Supplementary Information

Superconductivity in topological Ψ-graphene

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The Supplementary Materials include:

I. Tables S1, S2

II. Figures S1-S5

I. Tables

Table S1. Lattice parameters of Ψ-graphene optimized by VASP PBE.

Space-group symmetry	Lattice parameters	Wyckoff positions *x y z* in fractional coordinates
$Pmma$	$a = 4.833$ Å, $b = 25.000$ Å $c = 6.705$ Å	C1 2f: 0.25000 0.50000 0.12164 C2 4j: 0.51201 0.50000 0.21369 C4 4j: 0.59452 0.50000 0.41978 C5 2f: 0.25000 0.50000 0.90882

Table S2. Total energy by VASP geometric optimization.

Allotropes of graphene	Atomic number per unit cell	Total energy (eV/unit cell)	Total energy (eV/atom)
Graphene	2	-18.6646	-9.3323
SW-graphene	16	-147.0581	-9.1911
PHA-graphene	20	-182.6592	-9.1330
Ψ-graphene	12	-110.0880	-9.1740

II. Figures

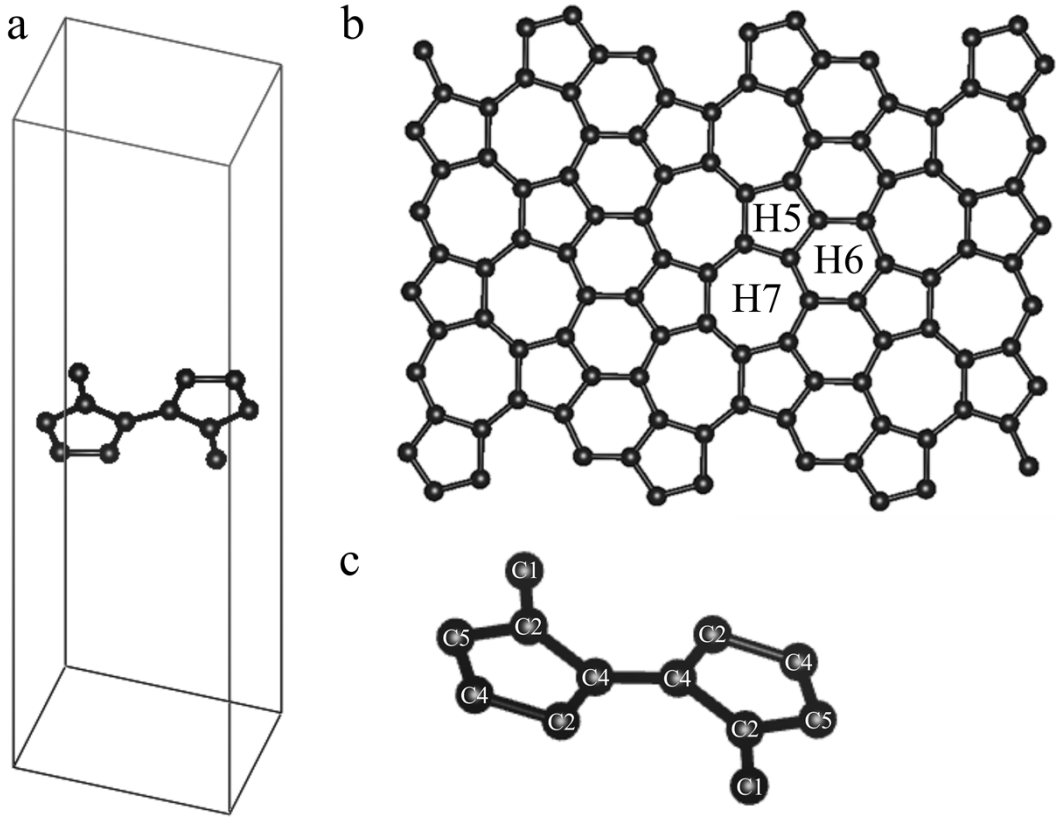

Fig. S1 (a) Unit cell structure of 25 Å vacuum layer. (b) Hollow sites for adsorption calculation. (c) Atom labels (C1, C2, C4 and C5) of the unit cell in VASP POSCAR.

