Atomistic Simulation Center Symposium
28.11.2022

14:00 – 14:10	Opening
14:10 – 15:30	**ML and Networks 1 (Thomas Kühne)**
14:10 – 14:50	**Markus Reiher**: Machine-learning enhanced exploration of chemical reaction networks
14:50 – 15:30	**Jörg Behler:** Atomistic Simulations with High-Dimensional Neural Network Potentials
15:30 – 15:50	**Coffee break**
15:50 – 17:10	**Quantum methods for many body systems (Andreas Görling)**
15:50 – 16:30	**Hilke Bahmann**: Application of flexible hybrid density functionals to molecule-solid interfaces in dye-sensitized solar cells
16:30 – 16:50	**Tobias Dornheim**: Ab initio path integral Monte Carlo simulation of electrons at extreme conditions
16:50 – 17:10	**Attila Cangi**: Accelerating Density Functional Theory with Neural Networks
17:10 – 17:30	**Coffee break**
17:30 – 18:50	**ML and Networks 2 (Tim Clark)**
17:30 – 18:10	**Karsten Reuter**: Exploring Catalytic Reaction Networks with Machine Learning
18:10 – 18:50	**Christoph Jacob**: Massively parallel quantum chemistry with the density-based many body expansion

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14:10 – 15:30	**Many Body and Complex systems (Carsten Bauer)**
14:10 – 14:50	**Carolin König**:Tailored quantum chemistry for electronic interaction energies, potential energy surfaces, and vibrational wave functions
14:50 – 15:10	**Dominik Munz**: Modelling Meets Chemical Synthesis: Zwitterions and Diradicals for Catalysis and Organic Electronic Materials
15:10 – 15:30	**Fakher Assaad**: The Algorithms for Lattice Fermions (ALF) Library: A toolbox to for simulations of strongly correlated electron systems
15:30 – 15:50	**Coffee break**
15:50 – 17:10	**Slow Dynamics in Liquid Matter (Felix Hoefling)**
15:50 – 16:30	**Jürgen Horbach**: Computer simulation of glassforming systems (under shear)
16:30 – 16:50	**Benjamin Dalton**: Extracting memory-dependent friction from large-scale protein folding simulations
16:50 – 17:10	**Roya Ebrahimi Viand**: Liquid flow through nanoporous media
17:10 – 17:30	**Coffee break**
17:30 – 18:50	**ML for Biomolecular Simulations (Petra Imhof)**
17:30 – 18:10	**Gerhard Stock**: Biomolecular Reaction Coordinates
18:10 – 18:50	**Marcus Weber**: Combining Molecular Simulation with Machine Learning
18:50-19:00	**Closing**

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