Comment on “d+id^{′} Chiral Superconductivity in Bilayer Silicene”

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Comment on "$d+id'$ chiral superconductivity in bilayer silicene"

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In Ref. [1], Liu *et al.* investigated the structural and electronic properties of the undoped bilayer silicene from first-principles. Their calculations show that the silicene bilayer is metallic with sizable pocket Fermi surfaces; based on this, their random-phase-approximation analysis suggests that the system is superconducting with the Cooper pairs mediated by the antiferromagnetic spin fluctuation on the border of spin density wave. Moreover, they claim that a high superconducting critical temperature is possible due to the tunable Fermi pocket vis strain.

Here we show that, however, their main conclusion is totally wrong since the ground state of the silicene bilayer is semiconducting with a substantial band gap of 0.55 eV; therefore the system cannot be a superconductor. This is because they didn't consider spin-polarization when carrying out electronic structure calculations.

Without spin-polarization, our density-functional-theory (DFT) calculations [2, 3] confirm that the AB bottom-top (AB-bt) structure as suggested by Ref. [1] is indeed energetically more favorable than other configurations. Our calculated phonon dispersion also shows that the AB-bt structure is stable. We find that equilibrium lattice constant is 3.854 Å, and the Si-Si bond length is 2.323 Å within each layer while it is 2.524 Å between two layers, in excellent agreement with their results.

The valence electrons of Si atoms within silicene monolayer are known to be sp^3-like hybridized [4]: three of the four sp^3-like orbitals form covalent bonds with neighboring atoms, while the last one (p_z orbital) could either form an extensive π-bonding network within a monolayer or bond with its adjacent counterpart of the other monolayer. The bilayer system could stay in a nonmagnetic or a magnetic ground state.

Liu *et al.* treated the silicene bilayer as two geometrically attached monolayers without magnetic ordering using both non-spin-polarized DFT calculations and the tight-binding analysis. Their results show that the silicene bilayer is intrinsically metallic, which in turn motivated them to pursue superconductivity. However, the spin degree of freedom is required to determine the electronic properties of silicene bilayer, since the formation of interlayer bonds might modify the π-bonding network, so that the electron in the p_z orbital of a Si atom with no interlayer bond might get unpaired and localized to carry a magnetic moment.

Here we employ spin-polarized DFT computations to examine all possible magnetic configurations. As shown in Fig. 1, we find that these magnetic moments prefer to couple ferromagnetically within each layer while antiferromagnetically across two layers, with the

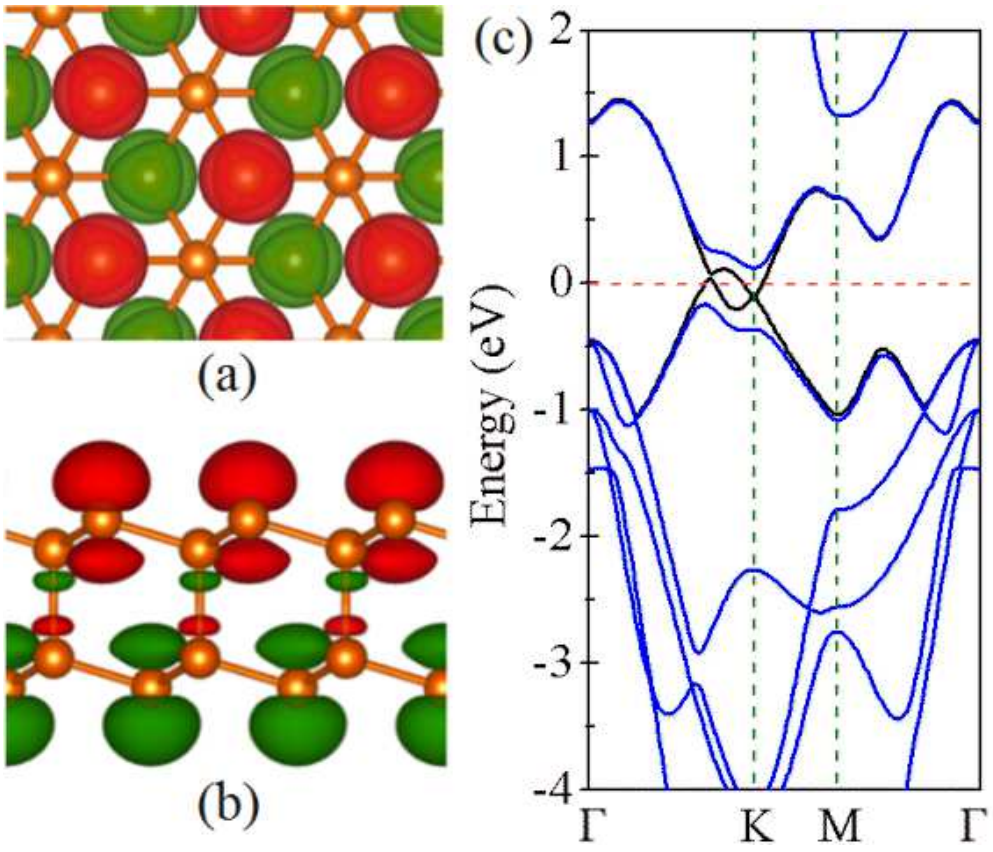

FIG. 1. (color online) (a) and (b) are the top view and side view for the spin-polarized electron density distribution of the silicene bilayer, respectively. The spin-up density is in red while spin-down in green, and the isosurface is plotted at the value of 0.25 electrons/Å^3. (c) The calculated DFT electronic band structure for the silicene bilayer with spin-polarization (in blue). The two bands near the Fermi level for the non-spin-polarized state are also plotted (in black) for direct comparison.

total energy lowered by 10 meV per unit cell due to magnetic ordering against that of the non-magnetic state. Therefore, the ground state of silicene bilayer is magnetic. Furthermore, the electronic band structure of the magnetic state, as plotted in Fig. 1(c), suggests that the silicene bilayer is a narrow-gap semiconductor, not an intrinsic metal. The fundamental band gap is calculated to be 0.55 eV using the many-body *GW* approximation [5, 6] (0.29 eV using DFT-GGA [3]). We thus conclude that there is no superconductivity at all in the silicene bilayer.

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[1] F. Liu, C.-C. Liu, K. H. Wu, F. Yang, and Y. G. Yao, Phys. Rev. Lett. **111**, 66804 (2013).

[2] G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15 (1996).

[3] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. **77**, 3865 (1996).

[4] G. G. Guzmán-Verri and L. C. Lew Yan Voon, Phys. Rev. B **76**, 075131 (2007).

[5] Mark S. Hybertsen and Steven G. Louie, Phys. Rev. B **34**, 5390 (1986).

[6] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002).