Testing Approximations in Quantum Monte Carlo on Silicon Single Self-interstitial Defects

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In quantum Monte Carlo (MC) simulations of solids, a number of controlled and uncontrolled approximations must be made to deal with fermion antisymmetry and improve efficiency. The uncontrolled errors are introduced by the fixed node, pseudopotential, and pseudopotential-locality approximations. Fixed-node error appears to be small when calculating silicon interstitial formation energies with different starting nodes. Comparison of formation energy convergence with cell size using LDA and HF pseudopotentials indicates that the pseudopotential error is small. Good agreement between variational MC and diffusion MC formation energies suggests error due to pseudopotential locality is also small. We estimate each uncontrolled approximation error is typically less than 0.2 eV in silicon interstitial calculations. The controlled errors are associated with Monte Carlo statistics, finite simulation cell size, finite time-step, population control, and numerical representation of orbitals. These errors can be reduced below 0.05 eV by spending more computer time. We compare the efficiency of different numerical orbital interpolation schemes and find B-splines require the least amount of memory for a given accuracy.