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Graphyne- and Graphdiyne-based Nanoribbons: Density Functional Theory Calculations of Electronic Structures¹ LIDA PAN, LIZHI ZHANG, BOQUN SONG, SHIXUAN DU, HONGJUN GAO, Institute of Physics, Chinese Academy of Sciences, Beijing — Graphdiyne, a carbon allotrope, which has the same symmetry as graphene and has butadiyne linkages between its nearest-neighbor hexagonal rings, has recently synthesized and fabricated on copper, showing experimentally the semiconductor property with conductivity of $2.516 \times 10^{-4} \text{ S m}^{-1}$, which is comparable to silicon. We investigate the configurations and electronic properties of graphyne and graphdiyne nanoribbons with armchair and zigzag edges by using first principles calculations. Our results show that all the nanoribbons are semiconductors with suitable band gaps similar to silicon. And their band gaps decrease as widths of nanoribbons increase. We also find that the band gap is at the Γ point for all graphdiyne ribbons and it is at the X point for all graphyne ribbons. Of particular interest, the band gap of zigzag graphyne nanoribbons show a unique "step effect" as the width increases. This property is good for tuning of the energy band gap, as in a certain range of the ribbon width, the energy gap remains constant and in reality the edge cannot be as neat as that in a theoretic model. Graphyne and graphdiyne with tunable gaps are promising candidates for future carbon-based electronic devices.

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