Combined LDA and LDA-1/2 method to obtain defect formation energies in large silicon supercells

Abstract
A source of uncertainty in the state of the art calculations of defect levels is the inaccurate prediction of band-gap energies. Several approaches were developed to surpass this problem. However, another source of uncertainty remains: the small number of clustered atoms imposed by the computational restrictions. In this work, the LDA-1/2 method is explored in an attempt to overcome both problems with a small computational cost. We considered the self-interstitial defects in silicon as a benchmark for calculating defect states and charge-transition levels of point defects in semiconductors. We found neutral formation energies, including reaction barriers, of 4.65, 4.49, and 4.87 eV, for hexagonal, split <110>, and C-3v configurations, respectively, in good agreement with most experimental results. (AU)