

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

A Quantum Monte Carlo Study of Molecular Titanium Systems¹

TODD D. BEAUDET, JEONGNIM KIM, KENNETH ESLER, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — We present a quantum Monte Carlo study of molecular TiH₂ and Ti-ethylene-hydrogen complexes which have been of recent interest for their relation to systems that can reversibly adsorb hydrogen.^{2,3,4} We study these systems using diffusion Monte Carlo with the fixed-node approximation and pseudopotentials. The symmetry and nodal structure used are determined by trial wave functions constructed of molecular orbitals from DFT. In the TiH₂ system, the four lowest states have different symmetries and are very close in energy due to the fact that the d-states are almost decoupled from the bonding. We show that partially occupying the relevant d-states at the DFT level allows for the construction of symmetry classified trial functions that are more directly comparable at the DMC level. This procedure has potential to be useful in analogous systems where d-state occupation results in nearly degenerate states of different symmetry.

¹Supported by NSF DMR03-25939.

²E. Durgun *et al.*, Phys. Rev. Lett. **97**, 226102 (2006).

³J. A. Platts, J. Mol. Struct. **545**, 111 (2001).

⁴B. Ma, C. L. Collins, H. F. Schaefer, J. Am. Chem. Soc. **118**, 870 (1996).

Todd D. Beudet
University of Illinois at Urbana-Champaign

Date submitted: 24 Nov 2009

Electronic form version 1.4