

Abstract Submitted  
for the MAR06 Meeting of  
The American Physical Society

Sorting Category: 17.5 (C)

**Energy Optimization of Many-Body Wave Functions:  
Application to Silicon Interstitial Defects<sup>1</sup>** W. D. PARKER, K.  
P. DRIVER, R. G. HENNIG, J. W. WILKINS, the Ohio State Uni-  
versity, C. J. UMRIGAR, Cornell University — Energy minimization  
[1], as opposed to the standard variance minimization [2], of the Jas-  
trow factor results not only in lower variational Monte Carlo (VMC)  
energies but also in lower diffusion Monte Carlo (DMC) energies for sys-  
tems 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 en-  
ergy 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 poly-  
nomial 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).

<sup>1</sup>Supported by DOE(DE-FG02-99ER45795), Ohio Supercomputing Cen-  
ter, NERSC, NSF(EAR-0530301,DMR-0205328) and Sandia National  
Laboratories

Prefer Oral Session  
 Prefer Poster Session

William Parker  
wparker@mps.ohio-state.edu  
the Ohio State University

Date submitted: 30 Nov 2005

Electronic form version 1.4