Research report

Computational Materials Science (2011-2016)

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

Citizen Cyber Science

Publications

Articles / published (peer reviewed)

C. Schütter, T. Husch, V. Viswanatan, S. Passerini, A. Balducci, **M. Korth**, Rational design of new electrolyte materials for EDLCs, *J. Power Sources* **2016,** *326,* 541. (Invited article.)

S. Brox, S. Röser, T. Husch, S. Hildebrand, O. Fromm, **M. Korth**, M. Winter, I. Cekic-Laskovic, Alternative single solvent electrolytes based on cyano-esters for safer lithium ion batteries, *Chem. Sus. Chem.* **2016,** *9,* 1704.

R. Wagner, B. Streipert, V. Kraft, A. R. Jimenez, S. Röser, J. Kasnatscheew, D. R. Gallus, M. Börner, C. Mayer H. F. Arlinghaus, **M. Korth**, M. Amereller, I. Cekic-Laskovic, M. Winter, Counterintuitive Role of Magnesium Salts as Effective Electrolyte Additives for High Voltage Lithium-Ion Batteries, *Adv. Mater. Interfaces* **2016,** *3,* 1600096.

P. Ray, S. Dohm, T. Husch, C. Schütter, K. A. Persson, A. Balducci, B. Kirchner, **M. Korth**, Insights into bulk electrolyte effects on the operative voltage of EDLCs, *J. Phys. Chem. C* **2016,** *120,* 12325.

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.)

M. Korth, Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: evaluation of electronic structure theory methods, *Phys. Chem. Chem. Phys.* **2014,** *16,* 7919.

M. Korth and W. Thiel, Benchmarking Semiempirical Methods for Thermochemistry, Kinetics, and Noncovalent Interactions: OMx Methods Are Almost As Accurate and Robust As DFT-GGA Methods for Organic Molecules, *J. Chem. Theory Comput.* **2011,** *7,* 2929–2936. (Computational chemistry highlight November 2012, most popular computational chemistry highlight #5 2012.)

M. Korth, S. Grimme and M. D. Towler, The Lithium-thiophene Riddle Revisited, *J. Phys. Chem. A* **2011,** *115,* 11734–9.