

Abstract Submitted
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Diffusion Monte Carlo Formation Energies of Silicon Self-Interstitial Defects KEVIN P. DRIVER, WILLIAM D. PARKER, PHILLIP R. PETERSON, RICHARD G. HENNIG, JOHN W. WILKINS¹, Dept. of Physics, The Ohio State University, Columbus, OH 43210, CYRUS J. UMRIGAR², Cornell Theory Center, Cornell University, Ithaca, NY 14853 — Silicon self-interstitial defects can hinder the fabrication of semiconductor devices. Several stable single-, di-, and tri-interstitial clusters found with *ab initio* and tight-binding simulations are believed to form in silicon³. Since experimental detection of self-interstitials remains a challenge, accurate theoretical methods are needed to study their properties. The first Diffusion Monte Carlo (DMC) calculations found single-interstitial defect formation energies to be about 1 eV higher than predicted by density functional theory (DFT)⁴. This indicates that DFT may be insufficient for the study of silicon self-interstitials. We confirm the discrepancy between DMC and DFT formation energies for three single-interstitial structures (X, H, and T) and extend the comparison to several di- and tri-interstitial clusters.

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³D. A. Richie et al. *Phys. Rev. Lett.* **92**, 45501 (2004).

⁴W.-K. Leung et al. *Phys. Rev. Lett.* **83**, 2351 (1999).

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