

Abstract Submitted
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Origin of the failed ensemble averaged rule for the band gaps of the disordered nonisovalent semiconductor alloys JIE MA, Lawrence Berkeley National Lab, HUI-XIONG DENG, Institute of Semiconductors, Chinese Academy of Sciences, JUN-WEI LUO, SU-HUAI WEI, National Renewable Energy Lab — Recent calculations show that the nonisovalent random alloy, such as $\text{Zn}_{0.5}\text{Sn}_{0.5}\text{P}$, has a band gap much smaller than their ordered phases; i.e., the band gap of random alloy is not the ensemble averaged value of the ordered structures, as observed in most isovalent semiconductor alloys and predicted by cluster expansion theory. We show that this abnormal behavior in nonisovalent alloys is caused by strong wavefunction localization of the band edge states. Moreover, we show that although the disordered phase of isovalent alloys are similar to the random phase, for nonisovalent alloys the disordered phase deviates significantly from the random phase, and the completely random phase is not achievable for nonisovalent alloys under equilibrium growth conditions.

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