

Exploring Intermolecular Correlation with SAPT, vdW-Corrected DFT, and Diffusion Monte Carlo Methods

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This talk will focus on several projects underway in the group in which weak interactions play a role. In particular, the results of symmetry-adapted perturbation theory (SAPT) for analyzing interactions in water clusters and the adsorption of water molecules on acenes will be presented. Benchmark interaction energies have also been obtained by means of quantum Monte Carlo calculations and used to assess the performance of various vdW-corrected DFT methods as well as of the RPA method.