

## Research report

### 2017 part I

#### 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.