

Diffusion Monte Carlo Study of Single-, Di-, and Tri-Interstitials in Silicon

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Silicon self-interstitial defects are known to hinder the fabrication and production of semiconductor devices. Stable configurations of the simplest defects, single-, di-, and tri-interstitial clusters, have been found in *ab initio* and tight-binding simulations¹. Experimental techniques do not yet have the resolution to study such defects. Therefore, we must rely on accurate theoretical methods to study their properties. Early Diffusion Monte Carlo (DMC) calculations² found single-interstitial defect formation energies to be about 1 eV higher than predicted by density functional theory (DFT). Our preliminary results confirm the discrepancy between DMC and DFT formation energies for three single-interstitial structures (X, H and T). However, making the comparison for several di- and tri-interstitial clusters, we currently find DMC and DFT are in closer agreement. This work is supported by the DOE (DE-FG02-99ER45795) and NSF. Computational resources provided by Ohio Supercomputer Center and NERSC.

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