

# Atomistic Simulation Center Symposium 28.11.2022

14:00 – 14:10

Opening

14:10 – 15:30

**ML and networks 1 (Thomas Kuehne)**

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 Goerling)**

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	<b>Many Body and Complex systems</b>
14:10 - 14:50	<b>Carolin König:</b>
14:50 - 15:10	<b>Dominik Munz:</b> Modelling Meets Chemical Synthesis: Zwitterions and Diradicals for Catalysis and Organic Electronic Materials
14:50 - 15:50	<b>Fakher Assaad:</b> The Algorithms for Lattice Fermions (ALF) Library: A toolbox to for simulations of strongly correlated electron systems
15:30 - 15:50	<b>Coffee break</b>
15:50 - 17:10	<b>Slow Dynamics in Liquid Matter (Felix Hoefling)</b>
15:50 - 16:30	<b>Jürgen Horbach:</b> Computer simulation of glassforming systems (under shear)
16:30 - 16:50	<b>Benjamin Dalton:</b>
16:50 - 17:10	<b>Roya Ebrahimi Viand:</b> Liquid flow through nanoporous media
17:10 - 17:30	<b>Coffee break</b>
17:30 - 18:50	<b>ML for Biomolecular Simulations</b>
17:30 - 18:10	<b>Gerhard Stock:</b> Biomolecular Reaction Coordinates
18:10 - 18:50	<b>Marcus Weber:</b> Combining Molecular Simulation with Machine Learning
18:50-19:00	<b>Closing</b>



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