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First-principles calculation of photocurrent in monolayer silicene sheet under small voltages

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ABSTRACT

We report a calculation of photocurrent in monolayer silicene generated by the illumination of linearly and circularly polarized lights based on density functional theory within the nonequilibrium Green's function formalism. In a photoenergy range from 0.1 to 2.0 eV, the silicene shows a robust photoresponse to the polarized light. There are two peaks located at 0.1 and 1.7 eV, corresponding to the strong photoexcitation in the M and K points in the Brillouin zone of the silicene. The peak photoresponse in the armchair direction is larger than that in zigzag direction, indicating the anisotropy in optics along these two directions. We also found that the photocurrent saturates at the voltages of 0.6 V for both the linear and circular lights in the zigzag and armchair directions.

1. Introduction

Recently, silicene, the counterpart of graphene, has become an intriguing material in the wake of extensive research on graphene. Recent experiments have demonstrated that black phosphorus-based transistors even have a mobility higher than that in graphene-based ones, and these high mobilities are accompanied by high on-off ratios [1,2]. However, researchers are fighting against the inherent black phosphorus unstability issues. Other 2-dimensional (2D) films with an intrinsic bandgap like MoS2, MoSe2, WSe2, etc. have extended the research of the 2D materials to a critical point. However, their carrier mobilities cannot compete with that of graphene.The siliceneis easily integrated with the present IC process and the promising 2D films for nano-electronics in silicon-based technology as the transistors, spintronic devices, and optoelectronic devices and sensors etc.

The silicene optical properties have been widely investigated. It has been reported that silicene behaves like a group IV material and its properties depend on the electronic structure, such as the bandgap, doping or passivation conditions [3–5]. The study on the valley spin polarization of the silicene makes it potential to be optically active in the infrared and THz ranges [6]. Ezawa et al. reported a sufficiently large on and off ratio of silicene-based device in an external electromagnetic field by controlling the electronic and magnetic properties of silicene [7].

In this work, we aim to give a theoretical understanding on the photocurrent of the silicene for its potential application in optoelectronic device. We calculated the photocurrent generated by the illumination of polarized light with the photo energies ranging from 0.1 to 2.0 eV under different bias voltages. The photocurrent shows two peaks located close to 0.1 and 1.7 eV, corresponding to the strong photo excitation in the M and K points in the Brillouin zone of the silicene. The photocurrent saturates at the voltages of 0.6 V for both the linear and circular lights in the zigzag and armchair directions.An evident anisotropy in photocurrent is also observed between the armchair and zigzag directions.

2. Methods

To study the photocurrent under the polarized light, we construct a two-probe system for the zigzag, and armchair directions, respectively. The left- and right-hand leads and the center region are composed of silicene atoms. We consider both the linearly polarized and circularly polarized lights which irradiate the silicene vertically. The photoenergy is from 0.1 to 2.0 eV which covers the light from the far- and near-infrared frequency to the red light in visible range. We calculate the photocurrent varying with polarized angles from 0° to 180° in a photoenergy interval of 0.1 eV for small bias voltages from 0.2 to 1.2 V. The calculated photocurrent is a normalized one, i.e., the photoresponse, as mentioned in our previous work [8].

The photocurrent calculations were based on a state-of-the-art theoretical approach where density function theory (DFT) is

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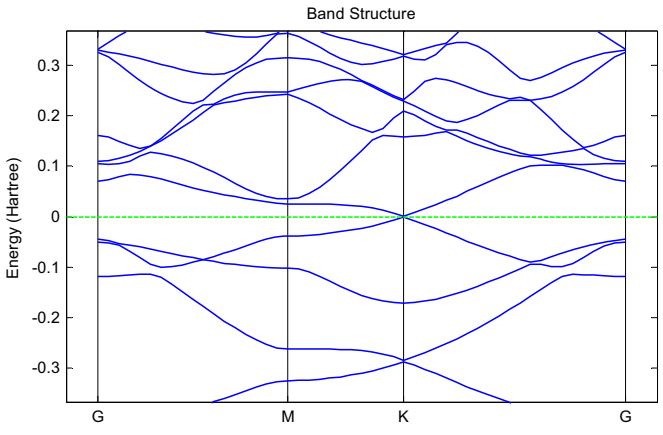

Fig. 1. Band structure of silicene.

combined with the Keldysh Nonequilibrium Green's Function (NEGF) theory [9,10]. In the subsequent NEGF-DFT numerical calculations, a double zeta polarized (DZP) atomic orbital basis was used to expand all the physical quantities; the exchange and correlation were treated at the level of the local density approximation and atomic cores are defined by the standard norm conserving nonlocal pseudopotentials. The whole system was obtained by DFT total energy relaxation. The tolerances were set as follows: 0.00001 eV/atom for the total energy, 0.05 eV/Å for the atomic force, and $1 \times 12 \times 12$ k-points were used in the irreducible Brillouin zone. The supercell were relaxed by optimizing the geometry to obtain the theoretical equilibrium structures.

3. Results and discussion

The optimized monolayer silicene cell parameters are 3.84 Å, in good agreement with the previous calculations [11]. The nearest-neighbour distance (NND) or bond length in the honeycomb lattice of siliceneis 2.41 Å, which is slightly less that of the bulk Si (2.43 Å).

