Research report

2015

Overview

PI

Jun.-Prof. Dr. M. Korth, Institute for Theoretical Chemistry, Ulm University, Germany

Research fields

Molecular materials for electrochemical energy storage

Multiscale modelling in computational materials science

Quantum Biochemistry

Citizen Cyber Science

Publications

Articles / published (peer reviewed)

T. Husch, **M. Korth**, How to estimate solid-electrolyte-interphase features when screening electrolyte materials, *Phys. Chem. Chem. Phys.* **2015,** *17,* 22799.

T. Husch, **M. Korth**, Charting the known chemical space for non-aqueous Lithium-air battery electrolyte solvents, *Phys. Chem. Chem. Phys.* **2015,** *17,* 22596.

C. Schütter, T. Husch, **M. Korth**, A. Balducci, Toward new solvents for EDLCs: From computational screening to electrochemical validation, *J. Phys. Chem. C* **2015,** *119,* 13413.

T. Husch, N. D. Yilmazer, A. Balducci, **M. Korth**, Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: computing infrastructure and collective properties, *Phys. Chem. Chem. Phys.* **2015,** *17,* 3394. (Computational chemistry highlight March 2015, top-scoring Altmetrics article in PCCP March 2015.)

N. D. Yilmazer, **M. Korth**, Enhanced semiempirical quantum-mechanical methods for biomolecular interactions, *Comp. Struct. Biotech. J.* **2015,** *13,* 169. (Invited mini-review.)

N. D. Yilmazer, P. Heitel, T. Schwabe, **M. Korth**, Benchmark of electronic structure methods for protein-ligand interactions based on highlevel reference data, *J. Theor. Comput. Chem.* **2015,** *14,* 1540001.

Book contributions (peer reviewed)

M. Korth, Computational Studies of Solid Electrolyte Interphase Formation. In: *Chemical Modeling: Volume 11*, M. Springborg, J.-O. Joswig, Ed., Royal Society of Chemistry, London, UK, **2015.** (Invited book chapter.)