



First-principles investigation of armchair stanene nanoribbons

M. Fadaie^{a,b}, N. Shahtahmassebi^a, M.R. Roknabad^a, O. Gulseren^{b,*}

^a Department of Physics, Ferdowsi University of Mashhad, Mashhad, Iran

^b Department of Physics, Bilkent University, Ankara, Turkey

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ABSTRACT

In this study, we systematically investigated the structural, electronic and optical properties of armchair stanene nanoribbons (ASNRs) by using the first-principles calculations. First, we performed full geometry optimization calculations on various finite width ASNRs where all the edge Sn atoms are saturated by hydrogen atoms. The buckled honeycomb structure of two dimensional (2D) stanene is preserved, however the bond length between the edge Sn atoms is shortened to 2.77 Å compared to the remaining bonds with 2.82 Å length. The electronic properties of these nanoribbons strongly depend on their ribbon width. In general, band gap opens and increases with decreasing nanoribbon width indicating the quantum confinement effect. Consequently, the band gap values vary from a few meV exhibiting low-gap semiconductor (quasi-metallic) behavior to ~ 0.4 – 0.5 eV showing moderate semiconductor character. Furthermore, the band gap values are categorized into three groups according to modulo 3 of integer ribbon width N which is the number of Sn atoms along the width. In order to investigate the optical properties, we calculated the complex dielectric function and absorption spectra of ASNRs, they are similar to the one of 2D stanene. For light polarized along ASNRs, in general, largest peaks appear around 0.5 eV and 4.0 eV in the imaginary part of dielectric functions, and there are several smaller peaks between them. These major peaks redshifts, slightly to the lower energies of incident light with increasing nanoribbon width. On the other hand, for light polarized perpendicular to the ribbon, there is a small peak around 1.6 eV, then, there is a band formed from several peaks from 5 eV to ~ 7.5 eV, and the second one from 8 eV to ~ 9.5 eV. Moreover, the peak positions hardly move with varying nanoribbon width, which indicates that quantum confinement effect is not playing an essential role on the optical properties of armchair stanene nanoribbons. In addition, our calculations of the optical properties indicate the anisotropy with respect to the type of light polarization. This anisotropy is due to the quasi-2D nature of the nanoribbons.

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1. Introduction

In recent years, graphene, first example of two dimensional (2D) materials, is attracting a lot of attention because of its exotic properties. Besides various nanostructures based on graphene, one-dimensional (1D) nanoribbons has been thoroughly explored. These 1D nanostructures exhibit interesting properties dependent on their size [1–3], topological shapes [4], geometry [2,5] and edge-passivation pattern [6,7]. The electronic structure of the graphene nanoribbons is extensively investigated; because of the finite width, quantum confinement effect leading to band gap opening is essential in graphene nanoribbons [8,9], and it has shown that band gaps are inversely proportional to the ribbons width [10]. In previous studies, armchair graphene nanoribbons

(AGNRs) are divided into three groups according to the modulo 3 of the number of rows of the carbon atoms along the nanoribbon edge, so these groups are labeled with $3M + 1$, $3M$ and $3M - 1$ where M is an integer. The electronic properties of these families and the gap openings of them strongly depend on the ribbon width [11–13]. The armchair graphene nanoribbons are metallic if the number of rows of carbon is $3M - 1$ while the AGNRs falling into $3M$ and $3M + 1$ family are semiconductor [7]. On the other hand, zigzag graphene nanoribbons are always metallic, however transverse electric field can be used to open and control their band gap [14,15]. Moreover, the zigzag graphene nanoribbons display remarkable edge ferromagnetism [16].

Aside from numerous both theoretical and experimental studies on the properties of graphene nanoribbons, there is a considerable effort to synthesize and to investigate various types of 1D nanostructures apart from GNRs. For instance, Cahangirov et al. investigated the nanoribbons from 2D silicene which is formed by silicon

* Corresponding author.

E-mail address: gulseren@fen.bilkent.edu.tr (O. Gulseren).

atoms, one row below the C of group IV of periodic table, analogous to graphene. They have shown that electronic and magnetic properties of armchair nanoribbons of silicene are strongly dependent on their width. Similar to the graphene nanoribbons, silicene nanoribbons are also sorted into three groups. Silicene nanoribbons (SNRs) falling in $3M + 1$ family and ‘low-width’ ribbons of $3M$ family are semiconductors, otherwise all the $3M - 1$ group SNRs have band gaps less than 0.1 eV, so they are low-band gap semiconductors, or quasi-metallic in practice. Comparison of the band gap variation of silicene and graphene nanoribbons shows that GNRs in general have larger band gaps [7]. Further to these inspiring theoretical predictions, experimental studies carried out by Nakano et al. reported the soft synthesis of a single Si monolayer sheet over a substrate, holds the promise for the synthesis of Si honeycomb nanoribbons [17,18].

In group IV of the periodic table, germanium comes down under the carbon and silicon, so one wonders the possibility of 2D structure from Ge atoms. In a following study, the armchair and zigzag nanoribbons from the low-buckled germanene have been studied by Cahangirov et al., and reported that these ribbons can exhibit fascinating electronic and magnetic properties [19]. Tin is the next group IV element under Ge in the periodic table. Stanene is a new 2D hexagonal material which is made of Sn atoms and it has been synthesized recently [20]. There are some very recent works that investigate the structural and mechanical properties of this new 2D nanostructure [21,22].

