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Full Length Article

Electronic structure tuning of stanene monolayers from DFT calculations: Effects of substitutional elemental doping

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ABSTRACT

Stanene is one of the most important quantum spin hall insulators and can be considered as an efficient material for the fabrication electronic and optoelectronic devices and next-generation integrated circuits. Density functional theory calculations were carried out to investigate the band gap variations in stanene, and the effects of elemental doping were taken into account. For the pristine stanene sheet, the valence and conduction bands of stanene consist of Sn 5p orbitals. The pristine stanene system is a zero band gap material with a Dirac cone located at the K point. The Al-doped, B-doped, N-doped and P-doped systems show metallic characteristics. In the Al-doped and B-doped stanene, the Fermi level is shifted towards the valence band edge, while in the N-doped and P-doped ones, the Fermi level shifts towards the conduction band edge. These doped systems behave as degenerate semiconductors, due to the significant shifts in the Fermi levels. Other doping elements such as Si and Ge were also considered in this study. Both Si and Ge-doped stanene show the properties similar to the pristine stanene, which is a consequence of the similar electronic structure of Si, Ge and Sn atoms. In the N-doped stanene, the Dirac cone vanishes, whereas in the other doping patterns, the Dirac cone exists around the Fermi level. The electronic band structure of the Si and Ge-doped systems is principally the same as that of pristine one. Our results thus suggest a theoretical basis for the potential application of such doped systems in electronic and optoelectronic devices.

1. Introduction

Over the past few years, a huge surge of interest has arisen in the design and development of novel two dimensional (2D) materials, which show satisfied properties for applications in next-generation nanoelectronic devices. In this regard, graphene [1], and its counterparts such as silicene [2–4], germanene [5,6], antimonene [7,8], and transition metal dichalcogenides [9,10] are receiving considerable attention because of their particular properties. Thus it is more and more important to synthesize atomically thin group-IV materials. Recently, various experimental techniques have been used for the realization of 2D materials [11–14]. Silicene and germanene based honeycomb-like buckled structures have been synthesized using molecular beam epitaxy method [11,15]. Different allotropes of atomically thin tin have been theoretically predicted by Garcia and co-workers [16]. They have suggested that the tin based allotropes exhibit properties similar to graphene. Zhu et al. proposed the successful synthesis of two-dimensional stanene by molecular beam epitaxy method (MBE), which unlocked up new areas in this regard, e.g., heterostructures of stanene and hydrogenated stanene (namely stanane) [17,18]. Additionally, Gao et al. have investigated the epitaxial growth of stanene over the surface of Ag atoms [19]. Stanene possesses excellent electronic and optical properties such as enhanced thermoelectricity [20], topological superconductivity and lack of an intrinsic band gap [21]. 2D materials such as stanene have been utilized in a wide range of applications such as photocatalyst [22,23], energy conversion or storage [24–26] and fabrication of nanoelectronic devices [27–30].

Comparing with graphene and silicene, the conductivity of stanene can reach 100% at room temperature [31,32], representing that the electronic properties of stanene can be efficiently modified. Thus, stanene can be considered as one of the most important members of atomically thin group-IV structures family. As mentioned above, stanene exhibits a buckled honeycomb-like structure, which can be attributed to the weak π- π bonding between two adjacent tin atoms. This buckled structure is the most stable structure compared to the other possible structures [33]. Electronic structure studies revealed that stanene has a zero band gap without addition of spin orbit coupling (SOC) effect. When the effects of SOC were taken into account, it exhibits a

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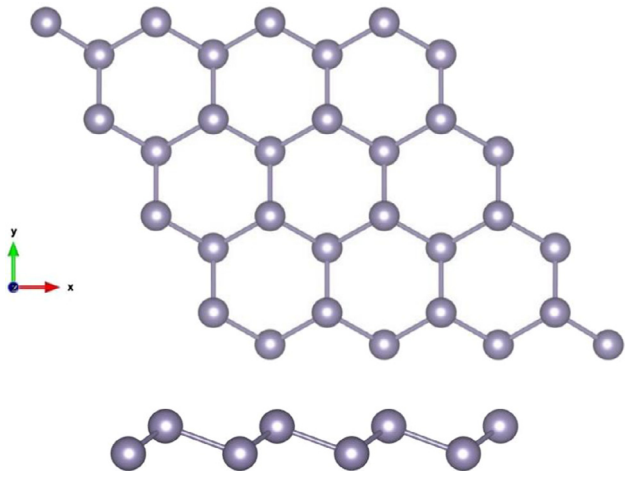

Fig. 1. Top and side views of the optimized structure of 4 × 4 × 1 supercell of stanene monolayer.

