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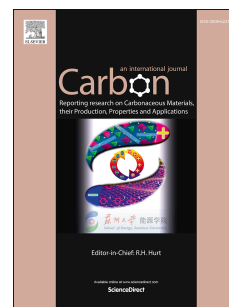
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Prediction of an ultrasoft graphene allotrope with Dirac conesXiaoming Zhang¹, Lin Wei^{1,2}, Jie Tan¹, Mingwen Zhao*¹

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Abstract

Searching for the Dirac materials with ultrasoftness is crucial for flexible electronics applications. Based on first-principles calculations, we propose a new carbon allotrope (named as ph-graphene) with a penta-hexagonal framework, which is energetically more favorable than the penta-graphene composing surely of pentagons and some of already-synthesized carbon allotropes. Ph-graphene has an in-plane stiffness of 27.75 GPa·nm, smaller than those of graphene and penta-graphene by one order. The famous isotropic Dirac cones are well preserved in the ultrasoft ph-graphene, exhibiting delocalized feature of p_z orbits with the Fermi velocity of 2.8×10^5 m/s. Additionally, surface hydrogenation alters drastically the electronic and mechanical properties of ph-graphene, resulting in electronic spin-polarization and anisotropic negative Poisson's ratios sequentially with the increase of hydrogenation concentrations.

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