Abstract Submitted
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Reassessing the Description of the Electronic Structure of a Semiconductor Alloy[1] YONG ZHANG, A. MASCARENHAS, National Renewable Energy Laboratory, L.-W. WANG, Lawrence Berkeley National Laboratory — Although an electronic state in an alloy like $Ga_xIn_{1-x}P$ is not a Bloch state, it is generally considered to be reasonably close to a Bloch state in the sense of a virtual crystal approximation (VCA), and it is often referred to as Γ-like, L-like, or X-like. We have find that within certain context one could call a band edge state as Γ-like, if the dominant component of its wavefunction is indeed the Γ state of the VCA, but globally the alloy states are in general very different from those of the VCA in two important aspects: (1) a Γ-like state, for instance, could in fact have a very small Γ component of the VCA state, and (2) if the corresponding VCA states are degenerate, for instance, a X-like band edge alloy state, there will be strong coupling among the degenerate valleys. These new insights have major impacts on our understanding of the optical and electronic properties[1], and the ordering effects [2] in a semiconductor alloy.
[1] Y. Zhang, A. Mascarenhas, and L.-W. Wang, Phys. Rev. Lett. 101, 036403 (2008).
[2]Y. Zhang, A. Mascarenhas, and L.-W. Wang, Phys. Rev. B (in press).

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