Guess Structures via System-Specific Force Fields**
Babushkina, Daria; Dang, Hai An; Feldmann, Gereon; Bannwarth, Christoph
RWTH Aachen, Germany
Method Development - Reaction Mechanisms and Catalysis

Thu 5 **Multiscale Mechanochemical Modeling of Spiropyran-Merocyanine Isomerization in Linear PMMA Polymers**
Dellwisch, Alexander[1]; Colombi Ciacchi, Lucio[2,3,4]; Neudecker, Tim[1,2,3]
1: University of Bremen, Institute for Physical and Theoretical Chemistry, Leobener Straße 6, D-28359 Bremen, Germany; 2: Bremen Center for Computational Materials Science, University of Bremen, am Fallturm 1, D-28359 Bremen, Germany; 3: MAPEX Center for Materials and Processes, University of Bremen, Bibliothekstraße 1, D-28359 Bremen, Germany; 4: Hybrid Materials Interfaces Group, Faculty of Production Engineering, Center for Environmental Research and Sustain Able Technology (UFT), University of Bremen, am Fallturm 1, D-28359 Bremen, Germany
Molecular Dynamics and Simulation

Thu 6 **A Scalable Automated Reaction Pathway Finder Using the NEB Method**
Meeder, Lynn; Mata, Ricardo
Georg-August-Universität Göttingen, Germany
Method Development - Reaction Mechanisms and Catalysis

Thu 7 **Bridging the Gap: Δ-Machine Learning for High-Level PES**
Pandey, Priyanka
Max Planck Institute for Multidisciplinary Sciences Göttingen/Universität Potsdam /Emory University
Machine Learning in Chemistry

Thu 8 **Investigating CO Release from Flavonol Using Ab Initio Methods**
Klíma, Marek; Filgas, Josef; Slavíček, Petr
University of Chemistry and Technology, Prague, Czech Republic
Reaction Mechanisms and Catalysis

Thu 9 **Simulations of Amorphous Polymer Structures**
Kreienbaum, Louis; Sebastiani, Daniel
MLU Halle, Germany
Molecular Dynamics and Simulation

Thu 10 **Bayesian Angular Overlap Model**
Scherz, Frederik[1]; Proppe, Jonny[2]; Krewald, Vera[1]
1: Technical University Darmstadt, Germany; 2: Technical University Braunschweig, Germany
Electron Structure Theory - Machine Learning in Chemistry - Spectroscopy and Properties - Method Development

Thu 11 **Towards an Automated Development of Multicomponent Coupled Cluster Algorithms**
Henninger, Steffen; Mata, Ricardo
Georg-August-University Göttingen, Germany
Electron Structure Theory - Method Development

Thu 12 **Excited States in Strong Magnetic Fields Using Equation-of-Motion-Coupled Cluster Methods**
Roeper, Christopher-Matthias[1]; Bonsignore, Manola[2,1]; Kitsaras, Marios-Petros[3,1]; Hollands, Mark[4]; Stopkowicz, Stella[1,5]
1: Department of Chemistry, Saarland University, 66123 Saarbrücken, Germany; 2: Dipartimento di Chimica E Chimica Industriale, Universitá di Pisa, Pisa I-56124, Italy; 3: Laboratoire de Chimie et Physique Quantiques UMR 5626, Université de Toulouse, CNRS, UPS, France; 4: Department of Physics, University of Warwick, Coventry CV4 7AL, UK; 5: Hylleraas Centre for Quantum Molecular Science, University of Oslo, 0315 Oslo, Norway
Electron Structure Theory - Method Development

Thu 13 **Bond Dissociation Energies of Diatomic 3D Transition-Metal Compounds: A Relativistic DFT Study**
Rodriguez Weber, Adrian; Kaupp, Martin
TU Berlin, Germany
Electron Structure Theory

Thu 14 **Impact of Systematic Isosteric (CH—>N) Replacement on the Molecule-Substrate Interaction**
Ulrich, Anna; Amirjalayer, Saeed
Universität Heidelberg, Germany
Molecular Dynamics and Simulation - Materials and Solid-State Theory

Thu 15 **Electron-Induced Chemistry: The Case of C5F10O and C3H2F4**
Ovad, Tomáš[1]; Fedor, Juraj[2]; Slavíček, Petr[1]
1: University of Chemistry and Technology, Prague, Czech Republic; 2: Jaroslav Heyrovský Institute of Physical Chemistry, Prague, Czech Republic
Molecular Dynamics and Simulation - Spectroscopy and Properties

