Supplemental Material for "A carbon allotrope with twisted Dirac cones induced by grain boundaries composed of pentagons and octagons"

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	Ring	E (eV/atom)	Electronic property
Graphyne	**6**	**0.64**	**semimetal**
Biphenylene	**4,6,8**	**0.468**	**metal**
TPH-graphene	**5,6,7**	**0.396**	**metal**
127-11-84-r568-1	**5,6,8**	**0.377**	**semimetal**
PHH-graphene	**5,6,7**	**0.319**	**semimetal**
Hopgraphene	**5,6,8**	**0.25**	**metal**
Phagraphene	**5,6,7**	**0.19**	**semimetal**
$(SF)_4$-graphene	**4,6,8**	**0.1732**	**semimetal**
SW graphene	**5,6,7**	**0.15**	**semimetal**
SW40	**5,6,7**	**0.13**	**semimetal**
Graphene	**6**	**0**	**semimetal**
[1]PHO-graphene	**5,6,8**	**0.3236**	**semimetal**
[2]PHO-graphene	**5,6,8**	**0.2704**	**metal**
[3]PHO-graphene	**5,6,8**	**0.2294**	**metal**
[4]PHO-graphene	**5,6,8**	**0.1982**	**semimetal**
[5]PHO-graphene	**5,6,8**	**0.1735**	**metal**
[6]PHO-graphene	**5,6,8**	**0.1546**	**semiconductor**
[7]PHO-graphene	**5,6,8**	**0.1394**	**semimetal**

Table.S1 Average atomic energy and electronic property of carbon allotropes.

