



Adsorption of alkali and alkaline-earth metal atoms on stanene: A first-principles study



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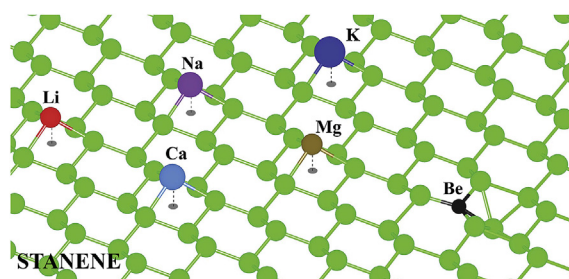
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HIGHLIGHTS

- Alkali and alkaline-earth metal atoms form stronger bonds with stanene compared to other group IV monolayers.
- Semi-metallic stanene becomes nonmagnetic metal for Li, Na, K, Mg, and Ca atoms adsorption.
- Semi-metallic stanene becomes nonmagnetic semiconductor with 94 meV band gap for Be atom adsorption.

GRAPHICAL ABSTRACT



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ABSTRACT

This paper presents a study on the adsorption of alkali and alkaline-earth metal atoms on single-layer stanene with different levels of coverage using first-principles plane wave calculations within spin-polarized density functional theory. The most favorable adsorption site for alkali atoms (Li, Na, K) were found to be the hollow site similar to other group IV single-layers, but the case of alkaline-earths on stanene is different from silicene and germanene. Whereas Mg and Ca are bound to stanene at hollow site, the bridge site is found to be energetically favorable for Be adatom. All adsorbed atoms are positively charged due to the charge transfer from adatom to stanene single-layer. The semimetallic bare stanene become metallic except for Be adsorption. The Beryllium adsorption give rise to non-magnetic semi-conducting ground state. Our results illustrate that stanene has a reactive and functionalizable surface similar to graphene or silicene.

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1. Introduction

After the synthesis of two dimensional (2D) single-layer (SL)

graphene [1,2], particularly 2D materials of group IV elements, such as silicene [3–6], germanene [7–11], and stanene [12–15], have attracted great attention due to their extraordinary electronic properties as well as their potential applications in nanoelectronic devices.

Stanene, a single-layer arrangement of tin atoms, has similar crystal and electronic structure with silicene and germanene systems. It shows a room temperature quantum spin Hall effect caused

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by spin-orbit coupling (SOC) [8]. The robustness and high resistance of silicene and germanene to oxidation are advantages which makes these materials desirable for technological applications [16]. Stanene is also predicted to possess these intriguing properties which need further investigation.

Previous experimental and theoretical studies have predicted that the electronic and magnetic properties of 2D single-layers are affected by the adsorption of foreign atoms [17–20]. For example, Li-covered graphene shows metallicity and high hydrogen storage capacity [21]. Moreover, doped-graphene has been found to show superconducting properties [22–24]. The semimetallic bare silicene can turn into metallic, half-metallic, or semiconducting material depending on the doped elements [18,25,26]. The tunable band gap of silicene upon adsorption of alkaline-earth metal atoms is highly desirable for use in nanoscale optoelectronic device applications. Similar with silicene, a band gap can be tuned by controlling the alkali metal atom coverage on germanene and this small band gap at Dirac point makes germanene a possible basis material for designing nanoscale electronic devices; such as high performance field effect transistors [19,20].

In this study, we investigated the adsorption of alkali and of alkaline-earth metal atoms on SL stanene at different level of coverage. The energetic preferences and electronic redecoration are studied in detail. The adsorption of adatoms on SL stanene give rise to crucial effects in the electronic properties. We found that semimetallic stanene becomes metallic, except the adsorption of Be, which is found to be nonmagnetic semiconductor having direct band gap of $E_g = 94$ meV. In this respect, functionalization of SL stanene through the adsorption of adatom appears to be promising way to extend the application of SL stanene.

