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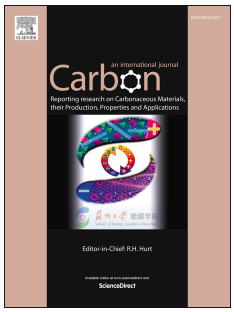

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Energetic and electronic structure of penta-graphene nanoribbons

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Abstract

Inspired by a very recent theoretical work on penta-graphene, a two dimensional (2D) carbon sheet [Proc. Nat. Acad. Sci. **2015**, *112*, 2372] composed of only carbon pentagons, we have made an attempt to see the stability and electronic properties of its one dimensional (1D) ribbons, naming penta-graphene nanoribbon (pentaGNR). Our first principle calculations predict that, pentaGNR is dynamically stable; it is mechanically flexible tolerating upto 11.5% of axial strain. We have also explored the electronic properties of the nanoribbons with different widths which show interesting charge separation for wider ribbons. The band gap of wider ribbons changes only marginally with further increasing the ribbon width which opens up the possibility of a stable nanoribbon with large band gap which is very useful for designing optoelectronic devices.

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