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Theoretical prediction of the structural, electronic,and thermal properties of $Al_{1-x}B_xAs$ ternary alloys

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Abstract: First-principles calculations are performed to study the structural, electronic, and thermalproperties of the AlAs and BAs bulk materials and $Al_{1-x}B_xAs$ ternary alloys using the fullpotential-linearized augmented plane wave method within the density functional theory.The structural properties are investigated using the Wu–Cohen generalized gradientapproximation that is based on the optimization of total energy. For band structurecalculations, both Wu–Cohen generalized gradient approximation and modified Becke-Johnson of the exchange-correlation energy and potential, respectively, are used. Thedependence of the lattice constant, bulk modulus, and band gap on the composition x wasanalyzed. The lattice constant for Al1 xBxAs alloys exhibits a marginal deviation from theVegard's law. A small deviation of the bulk modulus from linear concentration depen-dence was observed for these alloys. The composition dependence of the energy band gapwas found to be highly nonlinear. Using the approach of Zunger and coworkers, themicroscopic origins of the gap bowing were detailed and explained. The quasi-harmonicDebye model was used to determine the thermal properties of alloys up to 500 K.

Keywords : Band structures, First principle calculations, Ternary alloys, Thermal Properties