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; Kühne, Thomas D.
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[1]; Kärmer, Luisa[1,3]; Meiler, Jens[1,2,3,4,5]

1: Institute for Drug Discovery, University Leipzig, Leipzig, Germany; 2: Center for Scalable Data Analytics and Artificial Intelligence, ScaDS.AI Dresden/Leipzig; 3: School of Embedded Composite Artificial Intelligence SECAI, Dresden/Leipzig, Germany; 4: Department of Chemistry, Vanderbilt University, Nashville, Tennessee, United States of America; 5: Department of Pharmacology, Center for Structural Biology, Institute of Chemical Biology, Center for Applied Artificial Intelligence in Protein Dynamics, Vanderbilt University, Nashville, Tennessee, United States of America

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

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

Thu 99 **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