Thu 16 **Higher-Order Force Constants for Anharmonic Vibrational Frequencies of Molecules and Solids**
Pattani Ameerjan, Basila Bhanu[1]; Dononelli, Wilke[1,2,3]
1: Institute for Physical and Theoretical Chemistry, University of Bremen; 2: Bremen Center for Computational Materials Science, University of Bremen; 3: MAPEX Center for Materials and Processes, University of Bremen
Machine Learning in Chemistry

Thu 17 **Jahn-Teller and Spin-Orbit Effects in Methylhalide Cations**
Vossel, Maik; Eisfeld, Wolfgang
University Bielefeld, Germany
Electron Structure Theory - Molecular Dynamics and Simulation - Method Development

Thu 18 **Excited States Properties in Strong Magnetic Fields via Equation-of-Motion Coupled Cluster**
Bonsignore, Manola[1,2]; Röper, Christopher-Matthias[1]; Kitsaras, Marios-Petros[1,3]; Hollands, Mark[4]; Stopkowicz, Stella[1,5]
1: Department of Chemistry, Saarland University, 66123 Saarbrücken, Germany; 2: Dipartimento di Chimica E Chimica Industriale, Università di Pisa, Pisa I-56124, Italy; 3: Laboratoire de Chimie et Physique Quantiques UMR 5626, Université de Toulouse, CNRS, UPS, France; 4: Department of Physics, University of Warwick, Coventry CV4 7AL, UK; 5: Hylleraas Centre for Quantum Molecular Science, University of Oslo, 0315 Oslo, Norway
Electron Structure Theory - Method Development

Thu 19 **Random Phase Approximation at Finite Temperatures: Implementation with Localized Basis Sets**
Stein, Frederick
Helmholtzzentrum Dresden-Rossendorf E.V, Germany
Electron Structure Theory - Method Development - Materials and Solid-State Theory

Thu 20 **Open Quantum System Dynamics for Vibrational Strong Coupling: Resonantly Altered Reaction Rates**
Gundermann, Richard; Saalfrank, Peter
Universität Potsdam, Germany
Method Development - Reaction Mechanisms and Catalysis

Thu 21 **Exploring Heavy Atoms in Strong Magnetic Fields: A Study on ECP and X2C Methods for Noble Gas Atoms**
Appenzeller, Anja[1]; Klopper, Wim[1]; Pausch, Ansgar[2]
1: Karlsruhe Institute of Technology, Germany; 2: Vrije Universiteit Amsterdam, The Netherlands
Electron Structure Theory

Thu 22 **Computational Photochemistry of Bilirubin**
Peterka, Lukáš
University of Chemistry and Technology, Prague, Czech Republic
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Thu 23 **Electronic States of Diarylethene Switch on Gold Nanoclusters**
Mazarei, Elham; Titov, Evgenii
Potsdam University, Germany
Electron Structure Theory - Spectroscopy and Properties - Reaction Mechanisms and Catalysis

Thu 24 **Physics-Guided Machine Learning of Excited-State Properties for the Design of High-Performance TADF Emitters**
Sanyam, Sanyam
Indian Institute of Technology, Gandhinagar, India
Electron Structure Theory - Machine Learning in Chemistry - Method Development

Thu 25 **Multimer Embedding for Molecular Crystals up to Tetramer Interactions**
List, Alexander; Hoja, Johannes; Boese, A. Daniel
Department of Chemistry, University of Graz, 8010 Graz, Austria
Electron Structure Theory - Materials and Solid-State Theory

Thu 26 **Machine Learning Framework for Nanocrystalline Structure Determination from Total Scattering and Electronic Structure Calculations**
Diephaus, Philipp T.[1,2]; Gesing, Thorsten M.[1,2,3]; Dononelli, Wilke[1,3,4]
1: University of Bremen, Germany; 2: Institute of Inorganic Chemistry and Crystallography; 3: MAPEX Center for Materials and Processes; 4: Institute for Physical and Theoretical Chemistry
Machine Learning in Chemistry - Materials and Solid-State Theory

Thu 27 **Charge Transport Processes as Dynamics of Correlated Electron-Hole Pairs**
Conrad, Lawrence[1]; Paulus, Beate[1]; Tremblay, Jean Christophe[2]
1: Freie Universität Berlin, Germany; 2: Université de Lorraine, France
Method Development

Thu 28 **Promoting Photoreactivity via the Upper Polariton under Collective Strong Coupling**
Wallner, Lisamaria; Vendrell, Oriol
Universität Heidelberg, Germany
Molecular Dynamics and Simulation

Thu 29 **Hydrogen Isotopes Separation through Precision Membranes**
Mondonico, Daniela[1,2]; Joswig, Jan-Ole[2]; Heine, Thomas[1,2,3]
1: HZDR, Germany; 2: Technische Universitat Dresden, Germany; 3: Yonsei University, Seoul, Korea
Molecular Dynamics and Simulation

