Article

First-Principles Assessment of the Structure and Stability of 15 Intrinsic Point Defects in Zinc-Blende Indium Arsenide

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1. Defect Formation Energy in As-Rich Environment

The formation energy refers to the lowest formation energy among various charge states of $-4 \leq q \leq 4 + e$. Due to the influence of the chemical environment, the defect formation energy is a function of Fermi level E_F. The lowest formation energies as functions of E_F for each of fifteen defective configurations are presented in Figure S1 for As-rich environments.
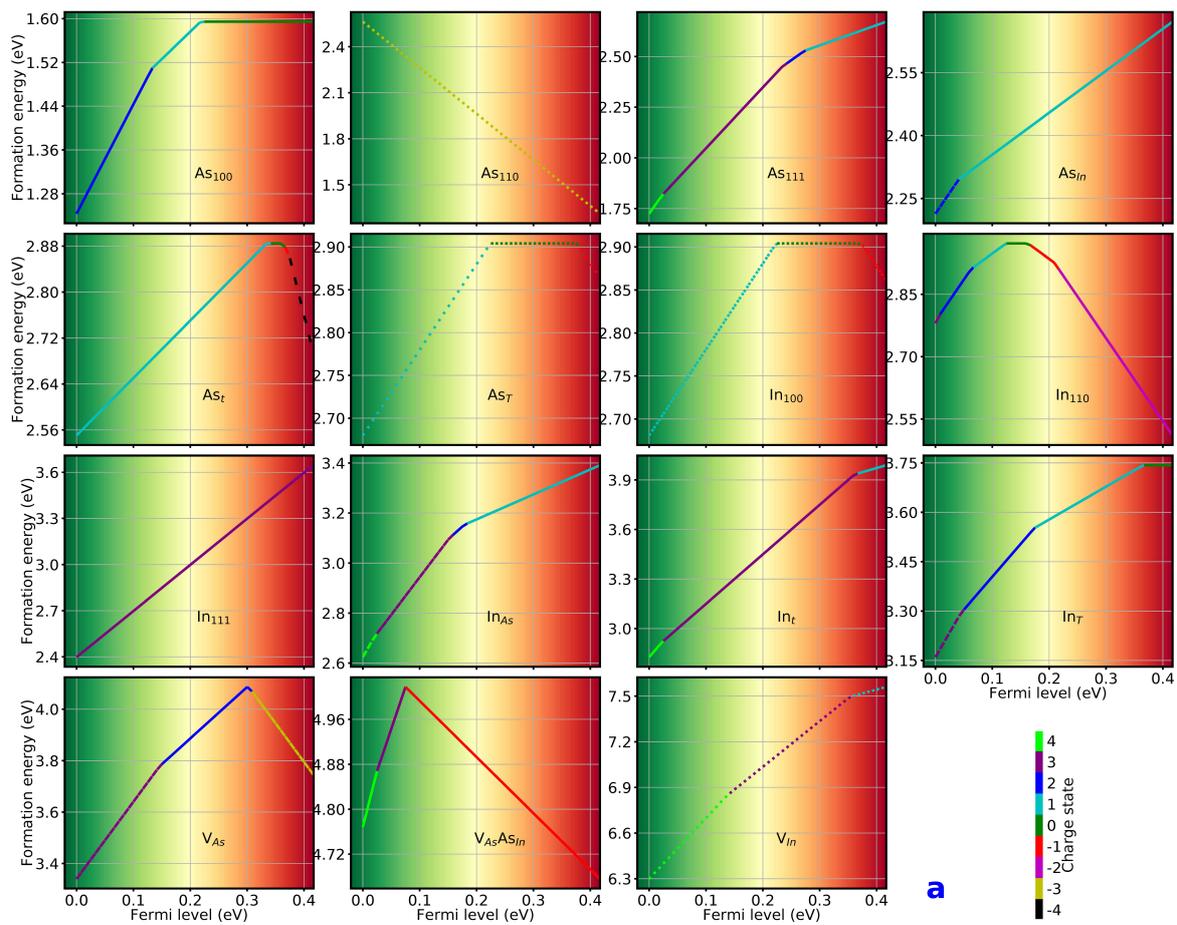
Figure S1. Formation energies as functions of E_F in the As-rich environments for fifteen different types of point defects in *zb*-InAs with all possible charge states from -4 to +4 marked by corresponding colors. The y-axis for each subplot is self-adapted for a better view. The different doping regimes near valance bands (*p*-type) and conduction bands (*n*-type) are displayed.

