# On the role of the basis set and electron correlation in the description of stacking interactions.

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Streszczenie

*Ab initio* SCF and Möller-Plesset electron correlations, up to fourth-order calculations, have been performed for a very simple model system of stacking interactions—the water dimer with parallel and antiparallel dipole-dipole orientations. The performance of a variety of basis sets in evaluating the basis set superposition error and the interaction energy has been systematically examined. It is shown that for a proper description of the stacking interaction the diffuse *sp*-functions as well as the multiple sets of polarization functions are required. Additional calculations were carried out with popular semi-empirical methods (MNDO, AMI and PM3). All of the applied semi-empirical methods greatly overestimate the interaction forces and give qualitatively incorrect results.

Słowa kluczowe

stacking interactions, ab initio calculations, diffuse functions, electron correlation, dispersion energy, BSSE

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