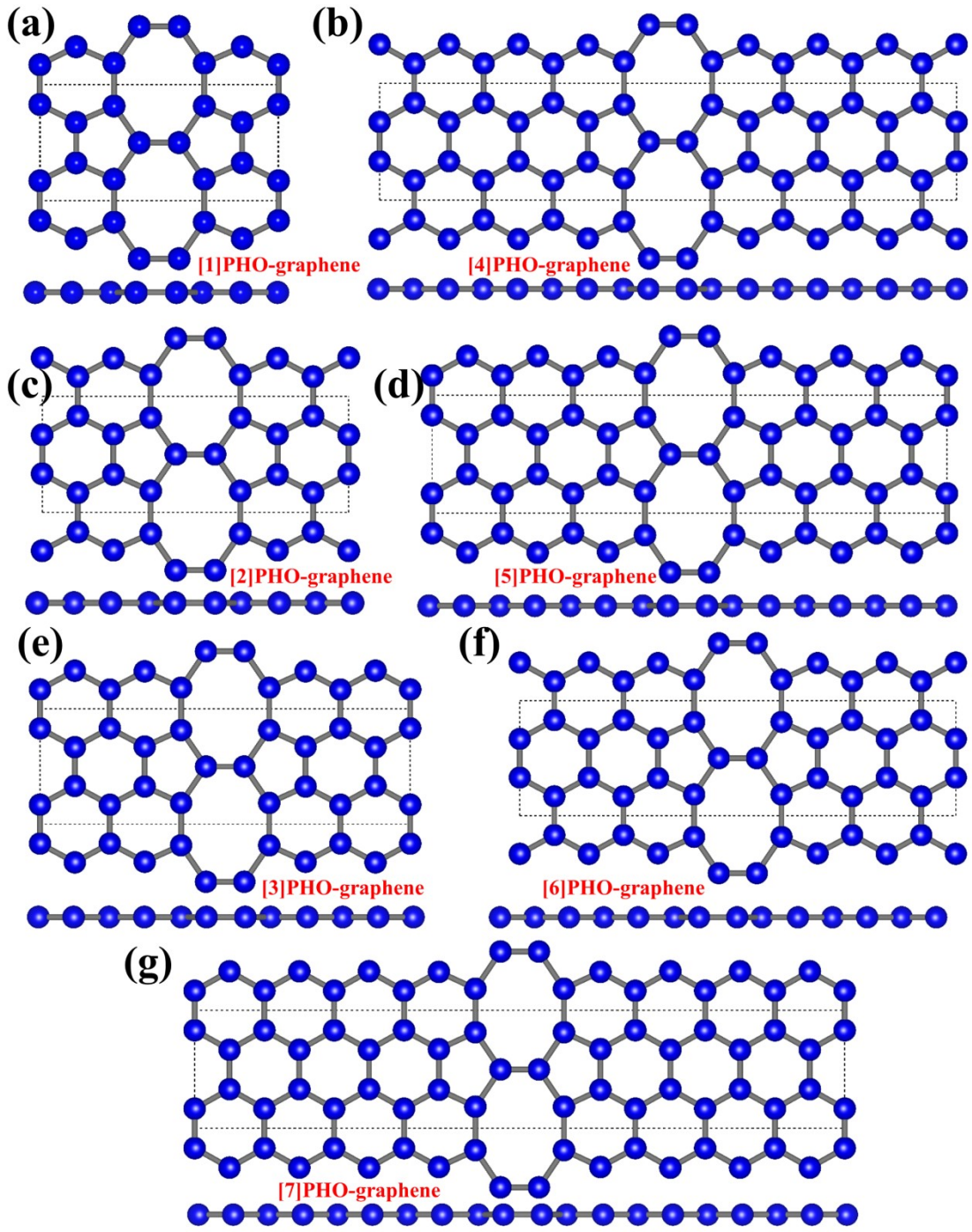

Fig.S1 The structure of [N]PHO-graphene. The rectangular primitive cell is represented by a black dash line.

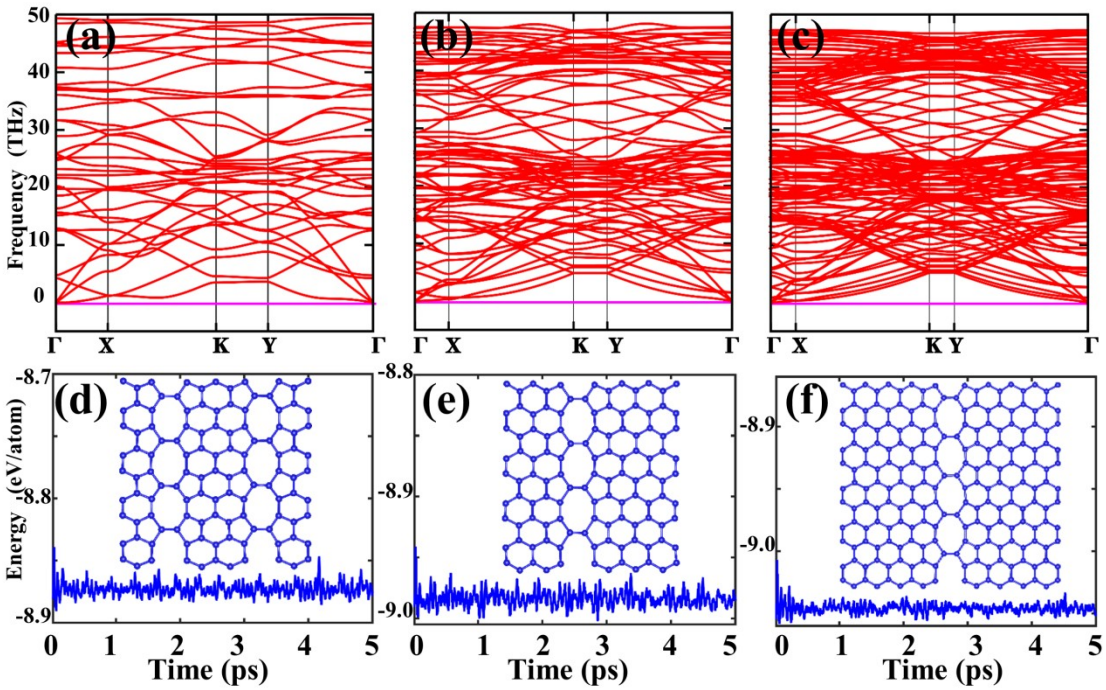

Fig.S2 Phonon spectrum of (a) [1]PHO-graphene, (b) [4]PHO-graphene and (c) [7]PHO-graphene. Molecular dynamics simulations of (d) [1]PHO-graphene, (e) [4]PHO-graphene and (f) [7]PHO-graphene.

