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Comparison of mechanical, optical and electronic transport properties of isotropic and anisotropic borophosphene

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Abstract

In this research, mechanical, optical and electronic transport properties of two phases of graphene-like borophosphene are investigated using the density functional theory. Graphene-like borophosphene, a honeycomb structure with an equal ratio of boron and phosphorus atoms, is introduced in two isotropic and anisotropic phases. For this purpose, band structure, partial density of states, Young's modulus, Poisson ratios, dielectric function, and current-voltage characteristics are calculated and compared. The results show that the anisotropic phase of the graphene-like borophosphene is semimetal and the isotropic phase is a semiconductor with a direct energy gap of 0.9 eV. Moreover, the Young's modulus has the highest values for both phases in the zigzag and armchair directions of crystal; the Poisson ratio has the lowest values in these two directions. Besides, the optical properties of these two structures, including electron energy loss spectroscopy, refractive index, extinction coefficient, optical conductivity and reflection coefficient, for the parallel and perpendicular polarization of electric fields with respect to the sheets are computed by real and imaginary parts of dielectric function, using random phase approximation. Plasmon's energies are obtained to be 2.24 and 8.88 eV in the armchair direction and 9.01 eV in the zigzag direction for the anisotropic phase; also, for the isotropic phase, these are 3.38 and 9.12 eV in both directions. Both phases are transparent with respect to the visible light polarized in the perpendicular direction to the crystal, and the reflection and absorption are zero. Due to the selective transmission / absorption / reflection of the electromagnetic wave in the crystals, this material is suggested as a suitable candidate in the fabrication of nano optoelectronic devices. Furthermore, Ohmic behavior is observed in the current-voltage characteristics of the isotropic phase after the threshold bias voltage of 0.9 V. As a result of the high Fermi velocity of the charge carriers in the anisotropic phase of borophosphene ($7.05\times10^5\ m/s$), this material can be used in nanoelectronic devices.

Keywords*:* graphene-like borophosphene, density functional theory, Young's modulus, dielectric function, electronic transport

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