Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Silicon-interstitials-based Benchmarking of DFT Exchange-correlation Potentials[1] K. P. DRIVER, W. D. PARKER, R. G. HENNIG, J. W. WILKINS, Ohio State U., C. J. UMRIGAR, Cornell U., R. MARTIN, E. BATISTA, B. UBERUAGA, LANL, J. HEYD, G. SCUSERIA, Rice U. — Diffusion Monte Carlo (DMC) benchmarks DFT functionals: LDA, GGA, and HSE [1]. Extensive DFT studies on single-, di-, and tri-interstitials [2] provide stable structures and converged energies. For single-interstitial formation energies, our DMC results confirm earlier work [3], with 1.5 and 1.0 eV underpredictions for LDA and GGA, respectively. We continue to observe this trend in most di- and tri-interstitials. Additionally, we find HSE reproduces DMC results for single-interstitals. Preliminary analysis indicates that large LDA and GGA discrepancies with DMC occur for highly distorted defect configurations.

[1] J. Heyd *et al.*, J.Chem.Phys. **118**, 8207 (2003).

[2] D. A. Richie *et al.*, Phys. Rev. Lett. **92**, 45501 (2004).

[3] W. -K. Leung *et al.*, Phys. Rev. Lett. **83**, 2351 (1999).

[1]Supported by DOE(DE-FG02-99ER45795), NSF (EAR-0530301, DMR-0205328), and Sandia National Laboratory. Computation performed at OSC and NERSC.

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Date submitted: 30 Nov 2005 Electronic form version 1.4