

## Research report

### Second funding period

(2015 – 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

Quantum Biochemistry

Citizen Cyber Science

#### Publications

**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 LiPF<sub>6</sub> 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.)

- N. D. Yilmazer, **M. Korth**, Prospects of applying enhanced semi-empirical QM methods for virtual drug design, *Curr. Med. Chem.* **2016**, *23*, 2101. (Invited review.)
- 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.
- N. D. Yilmazer, **M. Korth**, Recent progress in treating Protein-Ligand interactions with quantum-mechanical methods, *Int. J. Mol. Sci.* **2016**, *17*, 742. (Invited review.)
- 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.
- 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.)
- K. Vojinovic, N. W. Mitzel, **M. Korth**, R. Fröhlich, S. Grimme, Trifluoromethyl Silicon Compounds with Geminal Nitrogen Donor Centers. In: *Organosilicon Chemistry VI*, N. Auner, J. Weis, Ed., Wiley-VCH, Weinheim, Germany, **2005**.