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Density functional study of charged self-interstitials in silicon[1]

AMITA WADEHRA, JOHN W. WILKINS, Ohio State University, RICHARD G. HENNIG, Cornell University — The self-interstitials in silicon created by ion-beam processing determine migration rate of impurities, time evolution of dislocations and dopant-enhanced diffusion. The large mobility of interstitials makes their experimental observation difficult. Electron-assisted transport mechanism suggests that charged states with different migration barriers and minimum energy positions are responsible for this rapid migration. Therefore, it becomes necessary to identify the stable ground state charges for each geometry and electron chemical potential. Recent studies of energetics and migration of these defects have largely concentrated on neutral defects and a few on charged single interstitials. We present a density functional study of electronic structure and energetics of charged single-, di- and tri-interstitials in silicon. An analysis of stability of five different charged states in various geometries is provided through formation energies. The diffusion pathways of these charged interstitials are also discussed.

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