Accuracy of the pseudopotential and fixed-node approximations for C$_2$, Si$_2$ and defects in crystalline Si[1] 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.

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