Introduction to and Applications of Computational Quantum Chemistry for the Accurate Characterization of Non-Covalent Interactions in Molecular Clusters

Gregory S. Tschumper
Department of Chemistry and Biochemistry, University of Mississippi
University, Mississippi 38677–1848 USA
tschumpr@olemiss.edu http://quantum.chem.olemiss.edu

Non-covalent interactions, such as hydrogen bonding and London dispersion forces, play vital roles in a wide range of chemical, physical and biological phenomena. Examples include, but are certainly not limited to, molecular recognition and self-assembly processes as well as the structure and function of biological macromolecules. Reliable *ab initio* electronic structure calculations have provided much insight into the strength, anisotropy and nature of these relatively weak interactions [1]. The first half of this talk will provide a very basic introduction to fundamental principles and concepts associated with quantum mechanical (QM) electronic structure computations. This "crash course" in computational quantum chemistry will set the stage for the remainder of the lecture that will highlight some of our recent work characterizing small clusters of molecules held together by non-covalent interactions [2,3]. If time permits, recent developments in our n-body:Many-body QM:QM methods for non-covalent clusters [4,5] will also be discussed, including analytic 1st and 2nd geometrical derivatives (i.e., gradients and Hessians).

References (click on a reference to access the DOI link)

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