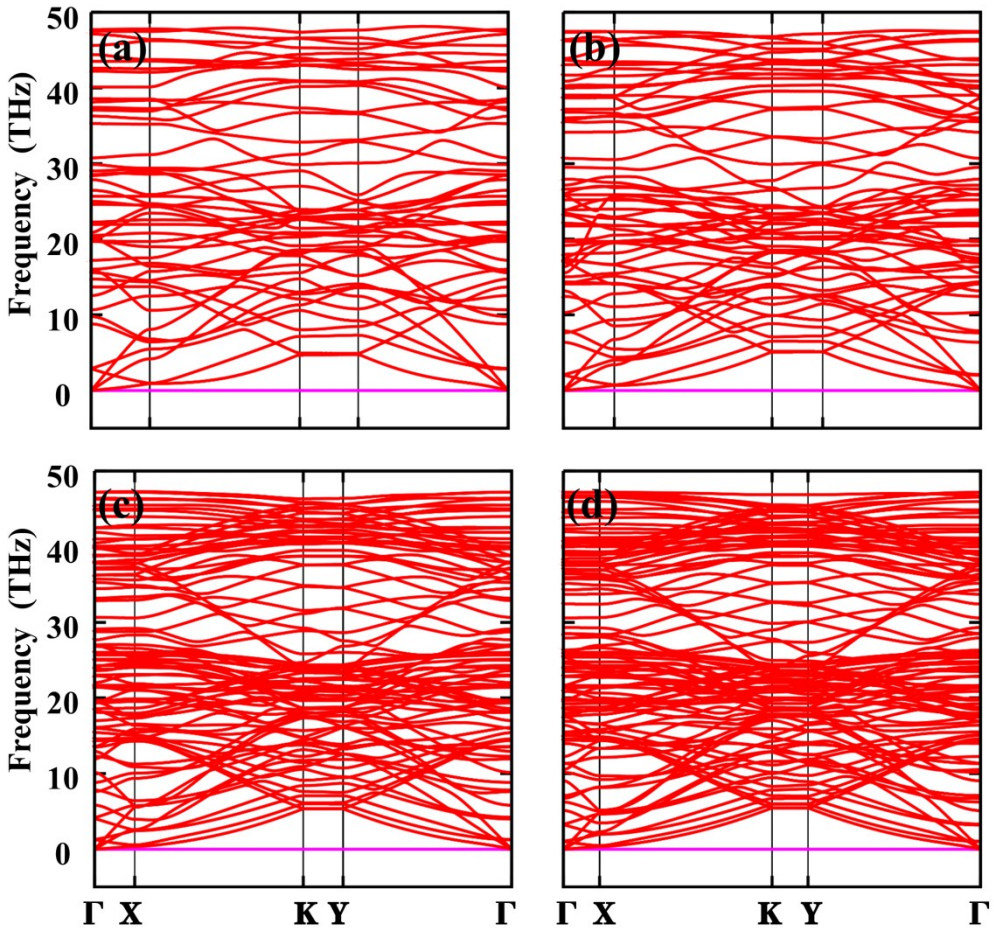

Fig.S3 Phonon spectrum of (a) [2]PHO-graphene, (b) [3]PHO-graphene, (c) [5]PHO-graphene and (d) [6]PHO-graphene.

