



Tunable electronic structures and magnetic properties in two-dimensional stanene with hydrogenation



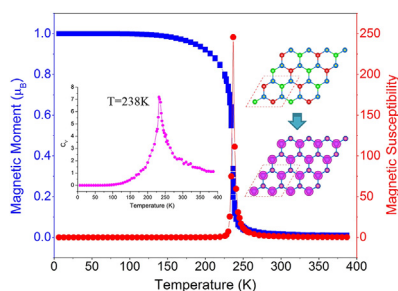
Sheng-shi Li, Chang-wen Zhang*

School of Physics and Technology, University of Jinan, Jinan, Shandong, 250022, PR China

HIGHLIGHTS

- Room temperature ferromagnetism in half hydrogenated stanene.
- The effects of the ratio of hydrogenation and electric field.
- Tunable band gaps of stanene by external factor.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:

Received 9 March 2015
 Received in revised form
 27 January 2016
 Accepted 2 February 2016
 Available online 12 February 2016

Keywords:

Nanostructures
 Semiconductors
 Ab initio calculations
 Electronic structure

ABSTRACT

Based on tight-binding model and first-principles calculations, we systematically investigate the geometric, electronic, and magnetic properties of hydrogenated stanene. The results indicate that the half-hydrogenation breaks the π -bondings of stanene, leaving π electrons in unsaturated Sn atoms localized and unpaired, which makes it transform into half-metal (HM) with room-temperature ferromagnetism. Especially, the magnetism of hydrogenated stanene can be effectively tuned by different rates of coverage for hydrogen atoms. While for the case of full-hydrogenated stanene, two different configurations exhibit the nature of semiconductor and semimetal, respectively, which is dependent on the arrangement of hydrogen atoms. We also find that the band gaps of stanene bilayer and monolayer can be effectively modulated by external electric field and strain. These findings demonstrate that hydrogenation is an efficient way to tune the electronic properties of stanene, and it provides a new perspective for the potential application in nanoelectronics.

© 2016 Elsevier B.V. All rights reserved.

1. Introduction

Graphene, a two-dimensional (2D) honeycomb carbon network, has motivated tremendous interest due to its exciting properties since experimental realization in 2004 [1–5]. The unique symmetry of honeycomb π -orbital network makes graphene exhibit peculiar

* Corresponding author.

E-mail address: zhchwsd@163.com (C.-w. Zhang).

properties, including massless Dirac fermions, high thermal conductivity, and half-integer Hall conductance et al. [6,7]. Nevertheless, graphene still faces many challenges, such as toxicity, difficulty in processing and incompatibility with current silicon-based electronic technology. So these problems have further encouraged significant efforts to look for other honeycomb-like structures made of group IV elements such as silicon (Si) and germanium (Ge) which are called silicene and germanene [8–12], respectively. Different from graphene, the most stable configuration of them prefers a low-buckled structure, which is mainly attributed to the

mixing of sp^2 and sp^3 hybridizations. Interestingly, their band structures still have a semi-metallic character [8,10–12], similar to the one of graphene. More recently, stanene, arranged in a single layer with tin (Sn) atoms, is predicted by Zhang et al. [13]. Furthermore, ultrathin tin film with the low-buckled configuration has been observed in molecular beam epitaxy (MBE) experiment [14]. Compared with C, Si and Ge atoms, Sn atom has a larger atomic radius and lower electronegativity, which may cause many distinct properties. For example, the functionalized stanene monolayer is a large-gap quantum spin Hall (QSH) insulator [15], which can be used to design and fabricate smaller, faster and more energy efficient electronic device.

It is generally known that the chemical modification is an effective route to change the electronic properties of 2D materials. Moreover, as a common avenue, hydrogenation has been used to decorate graphene [16], silicene [17–19], germanene [19], plum-bene [20], and group III-V film [21]. Indeed, sizable band gap opening has been observed in these 2D materials after hydrogenation, which has potential interests for spintronics and optoelectronics. Besides, a long-sought room-temperature ferromagnetic (FM) order can be realized in graphene and silicene by tuning the rate of the hydrogenation [17,18]. However, up to now, the electronic properties of stanene with hydrogenation have not been explored thoroughly. To address this issue, we perform density-functional theory (DFT) computations on stanene with hydrogenation. Our results reveal that hydrogenation can tune the band structure of stanene effectively. Remarkably, the long-range FM order at room-temperature can be achieved in half-hydrogenated stanene. In addition, external electric field (E-field) and elastic strain engineering provide a route to harness the band gap opening of stanene with hydrogenation. These findings may open a new path for the applications of stanene in spintronics and optoelectronics.