Thu 30 **Lineshapes in Pump-Probe Spectroscopy of Polaritons**
Philipp, Luca Nils[1]; Münzel, Eva[1]; Lüttig, Julian[2]; Mitric, Roland[1]
1: Universität Würzburg, Germany; 2: University of Michigan, Michigan, USA
Spectroscopy and Properties

Thu 31 **Computational Investigation of Relaxation Pathways in Organic Donor-Functionalized Doublet Emitters**
Pauls, Mike[1]; Arnold, Mona[2]; Schwarz, Denise[1]; Kühne, Alexander[2]; Bannwarth, Christoph[1]
1: RWTH Aachen University, Germany; 2: Ulm University, Germany
Spectroscopy and Properties

Thu 32 **Scalable Energy Decomposition Analysis in Solvated Systems with Machine Learning**
Tahmasbi, Hossein; Beerbaum, Michael; Brzoza, Bartosz; Cangi, Attila; Kühne, Thomas D.
Center for Advanced Systems Understanding (CASUS)-HZDR, Germany
Machine Learning in Chemistry - Method Development

Thu 33 **In the Footsteps of Lewis und Linnett: The PDA Method and Its Potential Value for Chemical Education**
Richter, Tamara; Heinz, Michel V.; Lüchow, Arne
RWTH Aachen University, Germany
Electron Structure Theory - Method Development

Thu 34 **Cr-Based MIL-100 for Ethylene Oligomerization: Mechanistic Insights and the Role of Metal Dopants**
Matsokin, Nikita; Fink, Karin
Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT), 76344, Karlsruhe/DE
Reaction Mechanisms and Catalysis

Thu 35 **QCXMS2 – A Program for the Calculation of Mass Spectra via Automated Reaction Network Discovery**
Gorges, Johannes; Grimme, Stefan
University of Bonn, Germany
Reaction Mechanisms and Catalysis

Thu 36 **Multi-Scale Modelling for an Accurate Prediction of Redox Potentials in Iron Coordination Compounds**
Jimenez-Munoz, Carlos Michael[1]; Björnsson, Ragnar[2]; Krewald, Vera[1]
1: Department of Chemistry, Quantum Chemistry, TU Darmstadt, Peter-Grünberg-Str. 4, 64287 Darmstadt, Germany; 2: Laboratoire de Chimie et Biologie des Métaux, Univ. Grenoble Alpes, CNRS, CEA, IRIG, 17 Rue des Martyrs, F-38054 Grenoble, Cedex, France
Electron Structure Theory - Molecular Dynamics and Simulation - Spectroscopy and Properties

Thu 37 **How Simple Can You Go? Machine Learning Molecular Dynamics with Minimal Physical Constraints**
Gugler, Stefan[1,2]; Eissler, Max[1,2]; Korjakow, Tim[1,2]; Ganscha, Stefan[5]; Unke, Oliver[5]; Muller, Klaus-Robert[1,2,3,4,5]
1: BIFOLD – Berlin Institute for the Foundations of Learning and Data; 2: Machine Learning Group, Technische Universität Berlin; 3: Department of Artificial Intelligence, Korea University; 4: Max-Planck Institute for Informatics; 5: Google DeepMind
Molecular Dynamics and Simulation - Machine Learning in Chemistry

Thu 38 **Electronic Structure of Multichromic Molecular Motors**
Obel, Oscar Berlin; Amirjalayer, Saeed
IWR, Heidelberg University, Germany
Electron Structure Theory

Thu 39 **Insights into Dermal Permeation of Skin Oil Oxidation Products from Enhanced Sampling Molecular Dynamics Simulation**
Thomas, Rinto[1]; Prabhakar, Praveen Ranganath[2]; Tobias, Douglas J.[2]; von Domaros, Michael[1]
1: Philipps-Universität Marburg, Germany; 2: University of California, Irvine, United States
Molecular Dynamics and Simulation

Thu 40 **Boundary Mechanisms in Adaptive Resolution Simulations**
Hille, Julian Friedrich; Klein, Rupert
Freie Universität Berlin, Institut für Mathematik, Arnimallee 6, 14195 Berlin, Germany
Molecular Dynamics and Simulation - Method Development

Thu 41 **The Strongest Lewis Acids: Fluoride Ion Affinity and NMR**
Lehmann, Morten; Kaupp, Martin
Technische Universität Berlin, Germany
Spectroscopy and Properties

Thu 42 **Zinc Half Cell Modifications: Dynamics and Electronic Changes**
Beerbaum, Michael; Prasad, Dr Mahabir
Helmholtz Zentrum Dresden-Rossendorf E.V, Germany
Molecular Dynamics and Simulation

