Research report

Computational Materials Science UPDATE (2011-2017)

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)

M. Korth, DFT: Not quite the right answer for the right reason yet, *Angew. Chem. Int. Ed.* **2017,** *56,* 5396–5398. (Invited contribution.)

M. Korth, DFT: Noch nicht ganz die richtige Antwort aus den richtigen Gründen, *Angew. Chem.* **2017,** *129,* 5482–5484. (Invited contribution.)

R. Wagner, V. Kraft, B. Streipert, J. Kasnatscheew, D. R. Gallus, M. Amereller, **M. Korth**, I. Cekic-Laskovica, M. Winter, Magnesium-based additives for the cathode slurry to enable high voltage application of lithium-ion batteries, *Electrochim. Acta* **2017,** *228,* 9.

C. Schütter, S. Passerini, **M. Korth**, A. Balducci, Cyano Ester as Solvent for High Voltage Electrochemical Double Layer Capacitor, *Electrochim. Acta* **2017,** *224,* 278.

S. Dohm, E. Spohr, **M. Korth**, Developing Adaptive QM/MM Computer Simulations for Electrochemistry, *J. Comput. Chem.* **2017,** *38,* 51.

D. S. Firaha, M. Thomas, O. Holloczki, **M. Korth**, B. Kirchner, Can dispersion corrections annihilate the dispersion-driven nano-aggregation of non-polar groups? An ab initio molecular dynamics study of ionic liquid systems, *J. Chem. Phys.* **2016,** *145,* 204502.

R. Wagner, **M. Korth**, B. Streipert, J. Kasnatscheew, D. R. Gallus, S. Brox, M. Amereller, I. Cekic-Laskovica, M. Winter, Impact of Selected LiPF6 Hydrolysis Products on the High Voltage Stability of Lithium-Ion Battery Cells, *ACS Appl. Mater. Interfaces* **2016,** *8,* 30871.

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. Advances in Engineering key scientific 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.)

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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.

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.)