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Diamagnetic response in zigzag hexagonal silicene rings

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ABSTRACT

Hexagonal silicene rings with unusually large diamagnetic moments have been found in a theoretical study of the electronic and magnetic properties. In the presence of effective spin–orbit coupling, the magnetic-field-driven spin-up electrons flow anticlockwise exhibiting colossal diamagnetic moments, while the spin-down electrons flow clockwise exhibiting colossal paramagnetic moments along the rings. The large diamagnetic moment is thus the result of competition of spin-up and spin-down electrons, which can be modulated by spin–orbit coupling strength and exchange field.

Since Kroto et al. speculated a large diamagnetic response in C_{60} [1], the studies for carbon nanostructures with large moments become a hot topic. However, the experimental and theoretical studies show that C_{60} exhibits a very small magnetic susceptibility [2–4]. Experimental results indicate that the magnetic susceptibility of a carbon nanotube is about -25 ppm emu/g [5,6], and that of graphite is about -30 ppm emu/g [6]. Recently, based on tight-binding theory, Liu et al. found that metallic carbon nanotori possess colossal paramagnetic moments as their strength is 3 orders of magnitude stronger than that of graphite at 0.1 T [7]. Meanwhile, we found odd–even width effect on persistent current in zigzag hexagonal graphene rings [8] and giant orbital paramagnetism in toroidal carbon nanopeapods [9].

Recently, silicene, the counterpart of graphene for silicon, has been synthesized [10–12] and attracts much attention [13–21]. Differing from graphene, silicene possesses a relative large intrinsic spin–orbit coupling (SOC) and a considerable bulk band gap with $E_g = 1.55$ meV at the Dirac point [16]. Thus silicene is a good candidate to realize the quantum spin Hall (QSH) state. By adjusting the Rashba SOC strength, a topological phase transition results in the quantum anomalous Hall state (QAH) [16], which is characterized by a full insulating gap in the bulk and chiral gapless edges. Unlike the quantum Hall (QH) effect, arising from Landau-level quantization in a strong magnetic field, the QAH effect origins from the joint effect of internal magnetization and SOC. Specially, the QAH effects have been found in TM (transition metal) atoms adsorbed silicene [18–20]. Because of these rich physical properties, one may anticipate an enhanced magnetic response of silicene ring systems through adjusting SOCs strength and exchange field.

In this letter, we have investigated the magnetic response of silicene rings under an applied magnetic field (with the magnetic field perpendicular to the plane of rings) based on tight-binding model. The geometry of silicene ring is shown in Fig. 1, which can be realized by etching a ring out of the silicene sheet. The inner and outer radii of rings are labeled by m and n, respectively. The schematic illustration in Fig. 1(a) is (5, 9) ring. Based on tight-binding calculations, we find that hexagonal silicene rings possess unusually large diamagnetic moments. Our investigation has elucidated succinctly the physics underpinning the unusual magnetic response of silicene rings, which is mainly due to the effective SOCs and exchange field.

In the tight binding approximation, the silicene Hamiltonian with SOCs and an exchange field can be written as [22,23]

$$\begin{aligned} H = &-t \sum_{\langle ij\rangle\alpha} c^\dagger_{i\alpha} c_{i\alpha} + it_0 \sum_{\langle\langle ij\rangle\rangle\alpha\beta} \nu_{ij} c^\dagger_{i\alpha} \sigma^z_{\alpha\beta} c_{i\beta} \\ &- it_{so} \sum_{\langle\langle ij\rangle\rangle\alpha\beta} u_{ij} c^\dagger_{i\alpha} (\sigma \times \hat{d}_{ij})^z_{\alpha\beta} c_{i\beta} \\ &+ it_R \sum_{\langle ij\rangle\alpha\beta} c^\dagger_{i\alpha} (\sigma \times \hat{d}_{ij})^z_{\alpha\beta} c_{j\beta} + M \sum_{i\alpha\beta} c^\dagger_{i\alpha} \sigma^z_{\alpha\beta} c_{i\beta}, \end{aligned} \tag{1}$$

