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

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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 formation energies of single-interstitials (X, H, and T) to be about 1 eV higher than predicted by density functional theory (DFT) using both 16- and 54- atom supercells [2]. Our results confirm the discrepancy for the single-interstitial structures in the 16-atom supercell. However, using a 64-atom supercell, we find that DFT formation energies of single-, di-, and tri-interstitials are in much closer agreement with DMC values. This work was supported by the DOE(DE-FG02-99ER45795) and NSF. Computational resources provided by Ohio Supercomputer Center and NERSC.

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