Abstract Submitted
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Quantum Monte Carlo backflow calculations of the benzene dimer[1] KATHLEEN SCHWARZ, Cornell University, Department of Chemistry and Department of Materials Science and Engineering, RICHARD HENNIG, Cornell University, Department of Materials Science and Engineering — Benzene dimers provide the prototypical system for weak pi-pi interactions that determine the bonding for various organic materials and carbon nanostructures. Several previous studies using coupled-cluster, symmetry adapted perturbation theory, and quantum Monte Carlo methods have determined the binding energies of various configurations of the benzene dimer. In this work we investigate the accuracy of different trial wave functions for variational and diffusion Monte Carlo calculations for a set of candidate ground state dimer geometries. We compare Slater, Slater Jastrow, Slater Jastrow Backflow, and Multi-determinant wave functions. The inclusion of backflow improves our VMC and DMC total energies more than orbital optimization, larger basis sets, and increasing the number of determinants in the trial wave function. Using Slater Jastrow Backflow wave functions, we calculate the binding energies of the benzene dimers.

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Kathleen Schwarz
Cornell University, Department of Chemistry and
Department of Materials Science and Engineering

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