

# Investigation of new two-dimensional materials derived from stanene



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## ARTICLE INFO

### Article history:

Received 30 January 2017

Received in revised form 21 May 2017

Accepted 25 May 2017

### Keywords:

2D materials

Stanene

Optical properties

DFT

## ABSTRACT

In this study, we have explored new structures which are derived from stanene. In these new proposed structures, half of the Sn atoms, every other Sn atom in two-dimensional (2D) buckled hexagonal stanene structure, are replaced with a group-IV atom, namely C, Si or Ge. So, we investigate the structural, electronic and optical properties of SnC, SnGe and SnSi by means of density functional theory based first-principles calculations. Based on our structure optimization calculations, we conclude that while SnC assumes almost flat structure, the other ones have buckled geometry like stanene. In terms of the cohesive energy, SnC is the most stable structure among them. The electronic properties of these structures strongly depend on the substituted atom. We found that SnC is a large indirect band gap semiconductor, but SnSi and SnGe are direct band gap ones. Optical properties are investigated for two different polarization of light. In all structures considered in this study, the optical properties are anisotropic with respect to the polarization of light. While optical properties exhibit features at low energies for parallel polarization, there is sort of broad band at higher energies after 5 eV for perpendicular polarization of the light. This anisotropy is due to the 2D nature of the structures.

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## 1. Introduction

In recent years, investigating the properties of the 2D structures and exploring for new stable 2D structures attract a lot of attention, so they are the focus of several studies. The first and the most remarkable material among them is graphene which is a flat honeycomb structure of carbon atoms with zero band gap and exotic topological, optical, and electronic properties [1–4]. Some of these exotic properties can be listed as half-integer and fractional quantum Hall effects [5,6], Shubnikov–de Haas oscillations with a  $\pi$  phase shift due to Berry's phase [6,7], mobility ( $\mu$ ) up to  $10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and near-ballistic transport at room temperature [8]. The novel properties and applications that emerge from 2D structure and confinement inspire the scientific community to study the other elements from the periodic table for possible graphene-like structures. For example, the 2D honeycomb structures derived from group IV elements, compounds of group III-V and II-VI are generating significant interest because of their possible unique properties that might lead several new applications. Consequently, stable 2D structures made of silicon [9–11], germanium [11] and tin [12–14] are reported, and they are named silicene, germanene and stanene, respectively. These monolayer

structures exhibit honeycomb lattice, however they are not entirely 2D but buckled structures. Recently, the 2D honeycomb structure of silicon has been realized by deposition on Ag (111) substrates [15]. Lately, experimental evidence of germanene grown by molecular beam epitaxy using a gold (111) surface as a substrate is published [16]. Moreover, boron nitride (BN), formed from the group III-V elements, in ionic honeycomb lattice is iso-structure of graphene but having insulator electronic structure, and it has also been produced [17].

Silicene and germanene have zero band gap as in the case of graphene. Even though, they have high carrier mobility, their metallic characteristics limit their application in nanoelectronics. However, stanene has a band gap in order of meV [18], so this aspect differs the stanene from the others and can make it a good candidate for several applications.

Understanding the properties of these new structures is very important, they may maintain very interesting chemical and physical properties which might lead to novel applications. In this study, we introduce new 2D hexagonal structures which are derived from stanene. First, we introduce our model and describe some numerical details. Then, structural properties are presented in details. Next, electronic properties are discussed. Last, the optical properties are studied for two direction of polarization of light. Finally, we summarize the properties of these new structures, and conclude.

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## 2. Computational details

We have performed first-principles calculations based on density-functional theory (DFT) using SIESTA package [19]. The Perdew-Burke-Ernzehof (PBE) [20] formalism of the generalized gradient approximation (GGA) is used for the exchange-correlation functional in our calculations. Because of the periodic boundary conditions, we employed a super-cell geometry in order to describe the isolated monolayer structures. A large vacuum spacing of about 20 Å is considered which ensures the interaction between the layers along z direction is negligible. We used the Monkhorst-Pack scheme for the k-point sampling. After extensive convergence test calculations, we set the k-point mesh to  $20 \times 20 \times 1$  and cutoff energy to 120 Ry. The convergence for energy is chosen as  $10^{-5}$  eV between two steps. All atomic positions were fully relaxed such that the maximum Hellmann-Feynman forces acting on each atom is less than 0.02 eV/Å upon ionic relaxation.

