Intermolecular Interactions in Molecular Systems with 1000 and More Atoms — A Challenge for Quantum Chemistry

Christian Ochsenfeld

Chair of Theoretical Chemistry, Department of Chemistry,
University of Munich (LMU), Butenandtstr. 7 (C), D-81377 Munich

www.cup.uni-muenchen.de/pc/ochsenfeld/

Quantum chemistry has evolved over the last decades to become a versatile tool for studying structures and properties of molecular systems. Despite this success, the applicability to large molecules is hampered by the strong polynomial increase of the computational effort with molecular size M. Therefore a central goal of our work is to overcome this scaling wall and to develop linear-scaling methods, which allow for quantum-chemical studies of molecular systems with 1000 and more atoms at Hartree-Fock (HF), Density-Functional Theory (DFT), and Møller-Plesset (MP2) levels. At the same time our methods guarantee fully-controlled numerical accuracies, so that no reliability is lost. While in general HF and todays DFT approaches provide often useful results for describing many molecular properties (e.g., NMR), they fail for the calculation of intermolecular interaction energies, since dispersion-type effects are not or not sufficiently accounted for. However, such interactions are crucial for many chemical and biochemical processes. Here, our new MP2 method for reducing the $\mathcal{O}(M^5)$ scaling to linear offers new possibilities, since it allows for the calculation of large systems such as, e.g., an RNA system with 1664 atoms and 19 182 basis functions. The presentation will give an overview on new possibilities of quantum-chemical methods for studying complex systems. Furthermore, examples for a fruitful interplay between theory and experiment will be presented, which allows to gain new insights into molecular processes: the calculation of intermolecular interactions within molecular recognition processes, RNA-catalyzed Diels-Alder reactions, and receptor-virus interactions.