Thu 43 **Positively Charged 2D Polymer Membrane for Aqueous Al Batteries**
Prasad, Mahabir; Kühne, Thomas D.
Center for Advanced Systems Understanding, Helmholtz-Zentrum Dresden-Rossendorf, Germany
Molecular Dynamics and Simulation

Thu 44 **Spectral Predictions of Large-Scale Molecular Assemblies Using Excitonic Models**
Mausenberger, Sascha[1,2]; Jacobi, Richard[1,2]; Mai, Sebastian[1]; González, Leticia[1,3]
1: Institute of Theoretical Chemistry, Faculty of Chemistry, University of Vienna, Währinger Straße 17, 1090 Vienna, Austria; 2: Doctoral School in Chemistry (DoSChem), University of Vienna, Währinger Straße 42, 1090 Vienna, Austria; 3: Vienna Research Platform on Accelerating Photoreaction Discovery, University of Vienna, Währinger Straße 17, 1090 Vienna, Austria
Electron Structure Theory - Spectroscopy and Properties

Thu 45 **Towards Accurate Continuum Solvation Models for Fast Semi-Empirical Methods**
Dahl, Robin[1]; Wittmann, Lukas[1]; Nottoli, Michele[2]; Stamm, Benjamin[2]; Grimme, Stefan[1]
1: Universität Bonn, Mulliken Center for Theoretical Chemistry, Bonn, Germany; 2: Universität Stuttgart, Institute of Applied Analysis and Numerical Simulation, Stuttgart, Germany
Electron Structure Theory - Method Development

Thu 46 **Currents and Crossroads: Open Quantum System Perspective on Electron Flow and Chemical Selectivity**
Chuang, Grace Hsiao-Han[1]; Eisfeld, Alexander[1]; Quapp, Wolfgang[2]
1: Max Planck Institute for the Physics of Complex Systems; 2: Leipzig University
Molecular Dynamics and Simulation - Method Development

Thu 47 **Automated Sampling of Enzymatic Reaction Pathways Using QM/MM Methods**
Epee Ndongue, Jules Cesar; Imhof, Petra
Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany
Method Development - Reaction Mechanisms and Catalysis

Thu 48 **From Densities to Energies: A Machine Learning Pipeline for SAPT Interaction Energy Predictions**
Oestereich, Toni
University Leipzig, Germany
Machine Learning in Chemistry - Method Development - Biochemical Systems

Thu 49 **Towards the Prediction of Molecular Spectra of Magnetic White Dwarfs**
Paulus, Elena[1]; Monzel, Laurenz[1]; Tellgren, Erik[2]; Stopkowicz, Stella[1,2]
1: Department of Chemistry, Saarland University, Saarbrücken, Germany; 2: Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo, Oslo, Norway
Electron Structure Theory - Molecular Dynamics and Simulation

Thu 50 **Geometric Deep Learning for Molecules and Reactions: Do We Always Need Equivariance?**
Briling, Ksenia R.[1]; van Gerwen, Puck[1]; Cho, Yuri[1]; Bunne, Charlotte[2]; Somnath, Vignesh Ram[2]; Laplaza, Ruben[1]; Krause, Andreas[2]; Corminboeuf, Clemence[1]
1: Laboratory for Computational Molecular Design, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland; 2: Learning & Adaptive Systems Group, Department of Computer Science, ETH Zurich, 8092 Zurich, Switzerland
Machine Learning in Chemistry

Thu 51 **Kinetics and Thermodynamics of Cyclic Allenes as Dienophiles in Diels-Alder Reactions with Furan**
Monz, Tobias-Erik[1]; Fuerst, Rita[2]; Hartmann, Peter E.[1]; Hoja, Johannes[1]; Unger, Elisabeth[2]; Boese, A. Daniel[1]
1: University of Graz, Austria; 2: Graz University of Technology, Austria
Reaction Mechanisms and Catalysis

Thu 52 **From Gold to Copper: Comparative DFT Study of NHC Adsorption and Self-Assembly for Area-Selective ALD**
Thiemann, Franz[1]; Tumino, Francesco[2]; Desroche, Emmett[2]; Crudden, Cathleen[2]; Melix, Patrick[1]; Tonner-Zech, Ralf[1]
1: Leipzig University - Wilhelm-Ostwald-Institut, Germany; 2: Queen's University - Department of Chemistry
Materials and Solid-State Theory

Thu 53 **Modeling Energy Transfer in Multi-Chromophoric Light-Harvesting Assemblies**
van Dam, Laurens; González, Leticia
University of Vienna
Molecular Dynamics and Simulation - Method Development - Biochemical Systems

Thu 54 **Electronic States of Diarylethene Switch on Gold Nanoclusters**
Mazarei, Elham; Titov, Evgenii
Potsdam University, Germany
Electron Structure Theory - Spectroscopy and Properties - Reaction Mechanisms and Catalysis

