

Poster abstract

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Title: Introducing BSSE as an extra energy term in molecular dynamics

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Summary (max 200 words):

A radial distribution function (RDF) is a useful tool for studying the structure of liquids. In quantum calculations the basis set superposition error (BSSE) is suspected to overestimate the attractive interaction between the molecules of the liquid. We focus on a specific category of molecules which interact with each other by hydrogen bonds, which occur in e.g. water, methanol or ethanol. In this paper, RDF's are studied with DFT-based molecular dynamics (MD) with high quality basis sets in order to examine the effect of BSSE on the structure of the fluid. After an initial MD simulation, static BSSE-computations are done on well-chosen pairs of molecules. On this data, an exponential model of the form $A \cdot \exp(-B \cdot r)$ is fitted to the BSSE for each type of interaction, where r is the distance between atom pairs, rendering values for the A and B parameters. Then, *a posteriori*, the resulting extra classical energy term is added in a final MD-run. The RDF's computed from the MD-run with and without the BSSE correction term are then compared.