

Research report

2011

Overview

PI

Jun.-Prof. Dr. M. Korth, Institute for Theoretical Chemistry, Ulm University, Germany

Research fields

Quantum Biochemistry

Citizen Cyber Science

Publications

Articles / published (peer reviewed)

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.