Formation Energies of Small Interstitial Clusters: DMC vs. DFT

Kevin P. Driver, William D. Parker, Richard G. Hennig, John W. Wilkins (Department of Physics, Ohio State University, Columbus, OH 43210), Cyrus J. Umrigar (Cornell Theory Center, Cornell University, Ithaca, NY 14853)

Fabrication defects in silicon can degrade performance of semiconductor devices. Diffusion Monte Carlo (DMC) calculations suggest that single-interstitial defects have a higher formation energy (about 1 eV) than predicted by density functional theory (DFT) [1]. Several stable single-, di-, and tri-interstitial structures have been found using *ab initio* and tight-binding molecular dynamics calculations [2]. As a first step in an ongoing DMC study of silicon interstitial defects, we confirm the discrepancy between DMC and DFT formation energies [1] for three single-interstitial structures (X, H and T). Currently, we are in the process of calculating DMC energies of three stable di-interstitial structures to compare with LDA and GGA results.

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