Supplementary Material for

"C-Me-graphene: An Ideal Two-dimensional Nodal Line Semimetal with Ultrahigh Young's Modulus"

In this Supplemental Material, we give detailed computational methods of first-principles calculations. The symmetry of structures, electronic bands, and mechanical property are also included.

COMPUTATIONAL METHODS

First-principles density functional theory (DFT) computations were conducted through the utilization of the Vienna ab initio simulation package (VASP)[1]. To delineate electron-ion interactions, we employed the Projector Augmented Wave (PAW) method[2]. The exchange-correlation function assumed the Perdew-Burke-Ernzerh (PBE) form under a generalized gradient approximation (GGA)[3]. We designated a cutoff energy of 520 eV for the plane wave. We sampled the Brillouin zone (BZ) of C-Me-graphene using $6\times6\times1$ Gamma-centered Monkhorst-Pack grids[4]. A 16Å vacuum was employed to eliminate the spurious interactions. For optimal structural configuration, a relaxation sequence was performed on all atoms until the resultant alterations in energy and force attained values of 10^{-6} eV per cell and 10^{-2} eV/Å correspondingly. To ascertain dynamical stability, phonon computations incorporated a $2\times2\times1$ supercell approach, facilitated by the PHONON algorithm[5,6]. Verification of thermal stability was achieved through executing molecular dynamics simulations with a one femtosecond time granularity over a span of five picoseconds, maintained at a steady temperature of 300 Kelvin[7]. The surface states calculation applied the iterative Greens method, facilitated by the WANNIERTOOLS software package[8]. The composition of the tight-binding Hamiltonian was formulated through the employment of maximally localized Wannier functions (MLWF) method, facilitated by the WANNIER90 software package[9,10].

