DFT TEST STUDY ON VAN DER WAALS DIMERS

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Potential energy surfaces are obtained in the framework of the supermolecule approach by using density functional theory and basis sets optimized in generalized gradient approximation exchange-correlation calculations supplemented by bond functions placed at the midpoint of the van der Waals bond. They are compared to surfaces obtained using single and double excitation coupled-cluster theory with noniterative treatment of triple excitations CCSD(T) and correlation-consistent basis sets supplemented by bond functions. Bonding properties and Vertical excitation electronic spectra of $N_2 - He$ and $CO^+ - He$ van der Waals molecules will be presented and compared to recent theoretical results.