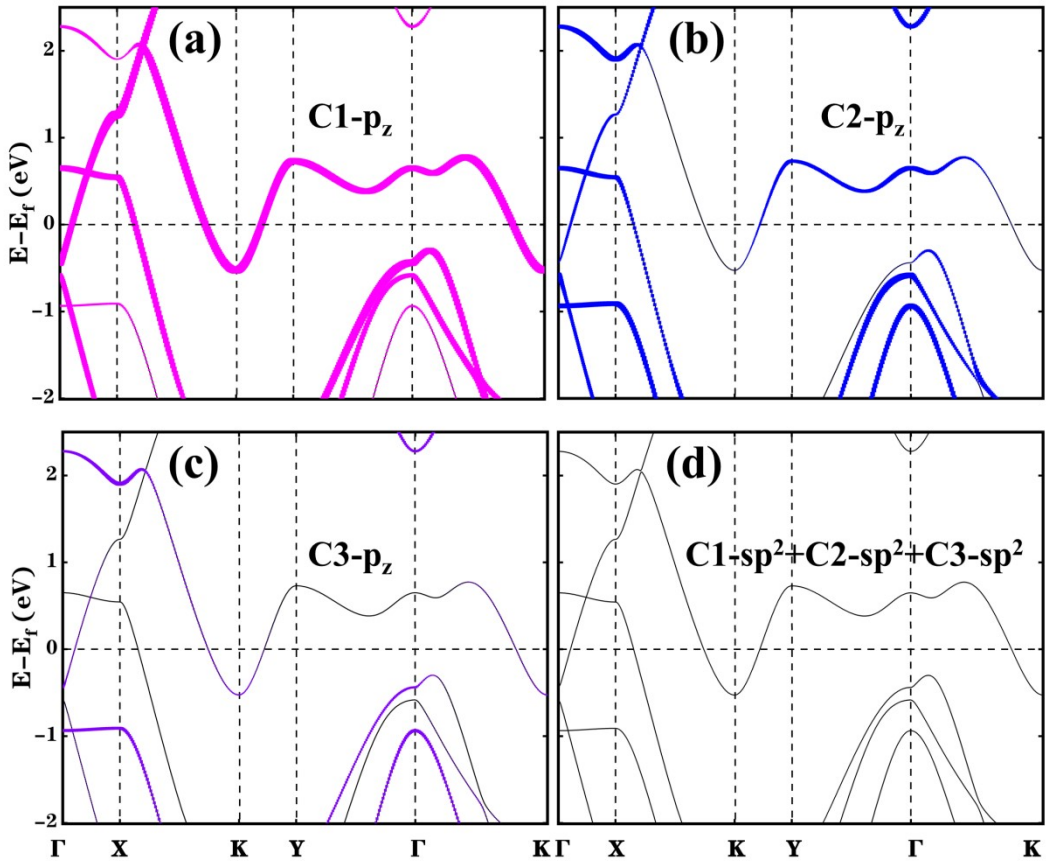

Fig.S4 The contribution of different carbon atoms to the bands around Fermi energy.

