Abstract Submitted
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Chemically accurate description of aromatic rings interaction using quantum Monte Carlo SAM AZADI, Department of Physics and Thomas Young Centre, University College London — We present an accurate study of interactions between benzene molecules using wave function based quantum Monte Carlo (QMC) methods [1]. We compare our QMC results with density functional theory (DFT) using various van der Waals (vdW) functionals. This comparison enables us to tune vdW functionals. We show that highly optimizing the wave function and introducing more dynamical correlation into the wave function are crucial to calculate the weak chemical binding energy between benzene molecules. The good agreement among our results, experiments and quantum chemistry methods, is an important sign of the capability of the wave function based QMC methods to provide accurate description of very weak intermolecular interactions based on vdW dispersive forces. \pardReferences:1] Sam Azadi, and R. E. Cohen, J. Chem. Phys. **143**, 104301 (2015).

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