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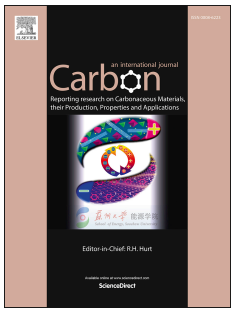

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Protomene: a new carbon allotrope

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Abstract

We introduce a new carbon allotrope named protomene. Its crystal structure is hexagonal, with a fully-relaxed primitive cell involving 48 atoms. Of these, 12 atoms have the potential to switch hybridization between sp^2 and sp^3, forming dimers. By means of DFT simulations, we have identified the equilibrium structure of protomene, and estimate that it is 2% less bound than diamond. We have also estimated the amplitude of its direct band gap to be 3 eV, and predicted the X-ray diffraction pattern and phonon modes.

1. Introduction

Driven by the discovery of some of the most interesting new materials, namely fullerenes, nanotubes and graphene, the quest for new allotropes of carbon has been an increasingly active field of research for several decades [1]. This broad interest is fueled by the wide range of structural and electronic properties of carbon allotropes. Indeed, carbon possesses three energetically competitive different types of orbital hybridization (sp, sp^2, and sp^3).

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