



Defect Physics in BaSi₂ absorber

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BaSi₂ is a low-cost, earth-abundant compound semiconductor from a silicide family. It has drawn an increasing amount of attentions recently as a candidate thin-film solar cell absorber material. Many promising properties such as ideal optical band gap (1.3 eV), high absorption coefficient ($>10^4$ cm⁻¹ for photon energies higher than 1.5 eV), long minority-carrier diffusion length (10 μm) and large quantum efficiency ($> 70\%$) have been reported till date [1-4]. Understanding the fundamental physical properties along with thermodynamic stability and formation mechanism of dominant intrinsic defects of material is crucial for designing and manufacturing efficient solar cells. Therefore, in this study, we investigate the neutral and charged native point defects of BaSi₂ by using first-principles density functional theory supercell approach.

From our detailed analysis on formation energies of native defects under appropriate chemical potential conditions of constituent elements, we found that predominant native defects in BaSi₂ are silicon vacancy V_{Si}, antisite Ba_{Si} and interstitial Si_i. On the other hand, antisite Si_{Ba} and interstitial Ba_i defects are unlikely to form as calculated defect formation energy is very high. Fig. 1 shows the calculated formation energies of all possible native charged point defects as a function of Fermi energy.

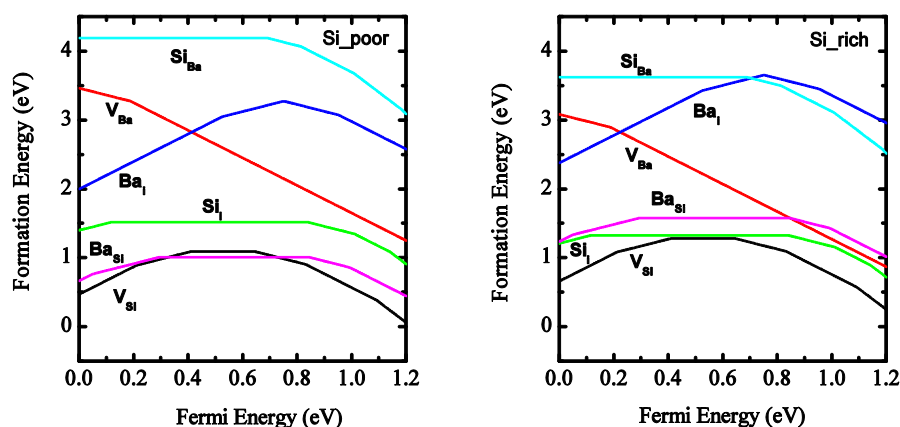


Fig. 1 Calculated formation energies as a function of the Fermi energy of intrinsic point defects in BaSi₂

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