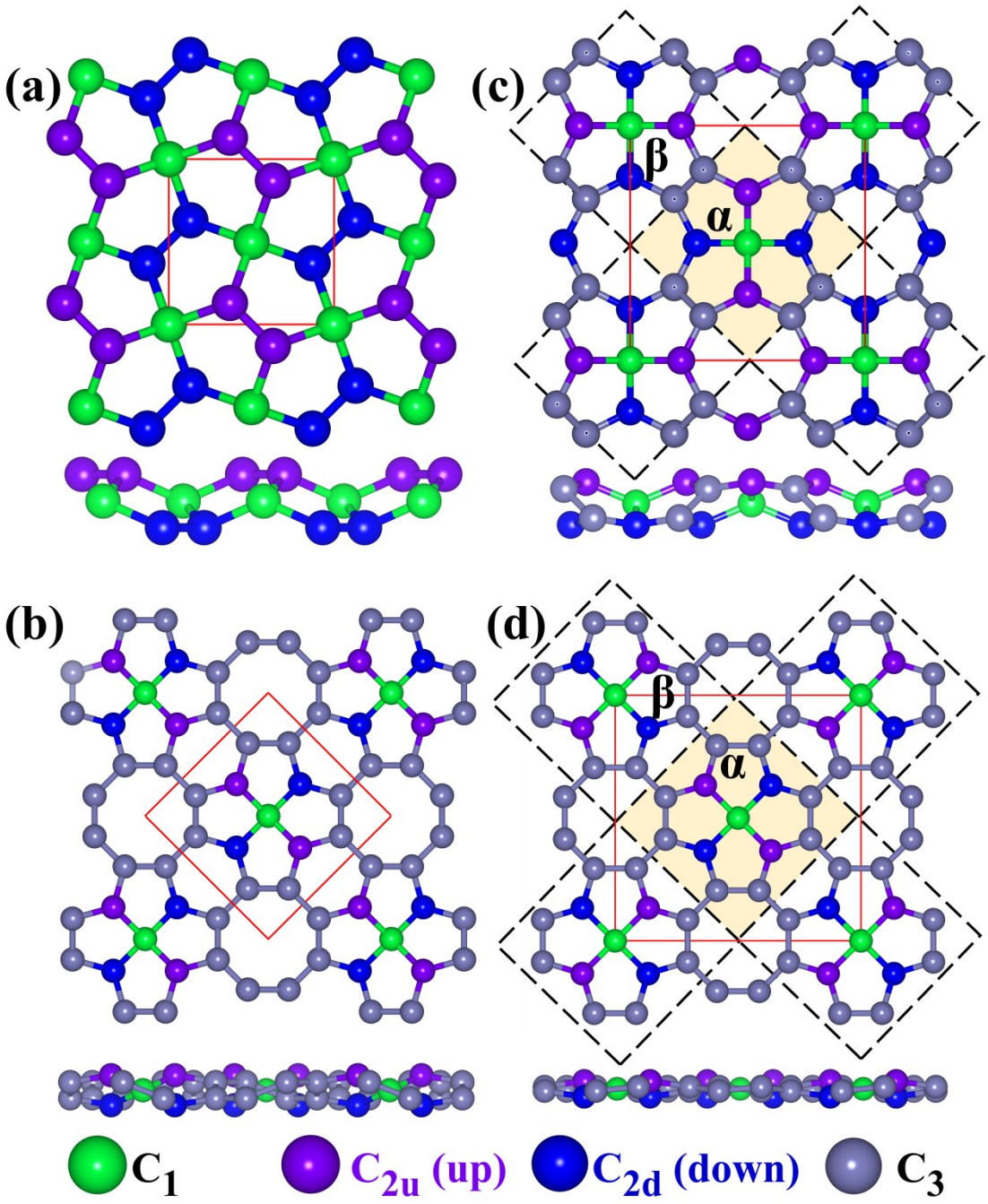

Fig. S1. The structures of (a) penta-graphene (b) Me-graphene (c) penta-octa-graphene and (d) C-Me-graphene. The solid red line represents the size of the unit cell. We have added the black dashed line to draw the regions of the two sublattices, where the middle yellowish area is the sublattice α, and the β sublattice is at four corners of the unit cell, each corner taking up only 1/4 of the β sublattice.

Table S1. The basic details of carbon allotropes with their space group, carbon rings, lattice constant, average atomic energy (E_A), and electronic property. SC and SM stand for the semimetal, semiconducting.

Name	Space group	Rings	Lattice constant(Å)	E_A (eV/atom)	Electronic property
penta-graphene	**P-42$_1$m**	**5**	**3.64**	**-8.3222**	**SC**
Me-graphene	**P-4m2**	**5,6,8**	**5.74**	**-8.8268**	**SC**
C-Me-graphene	**P4/nbm**	**5,6,8**	**8.31**	**-8.7373**	**SM** Nodal line
penta-octa-graphene	**P4/nmm**	**5,8**	**6.64**	**-8.6070**	**SM** Nodal line
graphene	**P6/mmm**	**6**	**2.47**	**-9.2197**	**SM** Nodal point
biphenylene	**Pmmm**	**4,6,8**	**a=3.75 b=4.51**	**-8.7594**	**Mental**

Table S2. Summary of the independent elastic constants(C_{ij}), Young's modulus(Y), and Poisson's ratio (v) of penta-graphene, Me-graphene, C-Me-graphene, penta-octa-graphene, and graphene.

Name	C_{11} (N/m)	C_{12} (N/m)	C_{66} (N/m)	Y (N/m)	v
penta-graphene[11]	**265**	**-18**	**152**	**263.8**	**-0.068**
Me-graphene[12]	**210**	**-0.4**	**103**	**210**	**-0.002**
C-Me-graphene	**261.2**	**74.6**	**112.6**	**Y(0°)=239.9 Y(45°)=269.6**	**v(0°)=0.286 v(45°)=0.197**
penta-octa-graphene[13]	**141.7**	**62.4**	**29.9**		**0.44**
Graphene[14]	**354.1**	**58.7**	**142.4**	**344.4**	**0.166**