2. Defect Formation Energy in In-Rich Environment

The lowest formation energies as functions of E_F for each of fifteen defective configurations are presented in Figure S2 for In-rich environments.
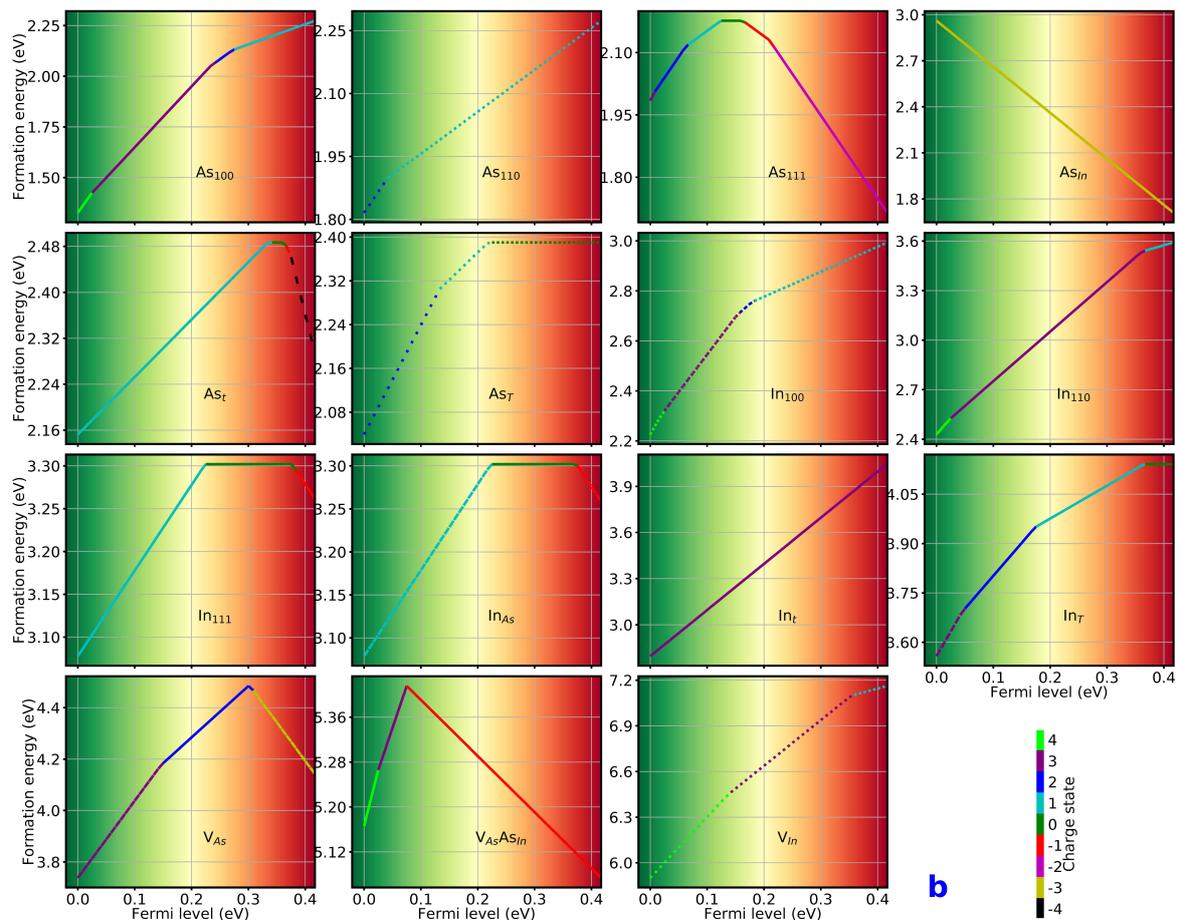
Figure S2. Formation energies as functions of E_F in the In-rich environments for fifteen different types of point defects in *zb*-InAs with all possible charge states from -4 to +4 marked by corresponding colors. The y-axis for each subplot is self-adapted for a better view. The different doping regimes near valance bands (*p*-type) and conduction bands (*n*-type) are displayed.