Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Multideterminant quantum Monte Carlo calculations of benzene dimers[1] RICHARD G. HENNIG, KATHLEEN A. SCHWARZ, Cornell University, Department of Materials Science and Engineering, CYRUS UMRIGAR, Cornell University, Department of Physics, JULIEN TOULOUSE, Universite Pierre et Marie Curie, France — Benzene dimers represent the prototypical system for weak π-π interactions that determine the bonding for various organic materials and carbon nanostructures. Several previous studies using coupled-cluster and quantum Monte Carlo methods have determined the binding energy of parallel, perpendicular and parallel-shifted configurations of the benzene dimer. Here we present multideterminant variational and diffusion Monte Carlo calculations for the various benzene dimer configurations. The total energy of the benzene dimers depends strongly on basis set size, orbital coefficients and number of determinants in the trial wave function. The binding energy converges faster than the total energy with basis set size and number of determinants due to partial cancellation of errors. While orbital optimization lowers the total energy, the large number of orbital parameters and hence large computational cost limits orbital optimizations to wave functions with small basis sets and small numbers of determinants. In comparison the optimization of the Jastrow and determinant coefficients can efficiently converge the energy of benzene dimers and enables accurate predictions of the binding energies.

[1] Funded by the DOE petascale initiative.

Richard Hennig
Cornell University

Date submitted: 29 Nov 2008

Electronic form version 1.4