

Research report

– 2010

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)

M. Korth, Third-generation Hydrogen-bonding Corrections for Semiempirical QM Methods and Force Fields, *J. Chem. Theory Comput.* **2010**, *6*, 3808–3816.

M. Korth, M. Pitonak, J. Rezac, P. Hobza, A Transferable H-Bonding Correction for Semiempirical Quantum-Chemical Methods, *J. Chem. Theory Comput.* **2009**, *6*, 344–352. (J. Chem. Theory Comput. most read article #9 in I/2010.)

M. Korth, S. Grimme, Mindless DFT Benchmarking, *J. Chem. Theory Comput.* **2009**, *5*, 993–1003. (J. Chem. Theory Comput. most cited article #15 over the first 3 years.)

M. Korth, A. Luechow, S. Grimme, Toward the Exact Solution of the Electronic Schroedinger Equation for Noncovalent Molecular Interactions: Worldwide Distributed Quantum Monte Carlo Calculations, *J. Phys. Chem. A* **2008**, *112*, 2104–2109.

S. Grimme, M. Steinmetz, **M. Korth**, Stereoelectronic Substituent Effects in Saturated Main Group Molecules: Severe Problems of Current Kohn-Sham Density Functional Theory, *J. Chem. Theory Comput.* **2007**, *3*, 42–45. (J. Chem. Theory Comput. most cited article #4 in 2007)

S. Grimme, M. Steinmetz, **M. Korth**, How to Compute Isomerization Energies of Organic Molecules with Quantum Chemical Methods, *J. Org. Chem.* **2007**, *72*, 2118–2126. (J. Org. Chem. most cited article #7 in 2007)

S. Grimme, C. Diedrich, **M. Korth**, The Importance of Inter- and Intramolecular van der Waals Interactions in Organic Reactions: the Dimerization of Anthracene Revisited, *Angew. Chem. Int. Ed.* **2006**, *45*, 625–629.

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**.