Thu 55 **Benchmark Comparison of IR Spectra Using the Pearson Correlation Coefficient**
Oung, Sangwar Wadtey; Jacob, Christoph R.
TU Braunschweig, Germany
Spectroscopy and Properties

Thu 56 **Revealing Allosteric Communication in the Tubulin Dimer through Molecular Dynamics and Network Analysis**
Teterina, Polina; Peter, Christine
University of Konstanz, Germany
Molecular Dynamics and Simulation - Biochemical Systems

Thu 57 **Active Learning Based Dataset Construction for Neural Network Potentials of Water in 2D Nanoconfinement**
Smith, Nathalie; Herrmann, Carmen
University of Hamburg, Germany
Molecular Dynamics and Simulation - Machine Learning in Chemistry

Thu 58 **Ligand Sphere Effects on Dinitrogen Activation in Bimetallic Complexes**
Singh, Shweta; Krewald, Vera
Technical University of Darmstadt, Germany
Electron Structure Theory

Thu 59 **Quantifying Mixing Dynamics via Configurational Entropy Measures**
Upterworth, Anna Luisa; Hanke, Till; Steinkopf, Tom; Sebastiani, Daniel
Martin-Luther-Universität Halle-Wittenberg, Germany
Molecular Dynamics and Simulation

Thu 60 **In Silico Studies Demonstrate That −OBO Units Bound to Stable Boron Cages in YB11(OBO)12- (Y=C/Si) Anions Provide a Desirable Borate-Rich Solid Electrolyte Interface in Calcium-Ion Batteries**
Sharma, Abhiruchi; Gupta, Puneet
Indian Institute of Technology Roorkee, Roorkee, Uttarakhand-247667, India
Electron Structure Theory - Molecular Dynamics and Simulation

Thu 61 **Prediction of Chirality Observables in Unsaturated Molecules Using Algebraic Models**
Gohain, Namrata; Berger, Robert
Philipps-Universität Marburg, Germany
Electron Structure Theory - Spectroscopy and Properties

Thu 62 **First-Principles Study of Lithium Ion Insertion at FEPO4 Surfaces**
Löseke, Julian; Brehm, Martin; Elgabarty, Hossam
Paderborn University, Germany
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Thu 63 **Opening the Digital Lab Door: Engaging High School Students with Computational Chemistry**
Peterknecht, Marina; Brossette, Jan
LMU, Germany
Reaction Mechanisms and Catalysis

Thu 64 **A Full Dirac-Coulomb Coupled-Cluster Approach by Means of Cholesky Decomposition.**
Cianchino, Davide[1]; Stopkowicz, Stella[1,3]; Gauss, Jürgen[2]
1: Fachrichtung Chemie, Universität des Saarlandes, Campus B2.2, D-66123 Saarbrücken, Germany; 2: Department Chemie, Johannes Gutenberg-Universität Mainz, Duesbergweg 10-14, D-55128 Mainz, Germany; 3: Hylleraas Centre for Quantum Molecular Sciences, Department of Chemistry, University of Oslo, P.O. Box 1033, N-0315 Oslo, Norway
Electron Structure Theory - Method Development

Thu 65 **Interface of the EC-RISM Solvent Model to TURBOMOLE to Include Solvent Granularity Effects in Energies and Gradients**
Haberhauer, Julia[1]; Kibies, Patrick[2]; Kast, Stefan[2]; Hättig, Christof[1]
1: Ruhr-Universit Bochum, Germany; 2: Technische Universität Dortmund, Germany
Electron Structure Theory - Spectroscopy and Properties - Method Development

Thu 66 **First-Principles Insights into Ni-Doped COFs for Efficient CO_2Electroreduction**
Lussari Vrech, Natalia[1]; Paulus, Beate[2]
1: Universitat Bremen, Germany; 2: Freie Universiat Berlin, Germany
Electron Structure Theory - Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Thu 67 **Girsanov Reweighting with Core Set Markov State Models**
Schäfer, Joana-Lysiane; Keller, Bettina
Freie Universität Berlin, Germany
Method Development

Thu 68 **Impact of Donor-Acceptor Functionalisation on 2H-MOS_2: A First-Principles Study**
Ray, Sreejita; Wang, Jhih-Syuan; Yin, Haixin; Paulus, Beate
Freie Universität Berlin, Germany
Materials and Solid-State Theory

Thu 69 **Towards Systematic Initiations of Minimum Energy Path Calculations**
Muecke, Maike; Mata, Ricardo
Georg-August-University Goettingen, Germany
Reaction Mechanisms and Catalysis