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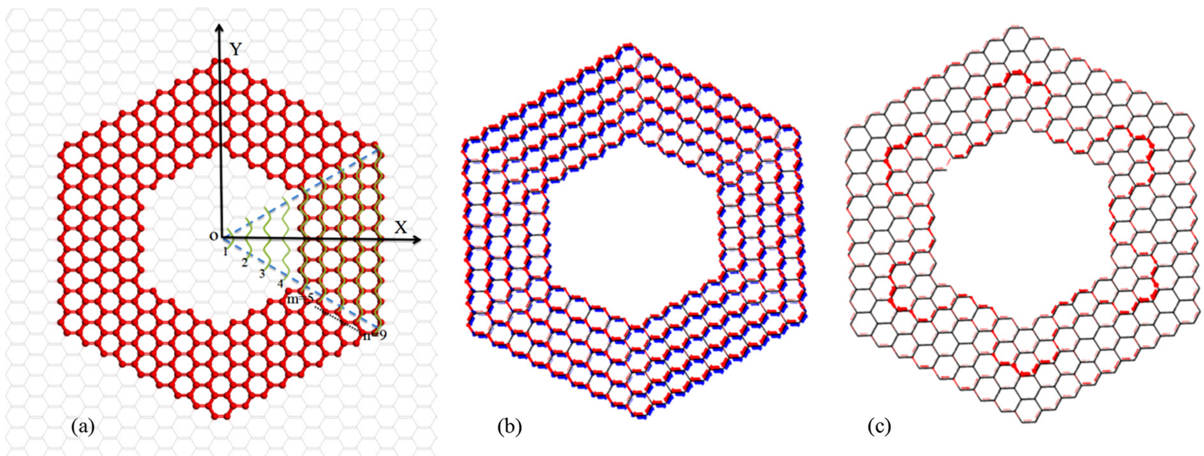

Fig. 1. (a) Schematic illustration of (5, 9) ring etched in silicene. (b) The geometric structure of (6, 13) ring and the corresponding ring current. The red arrows denote the ring current of spin-up electrons with their widths proportional to the current strength, while the blue arrows denote the ring current of spin-down electrons. (c) The pure current of spin-up and down electrons. The applied magnetic field is perpendicular to the plane of rings. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

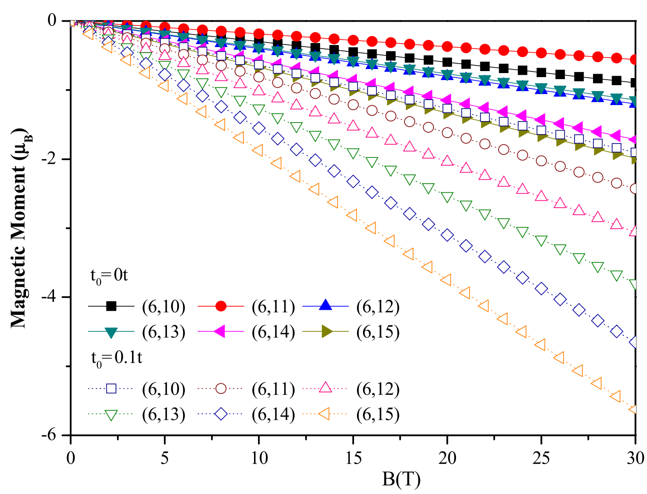

Fig. 2. Induced magnetic moment vs magnetic field strength of zigzag hexagonal silicene rings in the absence of effective SOCs (solid line) and presence of effective SOCs (dashed line), respectively.

