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A Quantum Monte Carlo Study of Molecular Titanium Dihydride[†] TODD D. BEAUDET, JEONGNIM KIM, KENNETH ESLER, RICHARD M. MARTIN, University of Illinois at Urbana-Champaign — Recently there has been interest in the possibility of reversibly storing molecular hydrogen on titanium decorated carbon-nanostructures[1]. As part of our research[2] in this area, we present DFT and QMC results for molecular TiH_2 using pseudopotentals. We identify the low energy symmetry-classified states and compare with previous work[3,4], where there is not a consensus on the symmetry and geometry of the ground state. At the DFT level, the TiH_2 d-states are nearly decoupled from the molecular geometry so that several d-state orderings are very close in energy. In our work we use diffusion Monte Carlo with the fixed-node approximation where the symmetry and nodal structure are determined by a trial function constructed of molecular orbitals from DFT. We will also discuss progress on Ti-carbon systems pertaining to hydrogen adsorption.

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