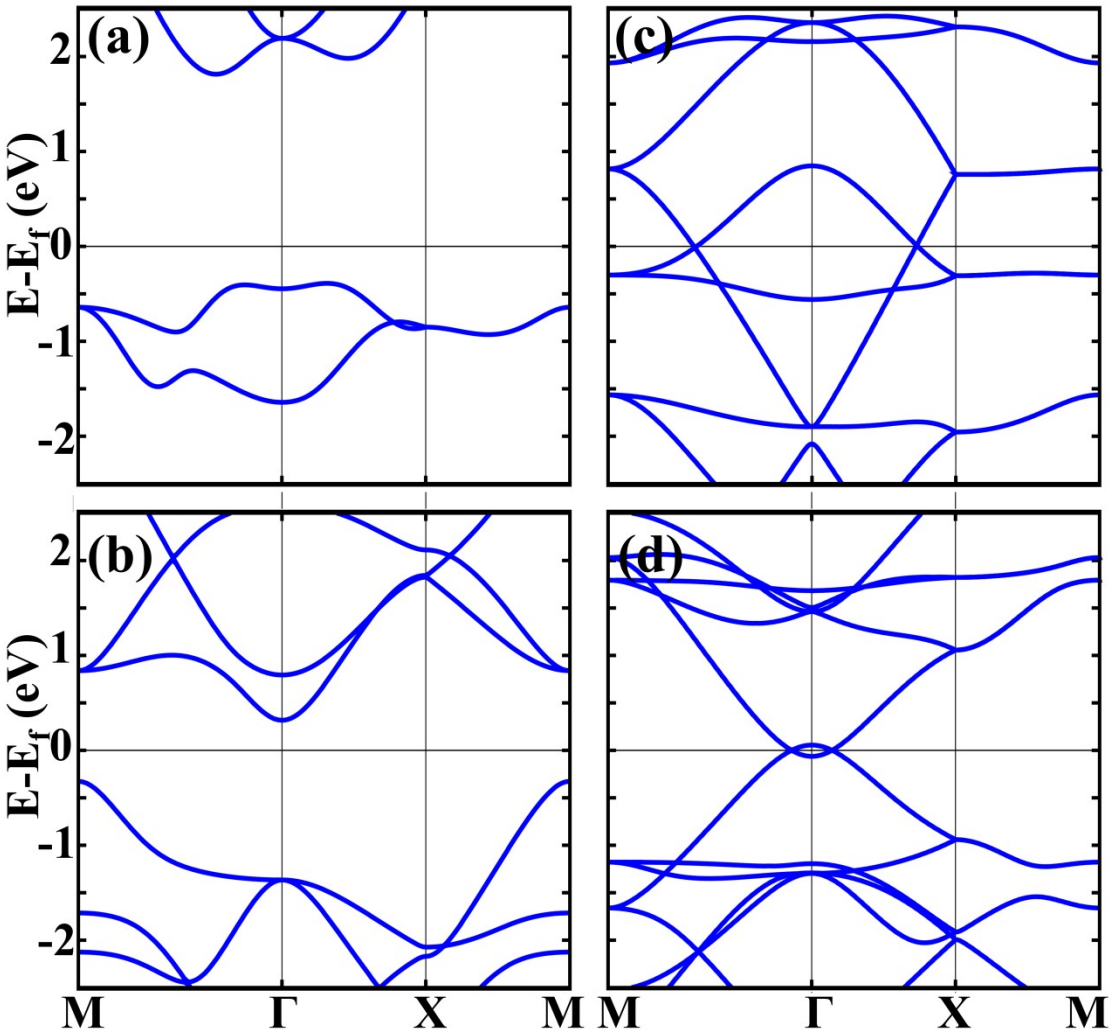

Fig. S2. The band structures of (a) penta-graphene (b) Me-graphene (c) penta-octa-graphene and (d) C-Me-graphene.

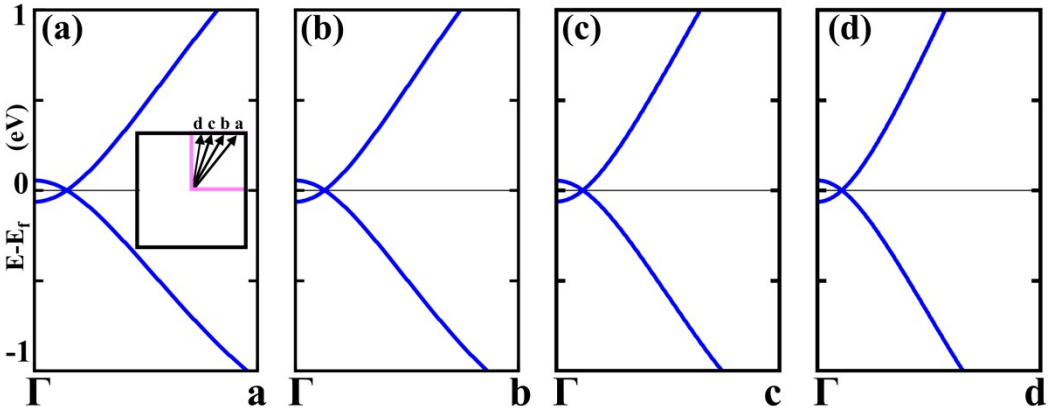

Fig. S3. Band structures for C-Me-graphene along the four general paths of Γ-a, Γ-b, Γ-c, and, Γ-d.