We have investigated the absorption properties of these new structures by calculating their frequency dependent complex dielectric function. The complex dielectric function is the linear response of a system due to external electromagnetic radiation and it is expressed the sum of real and imaginary parts as  $\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$ . Dielectric function calculations in SIESTA are based on the first order time dependent perturbation theory. Therefore, we first worked out the self-consistent ground-state energies and eigen functions which are used to calculate the dipolar transition matrix elements. Because of the Kramers-Kronig relation based on causality, we only need to calculate only one part, either real or imaginary, of the complex dielectric function,  $\epsilon(\omega)$ . The imaginary part,  $\epsilon_2(\omega)$ , is expressed by using the following equation

$$\epsilon_2(\omega) = \frac{e^2}{\pi m^2 \omega^2} \sum_{v,c} \int_{BZ} d\vec{k} |\langle \psi_{ck} | \hat{e} \cdot \vec{p} | \psi_{vk} \rangle|^2 \delta(E_c(k) - E_v(k) - \hbar\omega) \quad (1)$$

within the dipole approximation. Here,  $c$  and  $v$  letters refer to the conduction and the valence band states, respectively.  $E_{(c,v)}(k)$  and  $\psi_{(c,v),k}$  are the corresponding energy and eigenfunction of these states. The sum runs over every pair of valance (filled) and conduction (empty) band states and the integral is over all k-points in the Brillouin zone. The electronic dipole transition matrix element is

calculated between the pair of filled and empty states where  $\hat{e}$  is the polarization vector and  $\vec{p}$  is the momentum operator. Then, the real part of the complex dielectric function can be obtained from this imaginary part,  $\epsilon_2(\omega)$ , by using the Kramers-Kronig transformation:

$$\epsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \frac{\epsilon_2(\omega') \omega'}{\omega'^2 - \omega^2} d\omega' \quad (2)$$

where P denotes the principle part [21].

The optical properties, for example the absorption spectra, can be obtained by determining the transitions from occupied to unoccupied states within the first Brillouin zone. Accordingly, the imaginary part of the dielectric function is essential and enough to describe the optical absorption which is basically calculated from the transition rate between valance and conduction band states. Therefore, once the band structure of the system is determined, i.e. eigenvalues and the eigenfunctions, the all optical constants can be calculated from the imaginary part of the complex dielectric function [18]. Eq. (1) shows the connection of the band structure to  $\epsilon_2(\omega)$ , essentially to the optical properties. For example, the absorption coefficient  $\alpha(\omega)$  simply is

$$\alpha(\omega) = \frac{\omega}{cn(\omega)} \epsilon_2(\omega) \quad (3)$$

where  $c$  is the speed of light and  $n$  is the refractive index which can easily be calculated from  $\epsilon_1(\omega)$  and  $\epsilon_2(\omega)$  as

$$n = \sqrt{\frac{\epsilon_1^2 + \epsilon_2^2 + \epsilon_1}{2}}$$

Therefore,  $\epsilon_2(\omega)$  and  $\alpha(\omega)$  are rather similar for most of the practical cases.

In the present work, the dielectric function and then the absorption coefficient are calculated in the energy interval from 0 to 20 eV for two direction of light's polarization, parallel and perpendicular to the structures. For  $\epsilon_2(\omega)$  calculations, a denser k-point mesh, i.e.  $200 \times 200 \times 1$ , within the Monkhorst-Pack scheme is used for the Brillouin zone integrations.

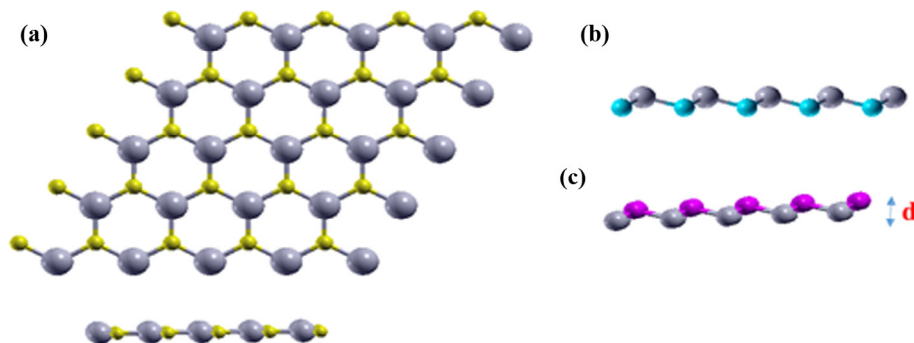


Fig. 1. (a) Top and side view of 2D SnC structure, and side view of (b) SnSi and (c) SnGe structures.

Table 1  
Geometrical parameters and cohesive energy of 2D SnX (X=C, Si or Ge) structures.

| Structure | Bond length (Å) | Lattice parameter (Å) | Buckling length (Å) | Cohesive energy (eV) |
|-----------|-----------------|-----------------------|---------------------|----------------------|
| SnC       | 2.11            | 3.66                  | 0.01                | 5.52                 |
| SnSi      | 2.58            | 4.29                  | 0.73                | 4.56                 |
| SnGe      | 2.63            | 4.35                  | 0.80                | 4.45                 |

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