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 **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 31 **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 32 **ChemLab Platform: Automating Quantum Chemical Research and Managing Computational Data**
Mikhailin, Aleksandr
Chemlab, Austria
Molecular Dynamics and Simulation

Mon 33 **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 34 **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 35 **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 36 **Quantum Dynamics Simulation of Exciton-Polariton Transport**
Krupp, Niclas
Heidelberg University, Germany
Molecular Dynamics and Simulation - Materials and Solid-State Theory

Mon 37 **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 38 **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 39 **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 40 **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 41 **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 42 **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 43 **Bringing Error Bars into Density Functional Theory**
Laqua, Henryk; Head-Gordon, Martin
UC Berkeley, United States of America
Electron Structure Theory - Method Development

Mon 44 **Decomposition of Magnetic Coupling in M-Oxo-Bridged Metal Complexes**
Krampe, Justin; Krewald, Vera
TU Darmstadt, Germany
Electron Structure Theory

Mon 45 **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 46 **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 47 **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 48 **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 49 **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 50 **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 51 **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 52 **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 53 **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 54 **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 55 **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 56 **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 57 **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 58 **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 59 **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 60 **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 61 **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 62 **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 63 **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 64 **Modelling Exciton Dynamics in Multiphotochromic Systems**
Titov, Evgenii
Universität Potsdam, Germany
Molecular Dynamics and Simulation - Spectroscopy and Properties

Mon 65 **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 66 **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 67 **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 68 **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 69 **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 70 **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 71 **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 72 **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 73 **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 74 **Community-Driven and Systematic Benchmarks to Advance and Democratize Nonadiabatic Molecular Dynamics**
Ibele, Lea
CNRS/Aix Marseille University, France
Molecular Dynamics and Simulation

Mon 75 **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 76 **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 77 **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 78 **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 79 **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 80 **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 81 **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 82 **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 83 **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 84 **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 85 **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 86 **Intrinsic Dimensionality of Molecular Properties**
Banjafar, Ali; von Rudorff, Guido
University of Kassel, Germany
Machine Learning in Chemistry - Method Development

Mon 87 **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 88 **Representative Random Sampling of Chemical Space**
Monterrubio Chanca, Diego Javier; von Rudorff, Guido
University of Kassel, Germany
Machine Learning in Chemistry - Method Development

Mon 89 **Spin-Isomers of Molecular Hydrogen in Weakly Bound Complexes**
Hartwig, Beppo; Hasselhorn, Jannes; Obenchain, Daniel
Georg-August-Universität Göttingen, Germany
Spectroscopy and Properties

Mon 90 **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 91 **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 92 **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 93 **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 94 **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 95 **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 96 **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 97 **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 98 **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 99 **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 100 **Noncollinear Density Functional Theory Made Simple**
Gaul, Konstantin
Helmholtz Institut, Johannes Gutenberg-Universität Mainz, Germany
Electron Structure Theory - Method Development

Mon 101 **Chemical Reaction Discovery with Periodic Boundary Conditions**
Meisner, Jan
Heinrich-Heine-Universität Düsseldorf, Germany
Molecular Dynamics and Simulation - Reaction Mechanisms and Catalysis

Mon 102 **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 103 **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 104 **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 105 **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 106 **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 107 **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]
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Molecular Dynamics and Simulation - Machine Learning in Chemistry - Materials and Solid-State Theory

Mon 108 **Development of SC-NEVPT2 Methods with SCI Wave Functions**
Ugandi, Mihkel
HU Berlin, Germany
Electron Structure Theory

Mon 109 **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 110 **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 111 **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 112 **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