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Structural, elastic, electronic and optical properties of the newly synthesized monoclinic Zintl phase $BaIn_2P_2$

Abstract

The present study explores the structural, elastic, electronic and optical properties of the newly synthesized monoclinic Zintl phase $BaIn_2P_2$ using a pseudopotential plane-wave method in the framework of density functional theory within the generalized gradient approximation. The calculated lattice constants and internal coordinates are in very good agreement with the experimental findings. Independent single-crystal elastic constants as well as numerical estimations of the bulk modulus, the shear modulus, Young's modulus, Poisson's ratio, Pugh's indicator of brittle/ductile behaviour and the Debye temperature for the corresponding polycrystalline phase were obtained. The elastic anisotropy of $BaIn_2P_2$ was investigated using three different indexes. The calculated electronic band structure and the total and site-projected *l*-decomposed densities of states reveal that this compound is a direct narrow-band-gap semiconductor. Under the influence of hydrostatic pressure, the direct D–D band gap transforms into an indirect B-D band gap at 4.08 GPa, then into a B–Γ band gap at 10.56 GPa. Optical macroscopic constants, namely, the dielectric function, refractive index, extinction coefficient, reflectivity coefficient, absorption coefficient and energy-loss function, for polarized incident radiation along the [100], [010] and [001] directions were investigated.

Keywords; Zintl phase $BaIn_2P_2$, Ab initio calculations, Elastic moduli, Electronic properties, Optical constants