Thu 70 **Mixed Metal Oxide in Gas Phase: The Study of the ALNI2O4+ Cluster**
de Lima, Lucas Welington[1]; C. Penna, Tatiana[2,3]; R. Asmis, Knut[3]; Sauer, Joachim[1]; Roemelt, Michael[1]
1: Humboldt-Universität zu Berlin, Germany; 2: Wilhelm-Ostwald Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany; 3: Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany
Spectroscopy and Properties

Thu 71 **MLH: An ML Model for Nuclear Hessians Based on GFN2-xTB Derived Atomistic Features.**
Feldmann, Gereon; Bannwarth, Christoph
RWTH Aachen University, Germany
Machine Learning in Chemistry - Method Development

Thu 72 **Multidimensional Lattice Models in the MCTDH Framework**
Niermann, Tristan; Manthe, Uwe
Universität Bielefeld, Germany
Method Development - Materials and Solid-State Theory

Thu 73 **Entropy Dependence on Smearing Radii**
Hanke, Till; Sebastiani, Daniel
MLU Halle, Germany
Method Development

Thu 74 **$Li^+$and K^+Diffusion at Interfaces in Si/C and SnS/SNS_2Anodes**
Kirsch, Christoph; Partovi-Azar, Pouya; Sebastiani, Daniel
Martin-Luther-Universität Halle-Wittenberg, Germany
Molecular Dynamics and Simulation

Thu 75 **Multiscale Modeling of Photosynthetic Light-Harvesting in Photosystem I**
Reiter, Sebastian[1]; Pointner, Ferdinand[1]; Gordiy, Igor[2]; de Vivie-Riedle, Regina[1]
1: Ludwig-Maximilians-Universität München, Germany; 2: ETH Zurich
Molecular Dynamics and Simulation - Biochemical Systems

Thu 76 **Design Principles for Efficient IR Luminescence in Pt/Pd(0) Complexes**
Guhl, Jasper[1]; Ruer, Paul[2]; Ralle, Philipp[2]; Steffen, Andreas[2]; Marian, Christel[1]
1: Heinrich-Heine-Universität Düsseldorf; 2: Technical University Dortmund
Spectroscopy and Properties

Thu 77 **Simulating Non-Equilibrium Solvent Dynamics Arount Nascent Aqueous Halogens Using QM/MM Molecular Dynamics**
Schneeberger, Michaela[1,4]; Bai, Mei[1,4]; Nurekeyev, Zhangatay[1,2,3]; Bressler, Christian[1,3]; Santra, Robin[1,2]; Thorwart, Michael[1]; Herrmann, Carmen[1]
1: Universität Hamburg, Germany; 2: Center for Free-Electron Laser Science CFEL, DESY, Germany; 3: European X-Ray Free-Electron Laser Facility GmbH, Germany; 4: The Hamburg Centre for Ultrafast Imaging CUI, Germany
Molecular Dynamics and Simulation

Thu 78 **Theoretical Study on the Electronic and Optical Properties of Some Polyborazine Structures**
Bahat, Mehmet; Kılınç, Hatice
Gazi University, Turkiye
Spectroscopy and Properties

Thu 79 **The CC2 Groundstate Is Significantly Improved by a Size-Consistent Brillouin-Wigner Partitioning**
Dittmer, Linus Bjarne[1]; Tkachenko, Nikolay[2,3]; Head-Gordon, Martin[2]; Dreuw, Andreas[1]
1: Interdisziplinäres Zentrum für Wissenschaftliches Rechnen, Universität Heidelberg, Germany; 2: Department of Chemistry, University of California, Berkeley, California 94720, United States; 3: Department of Chemistry and Biochemistry, University of Oklahoma, Norman, Oklahoma 73019, USA
Electron Structure Theory

Thu 80 **Investigation of Aggregation in N-Heteropolycyclic Aromatic Molecules via Vibrationally Resolved Electronic Absorption Spectra Simulations**
Tian, Lin
Interdisciplinary Center for Scientific Computing, Germany
Spectroscopy and Properties

Thu 81 **Machine Learning-Accelerated Quantum Mechanical Energy Function with Electron Density Based Energy Decomposition**

Hoffmann, Maximilian[1]; Kazimir, Aleksandr[1]; Oestereich, Toni[1]; Kaermer, Luisa[2]; Engelberger, Felipe[1]; Lamers, Christina[1]; Meiler, Jens[1,2]

1: University Leipzig, Germany; 2: Vanderbilt University, Nashville, Tennessee 37240, US

Machine Learning in Chemistry - Method Development

Thu 82 **Unveiling Patterns in AD-HoC Nickel Cross-Coupling with Machine Learning**

Bitterlich, Daniel[1]; Ghosh, Indrajit[2,3]; König, Burkhard[2]; Westermayr, Julia[1,4]

