## Comment on "Structural and Electronic Properties of *T* Graphene: A Two-Dimensional Carbon Allotrope with Tetrarings"

In Ref. [1], Liu *et al.* calculated the electronic properties of a two-dimensional tetrasymmetrical carbon allotrope named as *T* graphene. They claimed that buckled *T* graphene has Dirac-like fermions with a high Fermi velocity, contrary to planar *T* graphene. Herein, we show that their main conclusion is incorrect because buckled *T* graphene is indeed a normal metal as planar *T* graphene and thus does not possess Dirac-like fermions.

To reveal the nature of the electronic properties of *T* graphene, we independently performed density-functional calculations using the QUANTUM ESPRESSO package [2], and the obtained results are summarized in Fig. 1. The results indicated that planar *T* graphene is normally metallic [Fig. 1(c)] under the primitive unit cell, consistent with Ref. [1]. Interestingly, when we used a $\sqrt{2} \times \sqrt{2}R45°$ supercell to redraw the band structure of the same planar *T* graphene [Fig. 1(d)], a linear dispersion relation with crossing points appeared near the Fermi level. Obviously, such a variation originates from the band folding due to the use of a larger supercell: the *k* point of *X* under the primitive unit cell transforms into the point *M* under the supercell while *M* is folded back to Γ [Fig. 1(b)], so the bands along Γ*X* and *MX* under the primitive unit cell [Fig. 1(c)] merge into the bands along Γ*M* under the supercell [Fig. 1(d)], resulting in the crossing of linearly dispersive bands. More importantly, for buckled *T* graphene where the square C substructure displaces out of the plane in an ad-dimer way, the calculated band structure [Fig. 1(e), as well as the Fig. 2(c) of Ref. [1] ] is found to be essentially analogous to that of planar *T* graphene under the supercell [Fig. 1(d)], despite some differences owing to the corrugation of the buckled *T* graphene. These results demonstrate that the previously observed distinctions between planar and buckled *T* graphenes [1] are mainly an illusion due to the band folding.

In fact, the band crossing near the Fermi level in *T* graphene is totally different from the Dirac cone in graphene. Planar *T* graphene under the supercell and buckled *T* graphenes are bipartite (while planar *T* graphene under the primitive unit cell is not), so that their band structures are symmetric about the Fermi level under a tight-binding approximation. When the system is metallic as discussed here, such a symmetry naturally produces the band crossing at the Fermi level. However, it is different in nature from the Dirac cone as that in graphene. The crossings in *T* graphene form a line (a feature of normal metals) but not some discrete points (a feature of semimetals such as graphene). There is no conelike structure near the Fermi level. As a result, the density of states of *T* graphene is nonzero (as can be seen in the Fig. 2 of Ref. [1]). The band around a point on the crossing line (**P**) is expanded as $E_{\pm}(\mathbf{q}) \simeq \pm v_F|\mathbf{q} \cdot \hat{\mathbf{e}}_{\mathbf{P}}|$ with $\mathbf{k} = \mathbf{P} + \mathbf{q}$ and $\hat{\mathbf{e}}_{\mathbf{P}}$ being the normal direction of the crossing line at **P**, which varies with **P**. So the carriers of *T* graphene cannot be described by the Dirac equation (which is opposite to what was claimed in Ref. [1]) and novel physics revealed in graphene would not occur in *T* graphene. The lack of Dirac cone also explains why the quantum confinement effect does not open a band gap in the buckled *T* graphene nanoribbons [1].

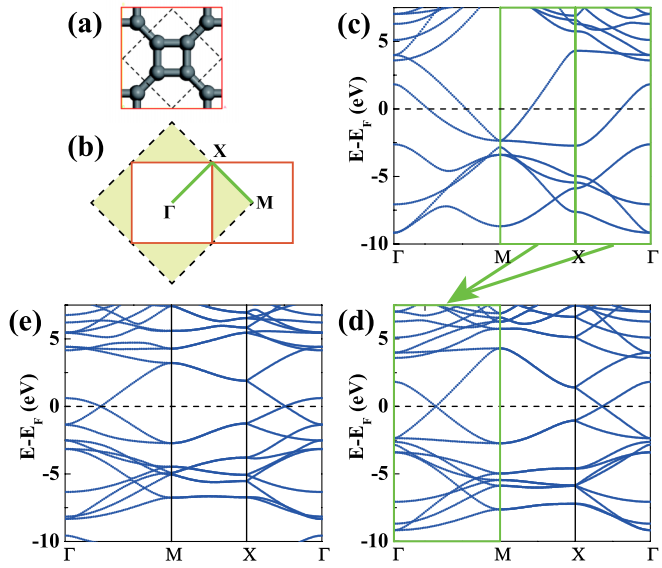


FIG. 1 (color online). (a) Atomic structures and (b) Brillouin zones for the primitive unit cell (black dashed frame) and $\sqrt{2} \times \sqrt{2}R45°$ supercell [red (or gray) solid frame] of planar *T* graphene. (c),(d),(e) The band structures of planar *T* graphene with the primitive unit cell and $\sqrt{2} \times \sqrt{2}R45°$ supercell, and buckled *T* graphene, respectively. The band folding process is schematically depicted by the green arrow.

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[1] Y. Liu, G. Wang, Q. S. Huang, L. W. Guo, and X. L. Chen, Phys. Rev. Lett. **108**, 225505 (2012).
[2] P. Giannozzi *et al.*, J. Phys. Condens. Matter **21**, 395502 (2009).

 