Density functional study of charged self-interstitials in silicon

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Silicon self-interstitials play a significant role in several solid-state processes such as dopant enhanced diffusion. The mobility of interstitials allows them to merge and combine with impurity atoms to form extended defects. Recent studies of energetics and migration of these defects have largely concentrated on neutral defects. We present a first-principles study of the energetics and electronic structure of charged single- and di-interstitial clusters in crystalline silicon in various geometries, providing formation energies and stability information. The results are in qualitative agreement with the existing literature [1]. Whereas charge is an important factor in determining the stability of single interstitials, the ground state of di-interstitials remains the same irrespective of the charge.

[1] Georgia M.Lopez and Vincenzo Fiorentini, Phys. Rev. B **69**, 155206-1 (2004).