An accurate water dimer interaction potential from symmetry-adapted perturbation theory calculations

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In recent years the symmetry-adapted perturbation theory (SAPT) ansatz of Jeziorski and coworkers has proven to be a valuable alternative to supermolecular calculations for the determination of accurate intermolecular potential energy surfaces. In particular it offers the advantage of breaking down the total interaction energy to not-multipole-expanded electrostatic, induction and dispersion energy contributions and their exchange corrections, thus providing the opportunity to fit analytic expressions to the individual physical terms. The poster presents our accurate SAPT calculations of the potential energy surface for the water dimer. Technical questions such as basis set requirements for the individual energy components and the influence of bond function locations upon them have been carefully investigated, allowing to improve the efficiency of the calculations. For some points on the potential energy surface the results are compared to the outcome of MP4 and CCSD(T) calculations.