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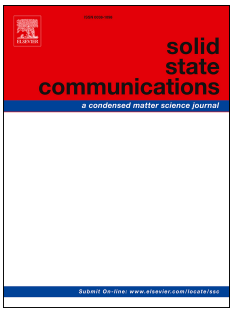

Optimized tight binding parameters for single layer honeycomb borophene

Liyan Zhu, Tingting Zhang

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Optimized tight binding parameters for single layer honeycomb borophene

Liyan Zhu[a,b], Tingting Zhang[a,b,*]

[a] *Department of Physics, Jiangsu Key Laboratory for Chemistry of Low-Dimensional Materials, Huaiyin Normal University, Huai'an, People's Republic of China*

[b] *Jiangsu Key Laboratory of Modern Measurement Technology and Intelligent Systems, Huaiyin Normal University, Huai'an, People's Republic of China*

Abstract

Motivated by experimental realization of honeycomb borophene (HB) on an Al(111) surface, we propose a non-orthogonal Slate-Koster tight binding (TB) model for single layer HB, of which parameters are optimized via a combination of the genetic algorithm and the simplex method using electronic structures obtained from density functional theory (DFT) as targets. Our proposed Slate-Koster parameters can well produce both energies and orbital compositions of electronic bands of a single layer HB. The direct calculation of band structure and atomic orbital resolved density of states show excellent agreement with DFT results. The highly accurate TB model would facilitate the future large-scale atomistic modeling on electronic, optical, and transport properties of HB based nano-materials.

Keywords: Borophene, tight binding, electronic band structure, density of states

1. Introduction

Since the successful exfoliation of graphene[1], exploration of two-dimensional (2D) materials has received extensive interest[2]. As a left neighbor of carbon, great effort has been devoted to searching 2D allotropes of boron[3], i.e. borophene. Extensive studies on small sized boron clusters suggest that the triangular motif is a building block for constructing large sized boron clusters.[4, 5] Inspired by these findings, a theoretical study proposed that the buckled triangular structure of borophene could be a stable allotrope of 2D boron.[6] However, the further investigation revealed that the cohesive energy of borophene can be remarkably enhanced by removing a few fractions of boron atoms to create hexagonal holes into the pristine triangular lattice.[7] For example, Tang et al.[7] proposed two energetically favorable 2D allotropes of boron with a porosity of 1/9 and 1/7, which are coined as α- and β-borophene. Currently, advanced algorithms, e.g., particle swarm optimization[8], cluster expansion[9], genetic algorithm[10], have been employed to search candidates of 2D boron. Besides the advance in theoretical studies, experimental realizations of 2D boron have been achieved on Ag(111) by Manix et al.[11] and Feng et al.[12], in which the rectangular and rhombohedral phases can match the allotropes of borophene with a hexagon hole density of 1/6 and 1/5, respectively.[13]

In addition to diversity in 2D allotropes, borophene also possesses many outstanding physical and chemical properties.[13] For example, Zhang and co-workers predicted a high and anisotropic in-plane modulus for borophene ranging from 189 to 399 N/m[14], which is comparable to that of graphene[15] and hexagonal boron nitride[16]. Besides superior mechanical strength, structure diversity renders many 2D allotropes with nontrivial electronic structures and emergent fermions, e.g., Dirac[17] and triplet[18] fermions. Furthermore, borophene was also predicted to be the first known materials with high-frequency plasmons in the visible regions[19]. Such intriguing properties make borophene a promising candidate for many applications, e.g., electronic and optoelectronic devices. On the other hand, the intriguing electronic properties

*Corresponding author
Email address: ttzhang@hytc.edu.cn (Tingting Zhang)