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Ab Initio Study of Electronic Structure and Transport of Graphyne and Graphdiyne

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Abstract : Graphene has attracted a tremendous interest in the field of nanoelectronics and spintronics due to its exceptional electronic properties. However, pristine graphene has no band gap, a feature needed in building some of the electronic elements. Recently, a growing attention has been given to a class of carbon allotropes of graphene with honeycomb structures, in particular to graphyne and graphdiyne. They are characterized with a single and double acetylene bonding chains respectively, connecting the nearest-neighbor hexagonal rings. With an electron density comparable to that of graphene and a prominent gap in electronic band structures they appear as promising materials for nanoelectronic components. We studied the electronic structure and transport of infinite sheets of graphyne and graphdiyne and compared them with graphene. The method based on the non-equilibrium Green functions and density functional theory has been used in order to obtain a full ab initio self-consistent description of the transport current with different electrochemical bias potentials. The current/voltage (I/V) characteristics show a semi-conducting behavior with prominent nonlinearities at higher voltages. The calculated band gaps are 0.52V and 0.59V, respectively, and the effective masses are considerably smaller compared to typical semiconductors. We analyzed the results in terms of transmission eigenchannels and showed that the difference in conductance is directly related to the difference of the internal structure of the allotropes.

Keywords : electronic transport, graphene-like structures, nanoelectronics, two-dimensional materials
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