Abstract Submitted
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A Quantum Monte Carlo study of Hydrogen Adsorption on Carbon and Transition Metal Systems[1] TODD D. BEAUDET, University of Illinois at Urbana-Champaign, Presently U. S. Army Research Laboratory, JEONGNIM KIM, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — We present a quantum Monte Carlo study of many molecular structures of Ti-ethylene with up to 5 H_2 molecules. These structures have been of recent interest due to energetics favorable for reversibly storing hydrogen.[2] Diffusion Monte Carlo is employed with the fixed node approximation and pseudopotentials that have been tested for H_2 adsorbed on benzene and calculations on TiH_2 molecules.[3] Many low energy configurations were studied by calculation of ground and excited states energy surfaces. The formation energies are comparable to other work[4] and indicate that at least 3 hydrogen molecules can be adsorbed with energies in the range considered relevant for practical hydrogen storage.

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[2]E. Durgun *et al.*, Phys. Rev. Lett. **97**, 226102 (2006).
[3]T. D. Beaudet, Doctoral Dissertation, University of Illinois at Urbana-Champaign (2010).
[4]Y. Y. Sun *et al.*, Phys. Rev. B **82**, 073401 (2010).

Todd D. Beaudet
University of Illinois at Urbana-Champaign,
Presently U. S. Army Research Laboratory

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