Research report

First funding period

(2011 – 2014)

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)

J. C. Kromann, A. Christensen, C. Steinmann, **M. Korth**, J. H. Jensen, A third-generation dispersion and third-generation hydrogen bonding corrected PM6 method: PM6-D3H+, *PeerJ* **2014,** *2,* e449.

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.

N. D. Yilmazer, **M. Korth**, Comparison of Molecular Mechanics, Semi-Empirical Quantum Mechanical, and Density Functional Theory Methods for Scoring Protein-Ligand Interactions, *J. Phys. Chem. B* **2013,** *117,* 8075. (Computational chemistry highlight November 2013.)

M. Korth, A quantum chemical view of enthalpy-entropy compensation, *Med. Chem. Commun.* **2013,** *4,* 1025.

M. Korth, Error estimates for (semi-)empirical dispersion terms and large biomacromolecules, *Org. Biomol. Chem.* **2013,** *11,* 6515.

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, Empirical Hydrogen-Bond Potential Functions – An Old Hat Reconditioned, *Chem. Phys. Chem.* **2011,** *12,* 3131–3142. (Invited mini-review, including original research.)

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

Book contributions (peer reviewed)

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.**