

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Sorting Category: 17.5 (C)

Accuracy of the pseudopotential and fixed-node approximations for C_2 , Si_2 and defects in crystalline Si¹ RICHARD G. HENNIG, Department of Physics, Ohio State University, CYRUS J. UMRIGAR, JULIEN TOULOUSE, Cornell Theory Center, Cornell University, JOHN W. WILKINS, Department of Physics, Ohio State University — Quantum Monte Carlo calculates binding energies and atomic structures for molecules and defect energies in solids. Accurate QMC calculations require the control of the pseudopotential and the fixed-node approximation. The calculated binding energies and bond lengths for the Si and C dimer and the energies of defects in crystalline Si test the accuracy of a range of pseudopotentials and optimized trial-wave functions. For the Si dimer and defects in crystalline Si different pseudopotentials provide similar results. The results for the Si dimer are comparable with experiments with HF pseudopotentials being most accurate. While a single determinant wave functions is sufficient for the Si dimer, the C dimer requires an optimized multi-determinant trial-wave function to achieve experimental accuracy.

¹Supported by NSF (DMR-0205328, EAR-0530301) and DOE (DE-FG02-99ER45795). Computational resources provided by NERSC, NCSA and OSC.

Prefer Oral Session
 Prefer Poster Session

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Date submitted: 03 Dec 2005

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