1: Leipzig University, Wilhelm Ostwald Institute for Physical and Theoretical Chemistry; 2: University of Regensburg, Institute of Organic Chemistry; 3: VSB - Technical University of Ostrava, Nanotechnology Centre, Centre for Energy and Environmental Technologies; 4: Center for Scalable Data Analytics and Artificial Intelligence (ScaDS.AI), Dresden/Leipzig

Machine Learning in Chemistry

Thu 83 **Simulations of Nuclear Dynamics Triggered by Core-Excitation in N2O**

Vaz da Cruz, Vinicius

Helmholtz-Zentrum Berlin, Germany

Molecular Dynamics and Simulation - Spectroscopy and Properties

Thu 84 **Spectral Signatures of Ultrafast Dynamics of Competing Reaction Pathways in Molecular Rings**

Erić, Vesna[1]; Montorsi, Francesco[2]; Djumayska, Simona[1]; Keefer, Daniel[1]

1: Max Planck Institute for Polymer Research, Germany; 2: University of Bologna, Bologna, Italy

Spectroscopy and Properties

Thu 85 **MD and QM/MM Investigation of the Deubiquitinylase OTU Cezanne-2 Mechanism**

Escorcia, Andrés M.; Ilter, Metehan; Stein, Matthias

Max Planck Institute for Dynamics of Complex Technical Systems, Germany

Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis - Biochemical Systems

Thu 86 **Two-Component Quantum Electrodynamic Corrections to Nuclear Magnetic Resonance Shielding Tensors**

Janke, Kjell[1]; Kozioł, Karol[2]; Aucar, I. Agustín[3,4]; Aucar, Gustavo A.[3]; Gaul, Konstantin[5]; Berger, Robert[1]

1: Fachbereich Chemie, Philipps-Universität Marburg, Hans-Meerwein-Straße 4, 35032 Marburg, Germany; 2: Narodowe Centrum Badań Jądrowych (NCBJ), Andrzeja Sołtana 7, 05-400 Otwock-Świerk, Poland; 3: Instituto de Modelado E Innovación Tecnológica (UNNE-CONICET), Facultad de Ciencias Exactas Y Naturales Y Agrimensura, Universidad Nacional del Nordeste, Avda. Libertad 5460, Corrientes, Argentina; 4: Van Swinderen Institute for Particle Physics and Gravity, University of Groningen, 9747 AG Groningen, The Netherlands; 5: Helmholtz Institut Mainz, 55099 Mainz, Germany

Electron Structure Theory - Spectroscopy and Properties

Thu 87 **Fluorination of Small Carbon-Based Molecules on a NIF2 Model Surface: A First-Principles Study**

Lindic, Tilen; Paulus, Beate

Physical and Theoretical Chemistry, Freie Universität Berlin, Germany

Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Thu 88 **Regressing the Self-Consistent Hamiltonian and Density from the Non-Self-Consistent Hamiltonian**

Richter, Simon Ullrich

Helmholz Zentrum Dresden-Rossendorf /CASUS, Germany

Electron Structure Theory - Machine Learning in Chemistry - Method Development

Thu 89 **Molecular Response Properties with ADC/ISR: From Symbolic Inputs to Efficient Algorithms**

Rehn, Dirk Robert

Heidelberg University, Germany

Electron Structure Theory - Spectroscopy and Properties

Thu 90 **Interpolation Mechanics – A Fast Way to Multi-State Dynamics**

Lindfeld, Valentin[1,4]; Brumboiu, Iulia[2]; Rhee, Young Min[3]; Norman, Patrick[4]

1: University of Muenster, Germany; 2: Nicolaus Copernicus University in Toruń, Poland; 3: Korea Advanced Institute of Science and Technology, South Korea; 4: Royal Institute of Technology, Sweden

Molecular Dynamics and Simulation - Method Development

Thu 91 **Stability, Reactivity of Small Molecular Ions as Probes of Fundamental Symmetries**

Zülch, Carsten[1]; Gaul, Konstantin[2]; Berger, Robert[1]

1: Philipps-Universität Marburg, Germany; 2: Helmholtz Institut, Johannes Gutenberg-Univetsität Mainz

Electron Structure Theory - Spectroscopy and Properties

Thu 92 **Density-Based Many-Body Expansion for Metal Clusters**

Focke, Kevin; Jacob, Christoph R.