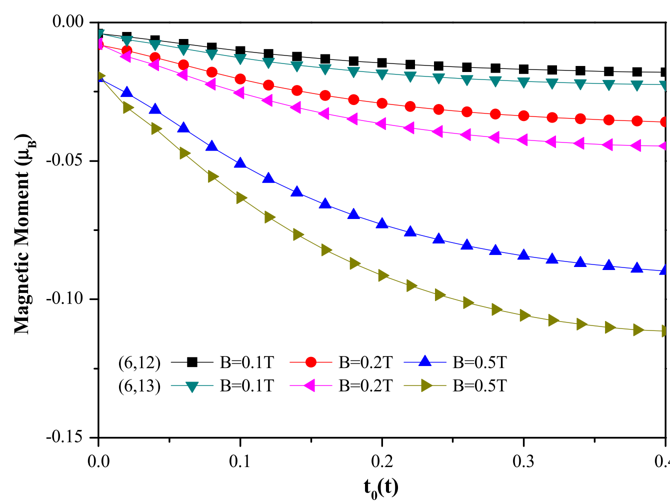

Fig. 3. Induced magnetic moment vs effective SOCs strength at the given magnetic field strength.

where $c^\dagger_{i\alpha}(c_{i\alpha})$ is a creation (annihilation) operator for an electron with spin α on site i, and $\langle ij\rangle\langle\langle ij\rangle\rangle$ run over all nearest or next-nearest neighbor hopping sites. The first term is the usual nearest neighbor hopping with the transfer energy $t = 1.6$ eV. The second term represents the effective SOC involving the next-nearest neighbor hopping with amplitude t_0. $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ is the Pauli matrix of spin. $\nu_{ij} = d_j \times d_i |d_j \times d_i|$, where d_i and d_j are two nearest neighbor bonds connecting the next-nearest neighbor sites. The third term is the intrinsic Rashba SOC, where $u_{ij} = \pm 1$ for the A (B) site, and $\hat{d}_{ij} = \hat{d}_{ij}/|d_{ij}|$ with the vector d_{ij} connecting two sites i and j. The fourth term is the extrinsic Rashba SOC, which induced by external electric field [24–26]. The last term is an exchange field M, which arises from the interaction with a magnetic substrate. The effect of the magnetic field enters the Hamiltonian via $H_{ij} = H^0_{ij} \exp\{i(2\pi/\phi)\int_i^j \vec{A}\, d\vec{r}\}$, where H^0_{ij} is the Hamiltonian matrix element for zero field, $\phi = hc/e$ the flux quantum, and $\vec{A}$ the vector potential [27,28]. The magnetic moment of a silicene ring was calculated in terms of the ring current I in the ring, namely, $M = IS$ where the current element between site i and j is $I_{ij} = \frac{4e}{\hbar}\,\mathrm{Im}\sum_n f(E_n) c^*_{in} H_{ij} c_{jn}$ with $f(E_n)$ being the Fermi factor, c_{in} the eigenvector corresponding to the eigenenergy E_n, and S the area enclosed by the rings.

The induced magnetic moment vs magnetic field for a wide variety of rings is shown in Fig. 2. As can be seen from Fig. 2, the zigzag hexagonal silicene ring exhibits diamagnetic response. In the absence of SOCs and exchange field, the magnetic moment of silicene rings decline linearly with the magnetic field strength, in which the total magnetic moment is the summation of magnetic moment of spin-up and spin-down electrons. The magnetic moment of spin-up electrons equals to that of spin-down electrons owing to doublet degenerate. Specially, we find that at the given magnetic field strength, the magnitude of magnetic moment of (6, 11) rings is lower than that of (6, 10) ring. Though there are more electrons in the surface of (6, 11) ring, the electrons have relatively small velocity compared with that of (6, 10) ring. This is the reason why the magnetic moment of (6, 11) ring is lower than that of (6, 10) ring.

In Fig. 3, we find the amplitude of total magnetic moment increases fast in the presence of effective SOC, which means that the amplitude of total magnetic moment can be adjusted by effective SOC strength. In the case of B = 0.5 T, the total magnetic moment of (6, 13) ring is $-0.01965u_B$ at $t_0 = 0t$ and $-0.1125u_B$ at $t_0 = 0.4t$, respectively. In Fig. 1(b), we find the magnetic-field-driven spin-up electrons flow anticlockwise and spin-down electrons flow clockwise around the rings. In the case of B = 0.1 T and