Abstract Submitted for the MAR08 Meeting of The American Physical Society

**Progress in the study of Molecular Hydrogen–Benzene binding**<sup>†</sup> TODD D. BEAUDET, MICHELE CASULA, JEONGNIM KIM, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — In this work we present a quantum Monte Carlo study of the hydrogen-benzene system where binding is very weak. We demonstrate that the binding is well described at both the VMC and DMC levels by a single determinant correlated geminal wave function<sup>1</sup> with an optimized compact basis set that includes diffuse functions. Agreement between VMC and fixed node DMC binding energies is found to be within 0.18 mHa, suggesting the calculations are well-converged with respect to the basis. This relative insensitivity to basis set and superposition error is an advantage of the QMC methods we employ. Comparison is made with a Slater-Jastrow wave function at the DMC level using a trial function comprised of PBE single-body orbitals, empirical models and previous work<sup>2</sup>. The physical underpinnings of the interaction will be discussed including the role of diffuse basis functions in this system. Progress on systems where binding is expected to be more favorable for practical hydrogen storage will also be presented.

<sup>1</sup> M. Casula, C. Attaccalite, and S. Sorella, J. Chem. Phys. 121, 7110 (2004).
<sup>2</sup> S. Hamel and M. Côté, J. Chem. Phys. 121, 12618 (2004).

 $^\dagger$  Supported by NSF DMR03-25939 and A6062 Army UMC00005071-3

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Date submitted: 27 Nov 2007

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