

Abstract Submitted
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Effective band structure of random III-V alloys¹ VOICU POPESCU, ALEX ZUNGER, National Renewable Energy Laboratory, Golden CO — Random substitutional alloys have no long range order (LRO) or translational symmetry so rigorously speaking they have no $E(k)$ band structure or manifestations thereof. Yet, many experiments on alloys are interpreted using the language of band theory, e.g. inferring Van Hove singularities, band dispersion and effective masses. Many standard alloy theories (VCA- or CPA-based) have the LRO *imposed* on the alloy Hamiltonian, assuming only on-site disorder, so they can not be used to judge the extent of LRO that really exists. We adopt the opposite way, by using large (thousand atom) randomly generated supercells in which chemically identical alloy atoms are allowed to have different local environments (a polymorphous representation). This then drives site-dependent atomic relaxation as well as potential fluctuations. The eigenstates from such supercells are then mapped onto the Brillouin zone (BZ) of the primitive cell, producing effective band dispersion. Results for (In,Ga)X show band-like behaviour only near the centre and faces of the BZ but rapidly lose such characteristics away from Γ or for higher bands. We further analyse the effects of stoichiometry variation, internal relaxation, and short-range order on the alloy band structure.

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Voicu Popescu
National Renewable Energy Laboratory, Golden CO

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