The purpose of the present work is study of the structural, electronic and optical properties of armchair stanene nanoribbons of widths ranging from $N = 7$ to $N = 17$ atomic rows employing first-principle simulations based upon density functional theory. In this paper, we first described the details of computational parameters which were used and the supercell model employed for the calculations. Then, we reported the structural and electronic properties of ASNRs, and discussed their band gap variation. Finally, the optical properties for two direction of light polarization are studied.

2. Computational method

All calculations were conducted using Siesta code based on density functional theory (DFT). We employed the generalized gradient approximation (GGA) within the Perdew–Burke–Ernzerhof (PBE) formalism [23] for the exchange–correlation potential in our calculations. Because of the periodic boundary conditions, a supercell geometry was adopted in order to avoid the spurious interaction between isolated nanoribbons, a large vacuum spacing of at least 20 Å for both layer–layer and edge–edge separations are introduced. Stanene nanoribbons were placed in the yz -plane. The Brillouin zone integrations were performed using $1 \times 20 \times 1$ k -point mesh within the Monkhorst–Pack scheme and cutoff energy of 950 eV (70 Ryd) was used after extensive test calculations with respect to convergence. All dangling bonds of the edge Sn atoms were passivated with H atoms. Then, all atomic positions were fully relaxed using a conjugate gradient technique. During these geometry optimizations, all the internal coordinates were relaxed until the Hellmann–Feynman forces were less than $0.005 \text{ eV \AA}^{-1}$.

In order to investigate the optical properties of stanene nanoribbons, we have calculated the complex frequency dependent dielectric function as well. The absorption spectra can be obtained by considering the transitions from occupied to unoccupied states within the first Brillouin zone. Dielectric function calculations in SIESTA are based on the first order time dependent perturbation theory. To this end, first the self-consistent ground-state DFT energies and eigenfunctions are computed and then they are used to calculate the dipolar transition matrix elements. Thus, the imaginary part of the dielectric function pinpoint the optical absorption

which is essentially calculated from the transition rate between valance and conduction band states.

We only need the calculation of imaginary part of the complex dielectric function which is expressed as sum of real and imaginary parts, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$. Within the dipole approximation, the imaginary part, $\varepsilon_2(\omega)$, is given by the following expression:

$$\varepsilon_2(\omega) = \frac{e^2}{\pi m^2 \omega^2} \sum_{v,c} \int_{\text{BZ}} d\vec{k} |\langle \psi_{ck} | \hat{e} \cdot \vec{p} | \psi_{vk} \rangle|^2 \delta(E_c(k) - E_v(k) - \hbar\omega) \quad (1)$$

where 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, c and v letters refer to the conduction and the valance band states respectively. $E_{(c,v)}(k)$ and $\psi_{(c,v),k}$ are the corresponding energy and eigenfunction of these states. The electronic dipole transition matrix element is between the pair of filled and empty states where \hat{e} is the polarization vector and \vec{p} is the momentum operator.

Having the imaginary part, $\varepsilon_2(\omega)$, allows the calculation of the real part of the complex dielectric function from causality, i.e. the Kramers–Kronig relations:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^{\infty} \frac{\varepsilon_2(\omega') \omega'}{\omega'^2 - \omega^2} d\omega' \quad (2)$$

where P denotes the principle part. Then, all optical constants can be calculated from the complex dielectric function once the band structure of the system is known [24]. Eq. (1) is the basic expression which connects the band structure to the optical properties. For example, the absorption coefficient $\alpha(\omega)$ is

$$\alpha(\omega) = \frac{\omega}{cn(\omega)} \varepsilon_2(\omega) \quad (3)$$

where n is the refractive index which can be calculated from $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$, and c is the speed of light. In most of the practical cases, the peaks and the structure of $\varepsilon_2(\omega)$ and $\alpha(\omega)$ are rather similar.

In the present work, dielectric functions are calculated for two different direction of light polarization, along ASNRs and perpendicular to stanene nanoribbons and also for unpolarized light. Dielectric function $\varepsilon(\omega)$ is calculated in the energy interval from 0 to 15 eV. For these calculations, a denser k -point mesh, i.e. $1 \times 200 \times 1$, within the Monkhorst–Pack scheme is used for the Brillouin zone integrations.

3. Results and discussions

3.1. Structural and electronic properties

Fig. 1(a) shows the top and side views of optimized 2D hexagonal sheet of stanene. In our previous work [22], we calculated its lattice parameter as $a = 4.68 \text{ \AA}$ and buckling height as $d_0 = 0.86 \text{ \AA}$, which are in a good agreement with other studies [21,25]. The armchair stanene nanoribbon structures are prepared from this infinite quasi-planar structure by keeping only N dimer lines along the ribbon direction which extends to infinity, imposed by periodic boundary condition along this direction. As indicated in Fig. 1(b), the ribbon width is shown by W_a and the buckling in the ribbons is labeled by d . Armchair type of bond structure appears along the both edges of the ribbon. All the edge Sn atoms are saturated by H atoms to avoid the effects of dangling bonds. In our calculations, we consider ASNRs with different widths, labeled by N as NASNR, and N is varied from 7 to 17. For example, the schematic structure of the 13ASNR is shown in Fig. 1(b) from top and side.

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