Scientific Program

Monday, July 3

09:00 – 13:00		Registration
13:00 – 13:20		Opening Words

		Session 1 – Chair: Karsten Reuter
13:20 – 14:00	I1	**Alexandre Tkatchenko** – University of Luxembourg, Luxembourg *Fully Quantum (Bio)Molecular Simulations: Dream or Reality?*
14:00 – 14:20	C1	**Jiří Czernek** – Institute of Macromolecular Chemistry, Czech Republic *Set40: the canonical CCSD(T)/CBS interaction energies for dimers comprising up to 40 atoms*
14:20 – 14:40	C2	**Jannis Erhard** – Friedrich Alexander Universität Erlangen, Germany *σ-Functionals: a Novel Family of Correlation Functionals Yielding Chemical Accuracy at Low Computational Cost*
14:40 – 15:00	C3	**Dmitry Fedorov** – University of Luxembourg, Luxembourg *Success of the Quantum Drude Oscillator (QDO) model in describing non-covalent interactions*
15:00 – 15:20	C4	**Milan Ončák** – Leopold-Franzens-Universität Innsbruck, Austria *Small Iron-Containing Ions: Spin-Orbit Coupling, Symmetry Breaking, and Signals from Space*
15:20 - 15:40		Coffee break

		Session 2 – Chair: Claudia Draxl
15:40 – 16:20	I2	**Karsten Reuter** – FHI Berlin, Germany *First-Principles based Modelling of Electrocatalysis Beyond the Potential of Zero Charge*
16:20 – 16:40	C5	**Oliver T. Hofmann** – Graz University of Technology, Austria *Designing Polymorphs: The Role of the Substrate for Intermolecular Interactions*
16:40 – 17:00	C6	**Dirk Andrae** – Freie Universität Berlin, Germany *Many-to-one Mapping in Electronic Structure Calculations for Molecules and Surfaces*
17:00 – 17:20	C7	**Peter Puschnig** – University of Graz, Austria *Benchmarking density functional methods with photoemission orbital tomography*
17:20 – 19:00		Free Time
19:00 – 22:00		Poster Session

Tuesday, July 4

		Session 3 – Chair: Gregory Beran
09:00 – 09:40	I3	**Claudia Draxl** – Humboldt-Universität zu Berlin, Germany *Level alignment and excitations at interfaces between molecules and 2D materials*
09:40 – 10:00	C8	**Christian W. Binder** – Graz University of Technology, Austria *Introducing Zorro – a novel code for molecular transport phenomena*
10:00 – 10:20	C9	**Héloïse Leboucher** – University of Toulouse - Paul Sabatier, France *Modeling the interaction between PAH clusters and water aggregates: structures and energetics*
10:20 – 10:40		Coffee break
		Session 4 – Chair: Alexandre Tkatchenko
10:40 – 11:20	I4	**Leeor Kronik** – Weizmann Institute of Science, Israel *Understanding structure-property relations in biological and bio-inspired molecular crystals from first principles*
11:20 – 11:40	C10	**Esteban Vöhringer-Martinez** – Universidad de Concepción, Chile *ffparAIM: A Python workflow for non-covalent force field parameter derivation and its applications.*
11:40 – 12:00	C11	**Matthias Stein** – Max Planck Institute for Dynamics of Complex Technical Systems, Germany *Non-covalent Interactions in Organometallic Crystals*
12:00 – 13:40		Lunch break
		Session 5 – Chair: Leeor Kronik
13:40 – 14:20	I5	**Barbara Kirchner** – University of Bonn, Germany *Liquid Phase Vibrational Spectra and Reducing Uncertainties in Ionic and Molecular Liquids simulation*
14:20 – 14:40	C12	**Ctirad Cervinka** – University of Chemistry and Technology, Prague, Czechia *Volatility of Ionic Liquids from First Principles: Where Experiments Can Hardly Reach*
14:40 – 15:00	C13	**Michael Hütter** – Universität Innsbruck, Austria *Master Equation Modeling of Water Dissociation in Small Ions: $Ag^+(H_2O)_n$, n = 4-6*
15:00 – 15:20	C14	**Maren Podewitz** – TU Wien, Austria *An Automated Approach to Quantum Chemical Microsolvation*
15:20 – 15:40		Coffee break