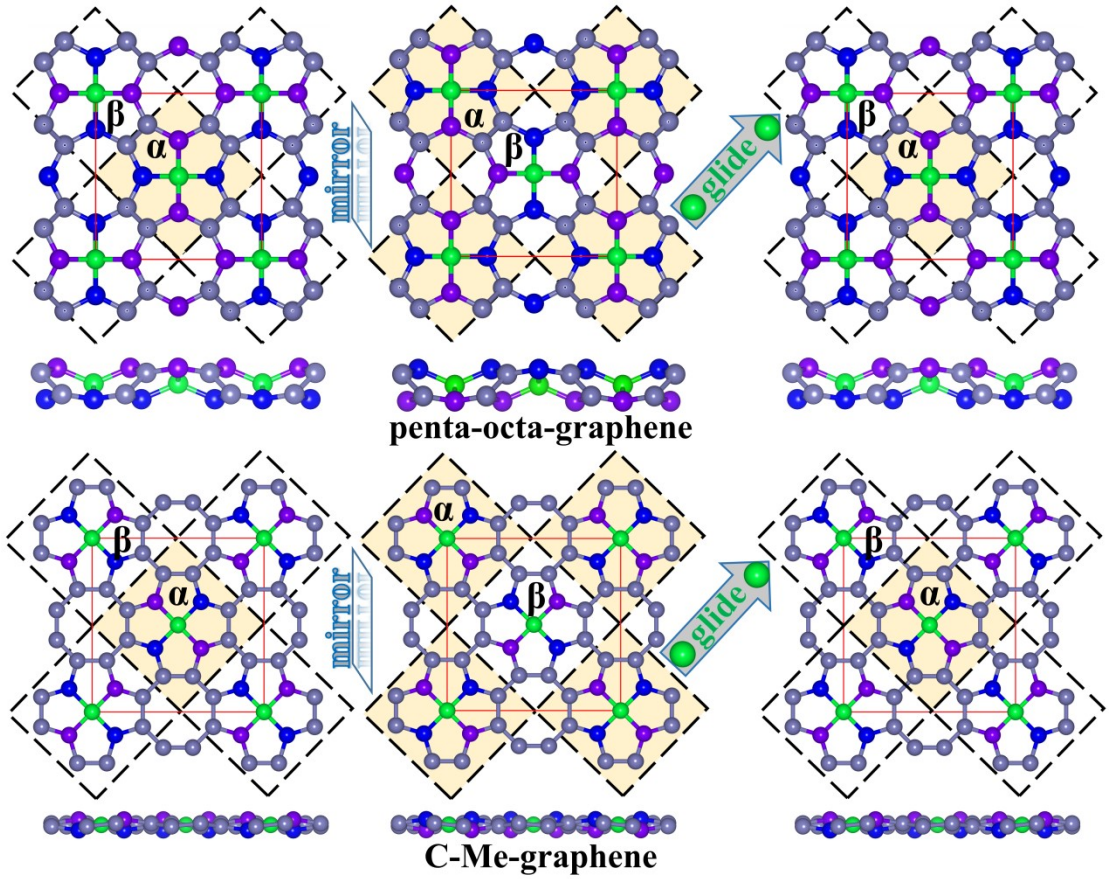

Fig. S4. The symmetries satisfied by the two structures of penta-octa-graphene and C-Me-graphene.

References

1 G. Kresse, J. Furthmüller, Phys. Rev. B, 1996, 54, 11169-11186.

2 P. E. Blochl, Phys. Rev. B, 1994, 50, 17953-17979.

3 J. P. Perdew, K. Burke, M. Ernzerhof, Phys. Rev. Lett., 1996, 77, 3865-3868.

4 J. D. Pack, H. J. Monkhorst, Phys. Rev. B, 1977, 16, 1748-1749.

5 K. Parlinski, Z. Q. Li, Y. Kawazoe, Phys. Rev. Lett., 1997, 78, 4063-4066.

6 A. Togo, F. Oba, I. Tanaka, Phys. Rev. B, 2008, 78, 134106.

7 M. P. L. Sancho, J. M. L. Sancho, J. Rubio, J. Phys. F, 1984, 14, 1205.

8 Q. Wu, S. Zhang, H.-F. Song, M. Troyer, A. A. Soluyanov, Comput. Phys. Commun., 2018, 224, 405-416.

9 A. A. Mostofi, J. R. Yates, Y.-S. Lee, I. Souza, D. Vanderbilt, N. Marzari, Comput. Phys. Commun., 2008, 178, 685-699.

10 N. Marzari, A. A. Mostofi, J. R. Yates, I. Souza, D. Vanderbilt, Rev. Mod. Phys., 2012, 84, 1419-1475.

11 S. Zhang, J. Zhou, Q. Wang, X. Chen, Y. Kawazoe, P. Jena, Proc. Natl. Acad. Sci. U. S. A., 2015, 112, 2372-2377.

12 Z. Zhuo, X. Wu, J. Yang, Nanoscale, 2020, 12, 19359-19366.

13 H. Gao, W. Ren, Carbon, 2020, 158, 210-215.

14 R. C. Andrew, R. E. Mapasha, A. M. Ukpong, N. Chetty, Phys. Rev. B, 2012, 85, 125428.