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Investigation of the mechanical and electronic transport properties of graphenelike 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-B₂O) 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-B₂O 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 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

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For full article, refer to the Persian section

strains, makes this material suitable for use in nanoelectronic devices.