		Session 6 – Chair: Barbara Kirchner
15:40 – 16:20	I6	**Feng Wang** – University of Arkansas, USA *MP2 and DFT based ensemble property predictions rival the accuracy of experimental measurements*
16:20 – 16:40	C15	**Gabriel Rath** – RWTH Aachen University, Germany *Configuration Integral Monte Carlo Integration (CIMCI): Anharmonic Thermochemistry with Low-Cost Hamiltonians*
16:40 – 17:00	C16	**Ramón Hernández-Lamoneda** – CIQ-IICBA/UAEM, Mexico *Local structure of liquid oxygen up to supercritical conditions from ab initio pair potentials*
17:00 – 17:20	C17	**Jasmina Savolović** – Institute for Medical Research and Occupational Health, Croatia *Structure Prediction of Physiological Bis(aminoacidato)copper(II) Species in Aqueous Solution: Bis(L-glutaminato)copper(II)*
17:20 – 18:30		Free Time
18:30 – 22:00		Conference Dinner

Wednesday, July 5

		Session 7 – Chair: Erin R. Johnson
09:00 – 09:40	I7	**Gregory Beran** – University of California Riverside, USA *Designing Organic Photomechanical Engines with Exceptional Work Capacities*
09:40 – 10:00	C18	**Reinhold Fink** – University of Tübingen, Germany *Orbital contributions explain strongly anisotropic exchange-repulsion energies and unexpected aggregate structures*
10:00 – 10:20	C19	**Georg Jansen** – Universität Duisburg-Essen, Germany *How intermolecular interactions modify the structure of $Te(BiR_2)_2$ in the solid phase*
10:20 – 10:40		Coffee break
		Session 8 – Chair: Anne-Marie Kelterer
10:40 – 11:20	I8	**Erin R. Johnson** – Dalhousie University, Canada *Numerical Atomic Orbital Implementation of the Exchange-Hole Dipole Moment Dispersion Model*
11:20 – 11:40	C20	**Jessica C. Hartmann** – Universität Innsbruck, Austria *Searching for the Origin of Magic Numbers amongst Sodium Chloride Clusters*
11:40 – 12:00	C21	**Ivor Lončarić** – Ruđer Bošković Institute, Croatia *Machine learning interatomic potentials for molecular crystals*
12:00 – 13:40		Lunch break

		Session 9 – Chair: Alexander F. Sax
13:40 – 14:20	I9	**Jan M. L. Martin** – Weizmann Institute of Science, Israel *Affordable approaches for benchmarking noncovalent interactions: localized coupled cluster theory and minimally empirical double hybrid DFT*
14:20 – 14:40	C22	**Almaz Khabibrakhmanov** – University of Luxembourg *Universal pairwise interatomic van der Waals potentials from quantum Drude oscillators*
14:40 – 15:00	C23	**Jan Řezáč** – Institute of Organic Chemistry and Biochemistry of the CAS, Czech Republic *Non-covalent interactions in semiempirical QM methods: from simple corrections to machine learning*
15:00 – 15:20	C24	**W. Andrzej Sokalski** – Wroclaw University of Science and Technology, Poland *Applications of the Theory of Intermolecular Interactions in the Rational Design of Inhibitors and Catalysts*
15:20 – 15:40	C25	**Igor Poltavskyi** – University of Luxembourg, Luxembourg *Force Field Analysis Software and Tools (FFAST)*
15:40 – 16:00		Coffee break

		Session 10 – Chair: Jan M. L. Martin
16:00 – 16:40	I10	**Konrad Patkowski** – Auburn University, USA *Making Symmetry-Adapted Perturbation Theory More Accurate and More Robust*
16:40 – 17:00	C26	**Michal Hapka** – University of Warsaw, Poland *Symmetry-Adapted Perturbation Theory Based on Multiconfigurational Wave Function Description of Monomers*
17:00 – 17:20	C27	**John Herbert** – The Ohio State University, USA *High-Order Many-Body Expansions Via a Bottom-Up Approach*
17:20 – 17:40	C28	**Johannes Hoja** – University of Graz, Austria *Anharmonic Vibrational Frequencies of Non-Covalently Bound Systems via Vibrational Perturbation Theory*
17:40 – 18:00		Closing Ceremony