TU Braunschweig, Germany

Electron Structure Theory - Method Development

Thu 93 **A Diels-Alder Reaction in Ionic Liquids in Comparison to Water**
Sariyar, Gülben; Brehm, Martin
Paderborn University, Germany
Molecular Dynamics and Simulation

Thu 94 **dxtb - an Efficient and Fully Differentiable Framework for Extended Tight-Binding**
Friede, Marvin[1]; Hölzer, Christian[1]; Ehlert, Sebastian[2]; Grimme, Stefan[1]
1: University of Bonn, Germany; 2: AI for Science, Microsoft Research
Electron Structure Theory - Machine Learning in Chemistry - Method Development

Thu 95 **Computational Investigation of the Oxygen Activation Mechanism on a Model pMMO Complex**
Sergel, Antonia; Roemelt, Michael
Humboldt Universitaet zu Berlin, Germany
Reaction Mechanisms and Catalysis

Thu 96 **Enhancing Phosphorescence in Pt(II) Complexes through Heavy-Atom Substitution**
Schwab, Dominik Alexander; Doltsinis, Nikos
Universität Münster, Germany
Electron Structure Theory - Spectroscopy and Properties - Reaction Mechanisms and Catalysis - Materials and Solid-State Theory

Thu 97 **Reactivity of P-Centered Biradicals with Isonitriles: A Computational Study**
Tayebi, Zahra
University of Rostock, Germany
Reaction Mechanisms and Catalysis

Thu 98 **Efficient Photo-Driven Electron Transfer from Amino Group-Decorated Adamantane to Water**
Wang, Xiangfei[1,2]; Remmert, Jonathan[3]; Paulus, Beate[1]; Bande, Annika[4]
1: Institute of Chemistry and Biochemistry, Freie Universität Berlin, Arnimallee 22, 14195 Berlin, Germany; 2: Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany; 3: Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany; 4: Institute of Inorganic Chemistry, Leibniz University Hannover, Callinstr. 9, 30167 Hannover, Germany
Spectroscopy and Properties - Reaction Mechanisms and Catalysis

9 Industry posters

Ind 01 **Boosting Thermophysical Property Predictions with Graph Neural Networks**
Richter, Martin
Dassault Systemes Deutschland GmbH, Germany

Ind 02 **ORCA Meets Python - the ORCA Python Interface OPI**
Neugebauer, Hagen; Plett, Christoph; Bursch, Markus
FACCTs GmbH, Germany

Ind 03 **NHR Atomistic Simulation Center (National Compute Resources and Expert Support)**
Ehtesabi, Sadaf
Paderborn Center for Parallel Computing (PC2), University of Paderborn, Paderborn, Germany

Ind 04 **Machine Learning-Based Correction for Spin-Orbit Coupling Effects in NMR Chemical Shift Calculations**
Bursch, Markus[1]; Kleine Büning, Julius B.[2]; Grimme, Stefan[2]
1: FACCTs GmbH, Germany; 2: University of Bonn

Ind 05 **Quantum Chemical Descriptors for Understanding Photostability of Small Molecules: A Protocol for Agrochemicals**
Alber, Yannic; Wagner, Silke; Cerezo-Galvez, Silvia; Timmermann, Christian; Anft, Thomas; Beck, Michael Edmund
Bayer AG, Crop Science Division, Germany

Ind 06 **Nature Communications**
Zobel, Patrick
Nature Communications, Germany

Ind 07 **Molpro quantum chemistry package**
Mata, Ricardo
Molpro; Universität Göttingen, Germany

Ind 08 **BASF**
Deglmann, Peter
BASF SE, Ludwigshafen, Germany

Ind 09 **TURBOMOLE**
Sierka, Marek
TURBOMOLE, Germany

Participants

10 Participants

Organizers

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Prof. Dr.	Paulus	Beate	Freie Universität Berlin	Germany

Speakers

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Prof. Dr.	Bande	Annika	Leibniz Hannover University, Helmholtz-Zentrum Berlin	Germany
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	Hermann	Jan	Microsoft Research AI for Science	Germany
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Dr.	Park	Chanbum	Ruhr-Universitaet Bochum	Germany
	Peterknecht	Marina	LMU München	Germany
Prof. Dr.	Podewitz	Maren	TU Wien	Austria
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Prof. Dr.	Stopkowicz	Stella	Universität des Saarlandes	Germany
Prof. Dr.	Tremblay	Jean C.	Université de Lorraine	France
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	Wesely	Sophia	Leipzig University	Germany
Dr.	Zarotiadis	Rhiannon Audrey	Simons Center for Computational Physical Chemistry, NYU	USA
	Zens	Clara	Friedrich Schiller University Jena	Germany

A

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	Adelsperger	Johannes	Uni Würzburg	Germany
Dr.	Alber	Yannic	Bayer AG	Germany
Dr.	Alizadeh	Vahideh	Max Planck Institute for the Structure and Dynamics of Matter	Germany
	Alvarez	Luis	Leibniz Universität Hannover	Germany
Prof. Dr.	Amirjalayer	Saeed	Heidelberg University	Germany
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