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Band crossing in isovalent semiconductor alloys with large size mismatch HUI-XIONG DENG, SU-HUAI WEI, National Renewable Energy Laboratory — Mixing isovalent compounds AC with BC to form alloys $A_{1-x}B_xC$ has been an effective way in band structure engineering to enhance the availability of material properties. In most cases, the mixed isovalent atoms A and B, such as Al and Ga in $Al_{1-x}Ga_xAs$ or As and Sb in $GaAs_{1-x}Sb_x$ are similar in their atomic sizes and chemical potentials; therefore, the physical properties of $A_{1-x}B_xC$ change smoothly from AC to BC. However, in some cases when the chemical and size differences between the isovalent atoms A and B are large, adding a small amount of B to AC or vice versa can lead to a discontinuous change in the electronic band structure. These large size- and chemicalmismatched (LSCM) systems often show unusual and abrupt changes in the alloys' material properties, which provide great potential in material design for novel device applications. In this report, based on first-principles band-structure calculations we show that for LSCM $GaAs_{1-x}N_x$ and $GaAs_{1-x}Bi_x$ alloys at the impurity limit the N (Bi)-induced impurity level is above (below) the conduction-(valence-) band edge of GaAs. These trends reverse at high concentration, i.e., the conduction-band edge of $GaAs_{1-x}Nx$ becomes an N-derived state and the valence-band edge of $GaAs_{1-x}Bi_x$ becomes a Bi-derived state, as expected from their band characters. We show that this band crossing phenomenon cannot be described by the popular BAC model but can be naturally explained by a simple band broadening picture.

Hui-Xiong Deng
National Renewable Energy Laboratory

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