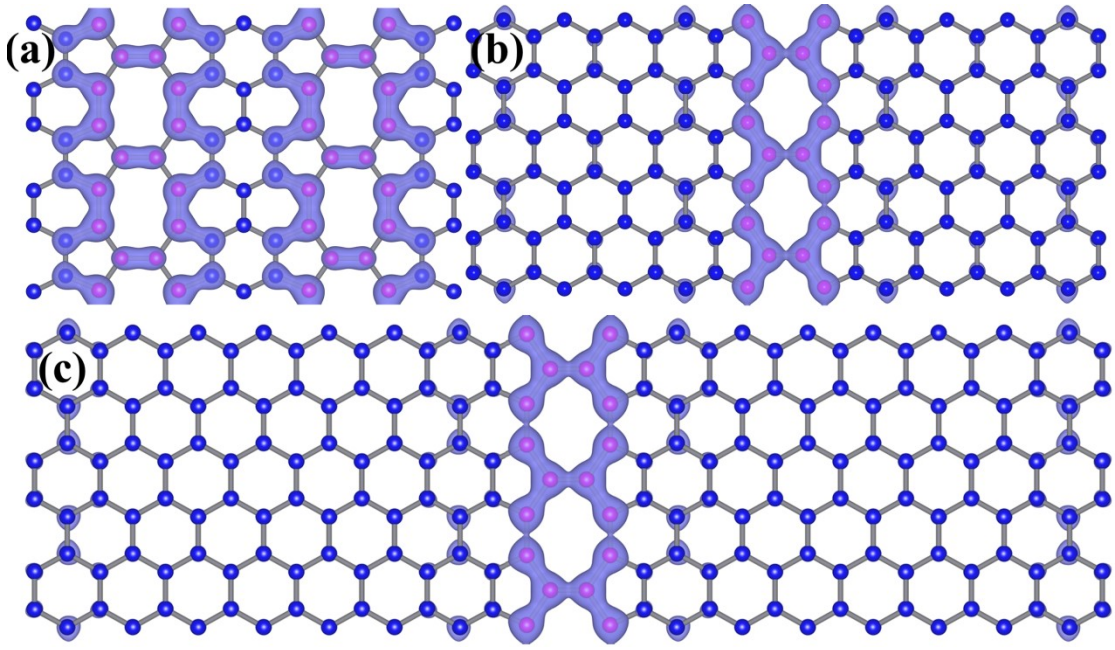

Fig.S5 The charge distribution near the Fermi energy of PHO-graphene, their behavior at the grain boundary is like a quasi-one-dimensional metallic wire.

