THREE-BODY EFFECTS IN DFT VIA MUTUAL POLARIZATION OF FRAGMENT DENSITIES

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The Pauli Blockade method allows calculations of noncovalent interactions via mutual polarization of fragment densities. When based on Kohn-Sham description of the monomers [1] Pauli Blockade may be recast into a rigorous dispersion-free DFT approach termed PBdf. We present an extension of the dispersion-free Pauli Blockade method to the three-body case. We compare the performance of PBdf to that of supermolecular DFT and wavefunction methods for a series of trimers ranging from the model He_3, Ar_3, Ar_2-HF and Ar_2-HCl complexes to the selected systems from the 3B-69 test set [2]. Both PBdf and supermolecular DFT results are analyzed using the partitioning of the nonadditive three-body energy into the exchange and deformation contributions [3]. The performance of different xc functionals is tested, including range-separated hybrids.

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