2. Computational methods

All the calculations were performed by the means of first-principles calculations as implemented in the Vienna Ab Initio

Simulation Package (VASP) [22,23]. Generalized gradient approximation (GGA) with the Perdew-Burke-Ernzerhof (PBE) [24,25] exchange correlation functional is adopted to describe the exchange–correlation interaction. Ion cores are modeled with projector augmented wave (PAW) potentials [26], while spin polarization corrections is also taken into account. To properly take into account the van der Waals (vdW) interaction in the stanene bilayer, the DFT-D2 [27] method is used throughout the calculations of bilayer. In addition, the Wannier functions technique is used on top of self-consistent first principles calculations to derive an accurate tight-binding Hamiltonian of the free standing stanene [28]. The plane-wave cutoff energy is to be 400 eV, and a supercell with 20 Å vacuum layer is used to simulate the isolated sheet. The Monkhorst-Pack (MP) [29] scheme was used to sample the Brillouin zone, which adopts the $11 \times 11 \times 1$ and $25 \times 25 \times 1$ k-mesh for the relaxation and self-consistent calculations, respectively. All the lattice constants and atom coordinates were optimized until the convergence of the force on each atom is less than 0.01 eV/Å. Since the DFT method has proven to be one of the most accurate methods for the electronic structure computations of solids [30–33], it can deal with this system well. To better evaluate the stabilities of these hydrogenated systems, the calculated formation energies can be expressed as:

$$E_f = E(\text{H@Sn}) - E(\text{Sn}) - N\mu(\text{H}) \quad (1)$$

where $E(\text{Sn})$ and $E(\text{H@Sn})$ are energies of the free-standing stanene (FSSn) and hydrogenated stanene, respectively. According to previous results [34,35], the $\mu(\text{H})$ is the chemical potential of hydrogen atom, which can be defined as $\mu(\text{H}) = E(\text{H}_2)/2$. Based on this definition, a smaller E_f stands for a stronger bonding interaction.

3. Results and discussion

3.1. Electronic properties of the free-standing stanene

Taking stanene monolayer as a starting point, we firstly investigate its geometric and electronic properties. The FSSn has a hexagonal honeycomb-like structure, which is similar to

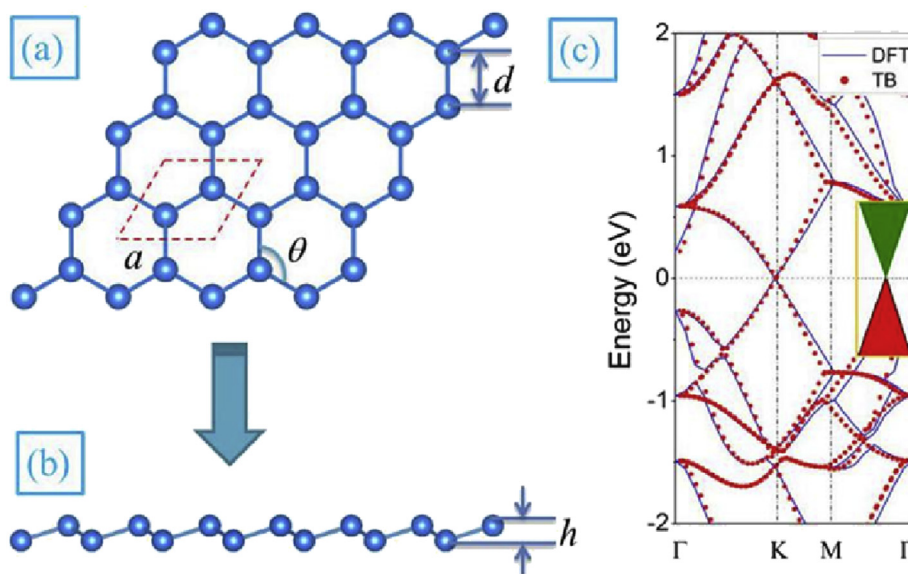


Fig. 1. Optimized geometric structures of stanene from top view (a) and side view (b). (c) The band structure calculated after structural relaxation along high symmetry directions: blue line and red dotted lines represent the result of DFT and TB, respectively. (For interpretation of the references to color in this figure caption, the reader is referred to the web version of this article.)

Download English Version:

<https://daneshyari.com/en/article/1520688>

Download Persian Version:

<https://daneshyari.com/article/1520688>

[Daneshyari.com](https://daneshyari.com)