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