

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Energy Optimization of Many-Body Wave Functions: Application to Silicon Interstitial Defects¹ W. D. PARKER, K. P. DRIVER, R. G. HENNIG, J. W. WILKINS, the Ohio State University, C. J. UMRIGAR, Cornell University — Energy minimization [1], as opposed to the standard variance minimization [2], of the Jastrow factor results not only in lower variational Monte Carlo (VMC) energies but also in lower diffusion Monte Carlo (DMC) energies for systems that employ a nonlocal pseudopotential. We apply this approach to solids: single-interstitials in silicon. Allowing the Jastrow for the defect atom(s) to differ from that for bulk atoms lowers the VMC energy but not the DMC energy, indicating the pseudopotential locality error is small. DMC energies from 8 and 64 atom cells (plus interstitial) computed with energy-optimized trial wave functions estimate a 0.2 eV finite-size error in the formation energy. Cubic spline and Lagrange polynomial representations of orbitals have comparable efficiency in memory usage, run time and accuracy. [1] C. J. Umrigar and C. Filippi, Phys. Rev. Lett. 94, 150201 (2005). [2] C. J. Umrigar, K. G. Wilson and J. W. Wilkins, Phys. Rev. Lett. 60, 1719 (1988).

¹Supported by DOE(DE-FG02-99ER45795), Ohio Supercomputing Center, NERSC, NSF(EAR-0530301,DMR-0205328) and Sandia National Laboratories

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Date submitted: 30 Nov 2005

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