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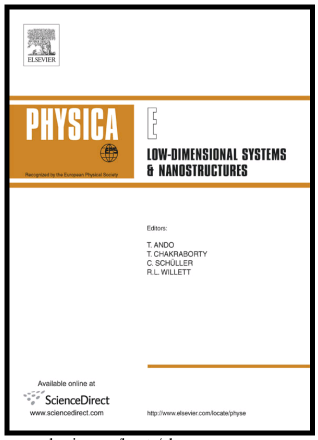

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A planar carbon allotrope with linear bipentagon-octagon and hexagon arrangement

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Abstract

A two-dimensional (2D) metallic carbon allotrope is proposed, which consists of linearly aligned bipentagon-octagon and hexagon rings in a planar sheet. The relatively high percentage of hexagon and the regular arrangement of the polygons make it energetically more favorable than most of other predicted 2D carbon allotropes. Phonon dispersions without negative frequencies also indicate its stability. Electronic structure calculations show that its metallic nature is mainly due to the atoms shared by the pentagon, hexagon and octagon. Its lattice thermal conductivity is only about one fifth of that of graphene. Armchair- and zigzag-edged nanoribbons of this structure are also studied. The former is metallic while the latter has a small band gap due to the spin-polarized edge states. The appropriate band gap and the significantly reduced thermal conductivity suggest potential applications in thermoelectricity.

Keywords: carbon allotrope, electronic structure, thermal transport, nanoribbon

1. Introduction

A carbon atom has the electron configuration of $[\mathrm{He}]2\mathrm{s}^2 2\mathrm{p}^2$ and can hybridize with other carbon atoms in sp, sp^2, or sp^3 bonding and form various allotropes of different dimensionalities and properties, such as zero dimensional (0D) fullerene[1], one dimensional (1D) carbon nanotube (CNT)[2], two dimensional (2D) graphene[3, 4], and three dimensional (3D) diamond. Among these allotropes, graphene which was believed not to exist naturally becomes the most studied one nowadays. This sp^2 hybridized planar monolayer possesses many interesting properties, such as

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