reasonable band gap of about 0.1 eV, being a fascinating property to help in the development of highly efficient integrated circuits [34]. Furthermore, the SOC effect of stanene makes that stanene acts like a quantum spin hall insulator (QSHI) [33]. It is worth noting that, doped QSHI materials exhibit time-reversal-invariant topological superconductivity [35]. Therefore, doped stanene monolayer could act as a potential candidate for a large variety of applications. Besides, the gapless nature of intrinsic stanene is a very important limitation, depressing its possible application in future semiconductor based microelectronic devices [36]. Hence, the investigation of the band gap opening in stanene has emerged new areas in stanene based science and technology. Recently, various methods have been tested to tune the electronic properties of stanene [37–41]. For example, Tang et al. studied the effects of functionalization on the electronic structure of stanene [40]. The prediction of van der Waals heterostructures of stanene with other 2D materials is also one of the most important approaches for tuning the electronic properties. Performing first-principles calculations, Wang and co-workers predicted a van der Waals heterostructure of stanene with hexagonal boron nitride (BN) sheet, which shows a significant band gap compared to the bare stanene [42]. It is

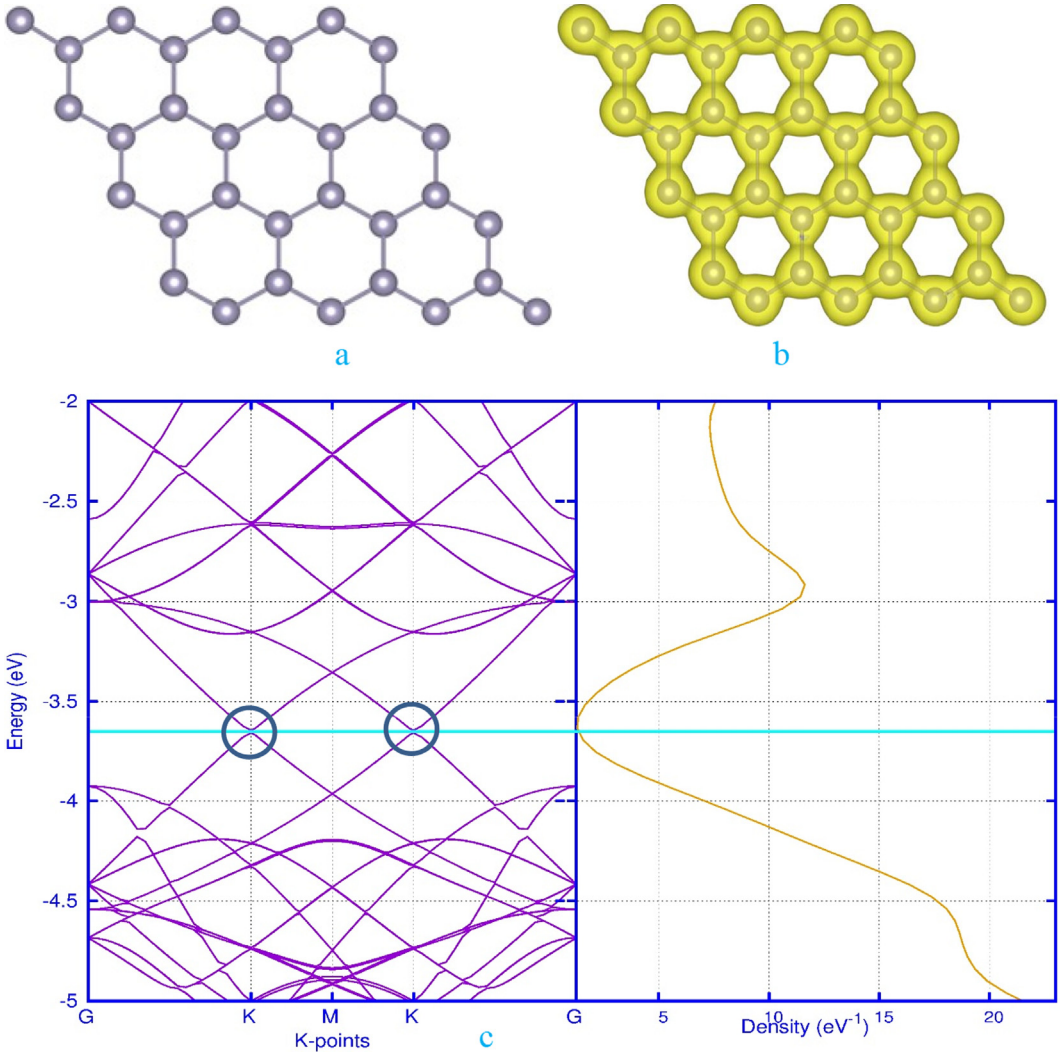

Fig. 2. (a) Optimized structure of pristine 4 × 4 × 1 supercell of stanene, (b) total electron density surface (Isosurface: 0.03 e. $Å^{-3}$), and (c) Band structure of pristine stanene monolayer along with the density of states. The Fermi level is indicated by a blue solid line. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)