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Investigation of the mechanical and electronic transport properties of graphene-like borophene oxide under small strains

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Abstract

The graphene-like phase of boron atoms has been recently synthesized on Al (111) substrate. This two dimensional material, which is unstable without substrate, is improved to a stable structure after being combined with oxygen. In this research, the mechanical and electronic transport properties of graphene-like borophene oxide (g-B_2O) have been investigated within density functional theory framework and non-equilibrium Green's function; for this purpose, total and partial density of states, energy band structure, charge density, elastic constants, Young's modulus, Poisson's ratio, quantum conductance, and current-voltage characteristics have been calculated by applying small uniaxial and biaxial strains. The results show that g-B_2O is a metal that has Dirac points with linear dispersion energy at positions above and below the Fermi level. In addition, the current-voltage curves display the Ohmic behavior of this material; they also exhibit that positive strain reduces the current density in armchair direction (I_x) and increases the current density in the zigzag direction of (I_y), as compared to that without strain . The positive biaxial and uniaxial strains in the armchair direction with an almost similar behavior have the most variations in I_x and I_y. Besides, the negative strain in the zigzag direction causes the most I_y increase. The negative uniaxial strain in the armchair direction and the negative biaxial strain with an almost analogous behavior caused the most (the least) changes in I_x (I_y). The anisotropic current density along zigzag and armchair directions, as well as the ability to control this anisotropy by positive and negative strains, makes this material suitable for use in nanoelectronic devices.

Keywords: graphene-like borophene, density functional theory, density of states, Young's modulus, electronic transport

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