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Tunable Electronic Properties of Graphdiyne Under Tension and Compression: A DFT Study

Graphdiyne, a carbon allotrope characterized by its unique two-dimensional structure, semiconducting behavior, and rich sp-hybridized carbon content, shows great promise for practical applications in fields such as energy storage, catalysis, and gas separation. Understanding the electronic properties of graphdiyne under tensile and compressive deformation is essential for its integration into flexible and stretchable electronic devices. Mechanical strain can significantly alter its band structure, offering a viable route to tune its conductivity and semiconducting behavior. Exploring these strain-induced effects enables the design of graphdiyne-based components with adjustable electronic performance, which is crucial for applications in nanoelectronics, strain sensors, and adaptive optoelectronic systems.

Using first-principles calculations based on density functional theory, this study systematically explores the effects of tensile and compressive deformation on the electronic properties of graphdiyne. The results indicate that graphdiyne possesses a direct and tunable band gap that responds to mechanical strain. Under uniaxial deformation, the band gap generally decreases as strain increases. In contrast, biaxial deformation leads to a band gap that increases with tensile strain and decreases with compressive strain. Band gap values obtained using the HSE06 functional are higher than those calculated with the GGA method, though both approaches yield similar band structure profiles and consistent trends in the band gap variation with strain. As deformation intensifies, charge transfer between carbon atoms in graphdiyne becomes more significant. Compressive strain enhances the structural stability of graphdiyne, while tensile strain reduces it. Compared to uniaxial strain, biaxial deformation exerts a stronger influence on the band gap and overall stability, but has a comparatively weaker effect on charge transfer.

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Primary author: Dr SAGHIR, Neelam (Department of Physics, University of South Africa (UNISA), 28 Pioneer Ave Florida Park Roodepoort, Johannes-burg, South Africa)

Co-authors: Prof. RAMPHO, G J (Department of Physics, University of South Africa (UNISA), 28 Pioneer Ave Florida Park Roodepoort, Johannes-burg, South Africa); Prof. KHENFOUCH, Mohammed (Department of Physics, Ibn Zohr University, Nouveau Complexe Universitaire Agadir 80000, Morocco)

Presenter: Dr SAGHIR, Neelam (Department of Physics, University of South Africa (UNISA), 28 Pioneer Ave Florida Park Roodepoort, Johannes-burg, South Africa)

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