2. Computational details

All numerical results were obtained by using Quantum Espresso Package [27] within density functional theory (DFT) using the generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhof (PBE) type functional for exchange and correlation including van der Waals interactions [28]. Spin-orbit interaction was not included in the calculations. Kinetic energy cutoff was taken as 816 eV. Brillouin-zone was sampled by special k-points according to Monkhorst-Pack method [29] by $(4 \times 4 \times 1)$ mesh points. A vacuum region of 13 Å was chosen in the direction of perpendicular to the stanene plane to ensure that the wave functions vanish at the edge of the cell as required in an isolated system. The convergence for energy was chosen as 10^{-5} eV between two successive iterations and the maximum Hellmann-Feynman force exerted on each atom was reduced to less than 0.05 eV/Å. The maximum pressure on the unit cell was reduced to less than 1 kbar. For partial occupations, Gaussian type smearing method was used with a smearing width 0.08 eV. The cohesive energy, E_{coh} was calculated as $E_{coh} = E_{stanene} - nE_{Sn}$ in terms of the total energy of the bare stanene ($E_{stanene}$) and the energy of isolated free atom of Sn (E_{Sn} , where n is the number of Sn atom in the cell). The adsorption energies of adatoms were obtained by $E_{ads} = E_{stanene+adatom} - E_{stanene} - E_{adatom}$. Here $E_{stanene+adatom}$, $E_{stanene}$, and E_{adatom} are the total energies of stanene + adatom, bare stanene, and isolated adatom calculated in the supercell, respectively.

The charge differences ($\Delta\rho$) were calculated by using the expression

$$\Delta\rho = \rho_{stanene+adatom} - \rho_{stanene} - \rho_{adatom} \quad (1)$$

where $\rho_{stanene+adatom}$, $\rho_{stanene}$, and ρ_{adatom} are the total charge on stanene + adatom system, bare stanene, and adatom, respectively. All charge densities were plotted by using VESTA program with

isosurfaces of 0.001 electron/Å³. The charge on atoms were calculated by Bader analysis [30].

3. Results

We first investigated a detailed analysis of pristine (1×1) hexagonal buckled stanene for the sake of the comparison before investigating the adsorption properties of single-layer stanene. Our results on optimized stanene structure yielded the lattice parameter $a = 4.595$ Å and the buckling parameter $\Delta z = 0.884$ Å with $d = 2.796$ Å distance between the nearest Sn atoms. The calculated value of the equilibrium cohesive energy for stanene is -5.556 eV per unit cell. All these results are in good agreement with literature [31,16].

Subsequently, we investigated the structural and electronic properties of the most stable adsorption configurations, which are determined from the minimum adsorption energies. It is known that alkali atoms have long range electrostatic interactions. Therefore, we enlarge the (1×1) stanene to (3×3) and (4×4) supercells to prevent the interactions between adatoms. The obtained lattice parameters of (3×3) and (4×4) stanene are $a = 13.785$ Å and $a = 18.380$ Å, respectively. Firstly, we determine the possible adsorption sites which are illustrated in Fig. 1 to

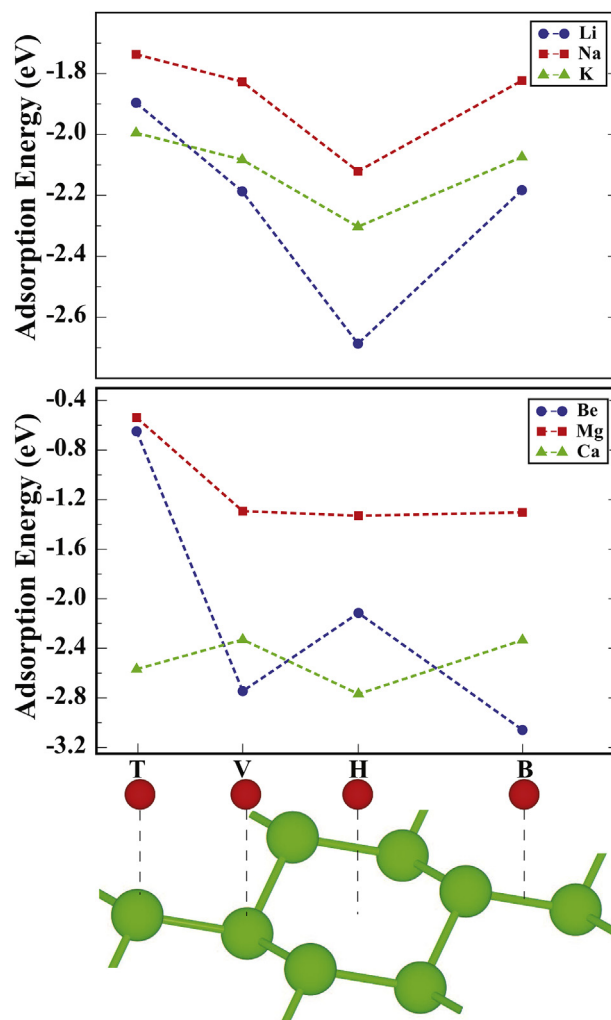


Fig. 1. Adsorption energies as a function of adsorption sites of alkali and alkaline-earth metal atoms on (4×4) stanene. The adsorption sites are illustrated on stanene sheet at the bottom side of graphs.

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