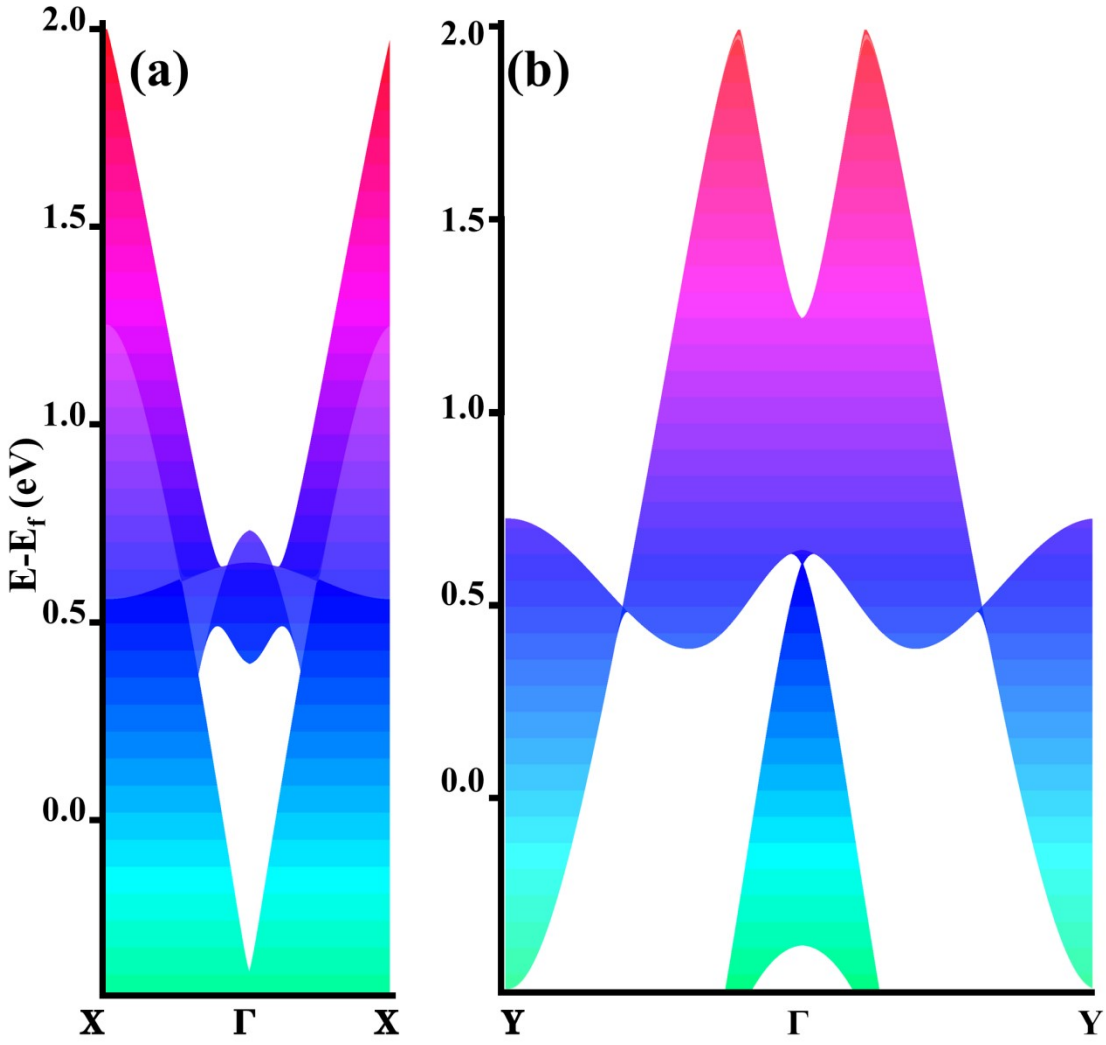

Fig.S6 The 3D band spectrum of [1]PHO-graphene. It can clearly observe the details of the bulk band.

