

**Diffusion Monte Carlo Formation Energies of
Silicon Self-Interstitial Defects**

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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 silicon [1]. 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) [2]. 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.

- [1] D. A. Richie, J. Kim, S. A. Barr, K. R. A. Hazzard, R. G. Hennig, and J. W. Wilkins. *Phys. Rev. Lett.* **92**, 45501 (2004).
- [2] W. -K. Leung, R. J. Needs, G. Rajagopal, S. Itoh, and S. Ihara. *Phys. Rev. Lett.* **83**, 2351 (1999).