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Electronic Structure of BGaP Alloys ERIK ALLDREDGE, KWISEON KIM, National Renewable Energy Laboratory, Golden, CO 80401 — We present the results of an *ab initio* investigation of zinc-blende BGaP alloys in the local density approximation. BP is a wide-band gap semiconductor with promising electronic and structural characteristics for potential optical and electronic applications. With an indirect gap of 2.0 eV, it has been considered as an optical window for silicon photoelectrochemical cells and has also been recently investigated as a thin buffer layer for the epitaxial growth of cubic GaN on silicon substrates. The use of boron, a first row element with deep atomic potentials and no p core electrons in III-V compounds results in signficiant differences in electronic structure. For example, the Γ conduction band minimum for BP is p- like (Γ_{15c}) in contrast to the s-like (Γ_{1c}) minimum typical of other III-V compounds such as GaP. We discuss the effect of this difference on the band structure of BGaP alloys and determine the bowing parameters for band gaps.

Erik Alldredge
National Renewable Energy Laboratory, Golden, CO 80401

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