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Uniaxial Strain Effects on Electronic Transport Properties of Hydrogenated beta12 Borophene: A First-Principles Study

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Abstract

In this study, the effect of uniaxial strain on the structural and electronic transport properties of pristine borophene and three of its hydrogenated configurations is investigated using density functional theory (DFT) calculations. Borophene is a two-dimensional structure composed of boron atoms that, due to lattice mismatch with the substrate during synthesis, may be subjected to small degrees of strain. Moreover, hydrogenation can increase its structural stability. Therefore, the simultaneous effects of small uniaxial tensile and compressive strains and hydrogenation on the band structure, partial density of electronic states, and current–voltage (I–V) characteristics of borophene are studied. The results indicate that the transport properties of both pristine and hydrogenated borophene display directional dependence, and this anisotropic behavior can be modified by applying strain. Analysis of the I–V characteristics at bias voltages below 1 V indicates that strain affects the degree of current anisotropy. For pristine borophene, the current anisotropy ratio at a bias voltage of 1 V is found to be 0.74, which varies significantly upon hydrogenation, leading to isotropic current behavior in one of the considered configurations. Additionally, comparison of the Poisson ratios along the armchair and zigzag directions reveals that hydrogenation softens the hydrogenated structures along the armchair direction compared with pristine borophene. The tunability of the I–V behavior under small strains highlights the high potential of these structures for applications in next-generation electronic devices.

Keywords: density functional theory, electronic transport, Borophene, Borophane, strain.

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