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A Quantum Monte Carlo study of Molecular Hydrogen adsorbed on Benzene TODD D. BEAUDET, JEONGNIM KIM, MICHELE CASULA, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign, SIMONE CHIESA, University of California at Davis — Many prospective hydrogen storage systems contain carbon scaffolding comprised of benzene-like structural units. The binding energy of H_2 with these benzene-like rings is below the $\sim$ 0.2-0.4 eV/H_2 target necessary for reversible adsorption[1]. Here we study the hydrogen-benzene system using quantum Monte Carlo (MC) methods suitable for resolving small energy differences. Potential energy curves are calculated using correlated umbrella sampling and variational MC. Reptation MC calculations are also in progress. A Jastrow correlated geminal wave function previously applied to benzene[2] is compared to Slater-Jastrows with orbitals derived from the PBE and B3LYP density functionals. We compare our results to previous work[3] and discuss our progress on larger systems that may have the desired binding affinity.

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