Hydrogen bonding in small model peptides; The DFT and MP2 study

Gracie Smith

Martina Kaledin
Kennesaw State University

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Gracie Smith, Martina Kaledin

Department of Chemistry & Biochemistry, Kennesaw State University, 370 Paulding Ave NW, Box # 1203, Kennesaw, GA 30144

Abstract

Formamide is a small model compound for the study of the peptide bond. The peptide bond links amino acids together, specifies rigidity to the protein backbone, and includes the essential docking sites for hydrogen-bond-mediated protein folding and protein aggregation, namely, the C=O acceptor and the N-H donor parts. Therefore, the infrared C=O (amide-I) and N-H (amide-A) vibrations provide sensitive and widely used probes into the structure of peptides. This computational chemistry work, we study hydrogen bonds in formamide dimer isomers. We evaluate the accuracy of the density functional theory (DFT) and many-body perturbation theory to the 2nd order (MP2) methods in the prediction of structural parameters and vibrational frequencies of formamide and formamide dimer. Also, we assess the importance of basis set superposition error when evaluating binding energy of formamide dimer isomers. This project introduces undergraduate students to methods and tools of computational chemistry.