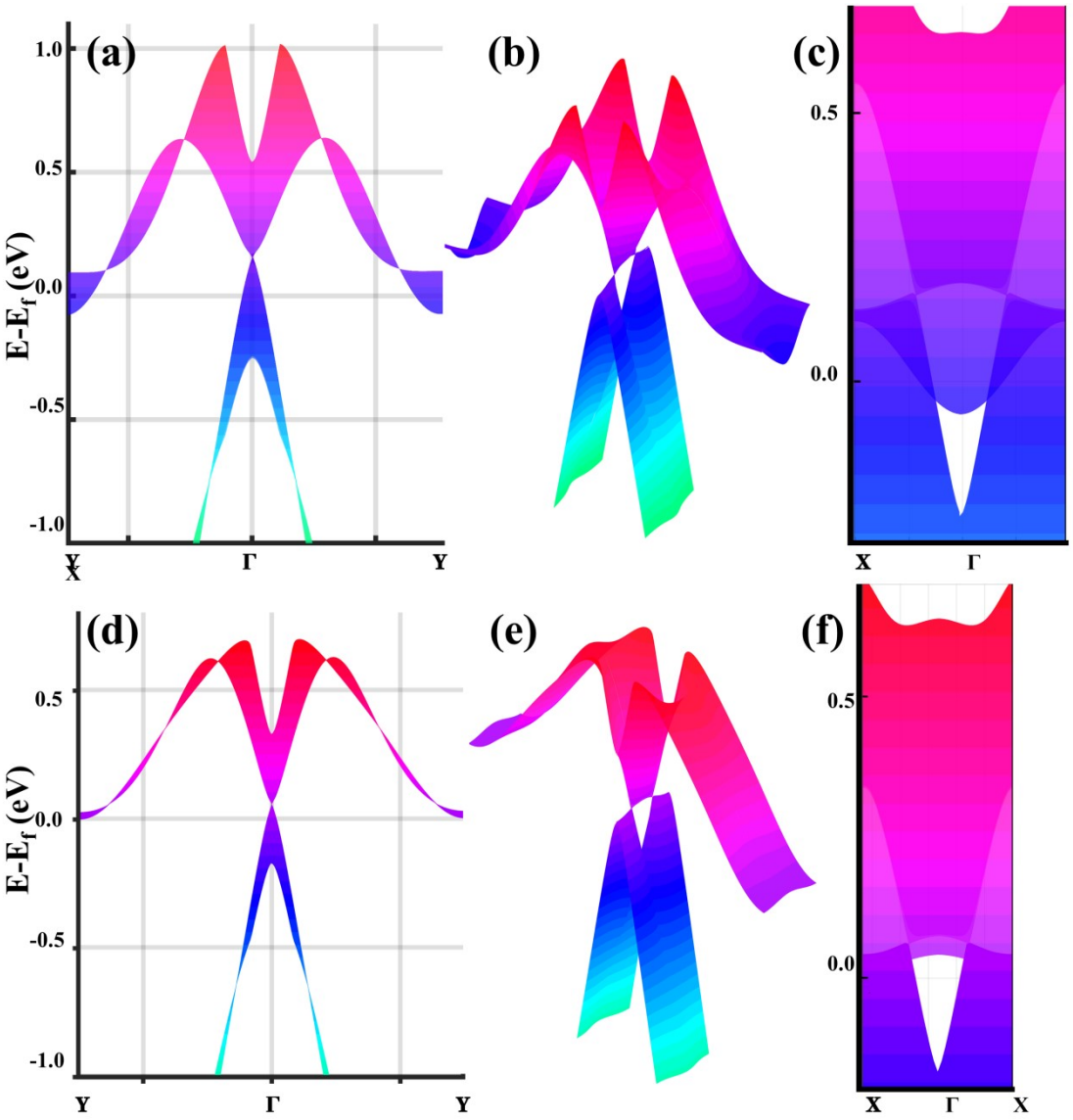

Fig.S7 The 3D band spectrum is implemented from three distinct perspectives of [4]PHO-graphene and [7]PHO-graphene to display the distorted Dirac cone features.

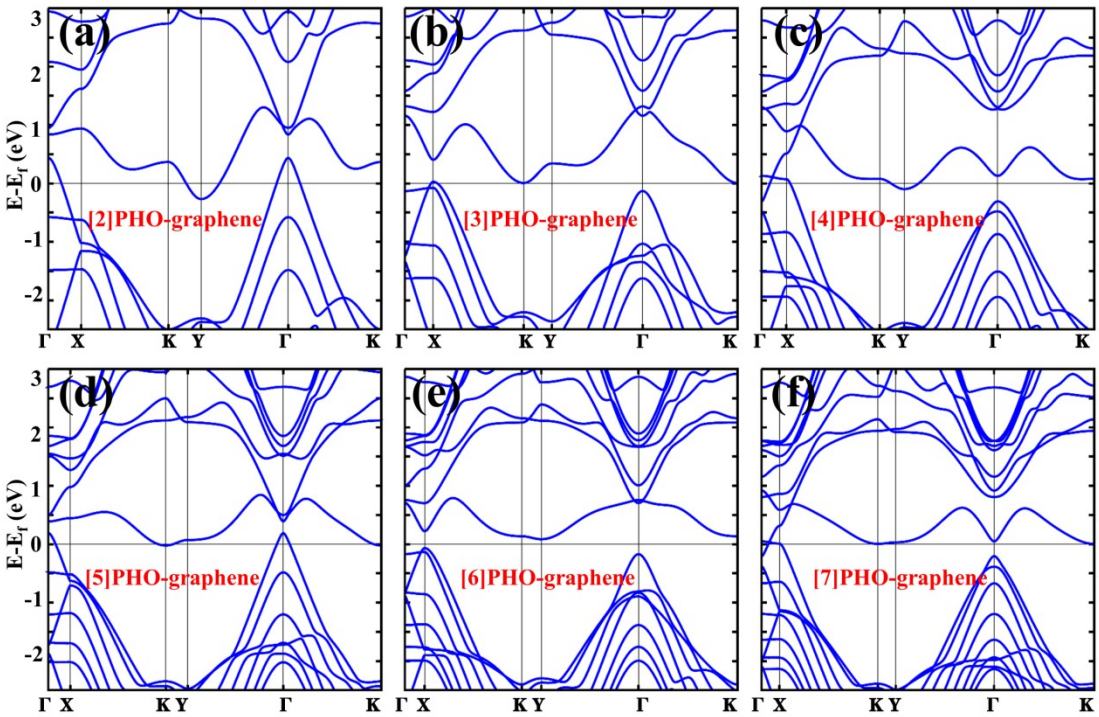

Fig.S8 It can be clearly observed that the electronic properties of PHO-graphene switch between metals, semimetals and even semiconductors.