3.1. Photocurrent in the zigzag direction

The electronic band structure of the relaxed silicene was plotted in Fig. 1. The monolayer silicene is a zero-gap semiconductor, for which we obtained a very slight bandgap of 2.68 meV at K point, which is smaller than the result from the calculation using the GGA Perdew-Burke-Ernzerhof exchange-correlation functional (66 meV) [12]. The difference between our calculated bandgap and those previous theoretical calculations should be attributed to the different energy functional [12] and/or the spin-orbital interaction [6]. In addition, there is a energy gap of about 1.7 eV located at M point, at which a robust optical absorption has been predicted in previous calculations [5].

The photocurrent generated by the illumination of the linear light in the zigzag is given in Fig. 2. We found that at different bias voltages the photoresponse in the zigzag direction varies in terms of Cos(2Θ) for the photoenergies in the range of 0.1 eV to 2.0 eV. Fig. 2 plots three curves at 0.6 V for photoenergies of 1.2, 1.4 and 1.6 eV, respectively, as examples.This behavior of the photoresponse is a direct result of the Fermi's golden rule which describes the photoexcitation of the electrons between different states. Fig. 3 shows the maximum photoresponse for different photoenergies at different bias voltages. We observed that the photoresponse increases from 0.2 V to 0.6 V, and then it saturates, as the curves of 0.6 to 1.2 V are almost coincides. It is worth to note

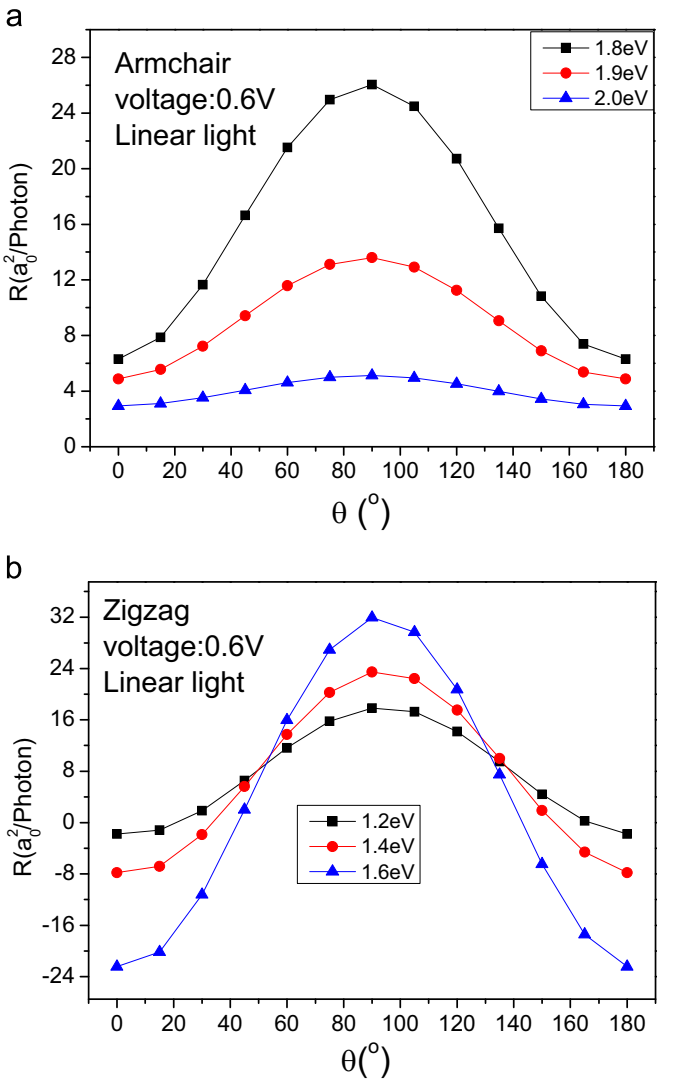

Fig. 2. The calculated photoresponse for the linearly polarized light. (a) The calculated photoresponse in the illumination of the linearly polarized light at different photon energies in the armchair direction and (b) The calculated photoresponse in the illumination of the linearly polarized light at different photon energies in the zigzag direction.

that there were two obvious peaks in the curves: the one is around 0 to 0.1 eV and the other is located around 1.7 eV, which should be attributed to the photoexcitation at the two high symmetry k points in the Brillouin zone of silicene, i.e., the K and M points, respectively. The reboust photoexcitation in silicene at these two symmetry points was also reported in previous calculations [5], which is in good agreement with our calculations. For the circular light, the photoresponse is basically of the same trend as that for the linear light, as shown in Fig. 3(b). The photoresponse varies as Cos(2Θ) for different photoenergies.

3.2. Armchair direction

In the armchair direction, the photoresponse also has a shape of Cos(2Θ) for the photoenergies in the range of 0.1 eV to 2.0 eV, as shown in Fig. 4. There are two peaks in the maximum photoresponse. One is located close to 0 eV and another covers the energy range from 1.4∼1.7 eV. This should also be ascribed to the strong photoexcitation at the K and M symmetry points of the Brillouiin zone. We found that for the second peak the photoresponse reaches maximum at about 0.6 V bias voltage and then