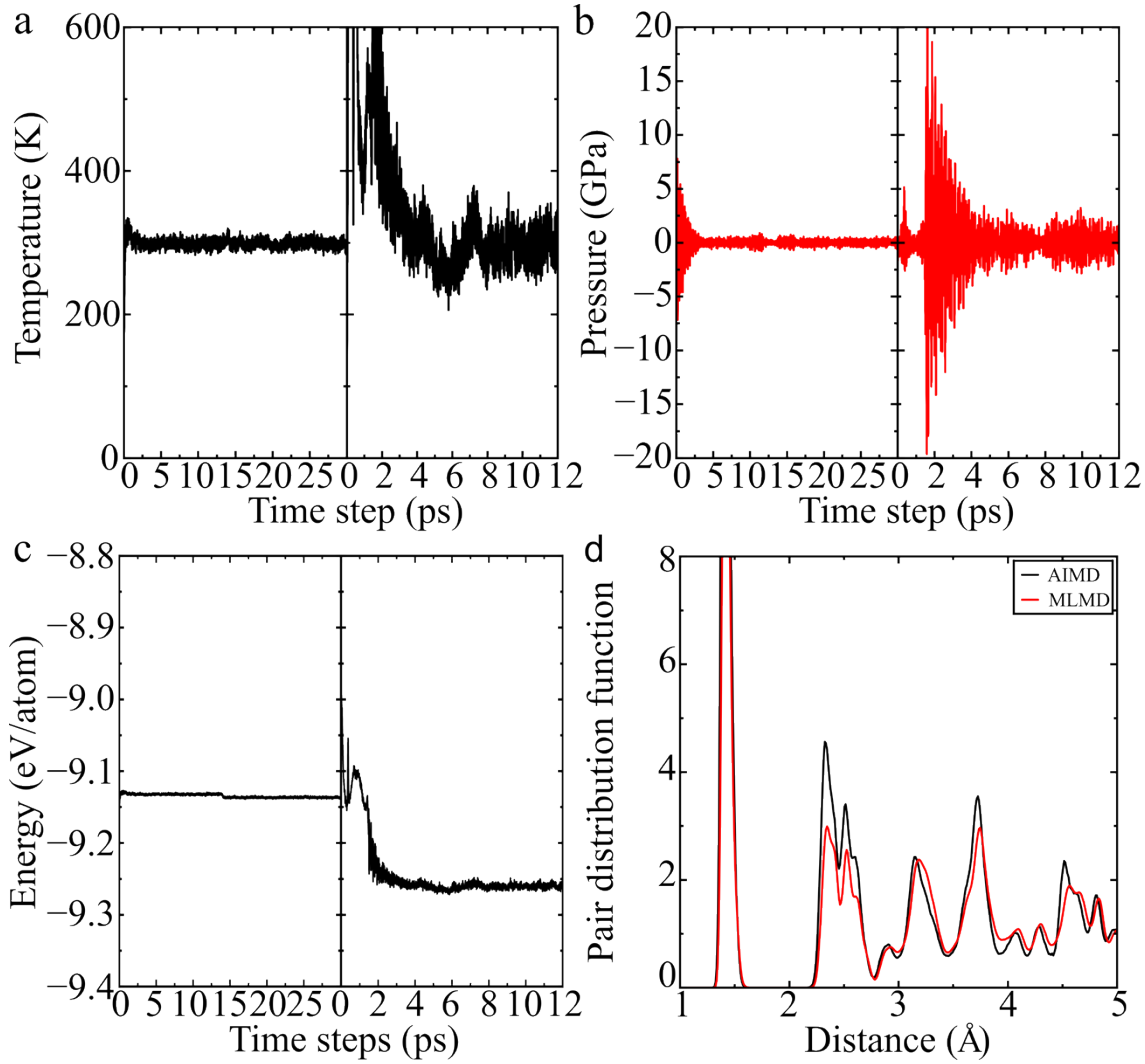

Fig. S2 The evolution of (a) temperature, (b) pressure parameter and (c) total energy during MLMD (30 ps, left panel) and AIMD (12 ps, right) simulations at 300 K. (d) The pair distribution function [$g(r)$] versus atomic distance at 300 K.

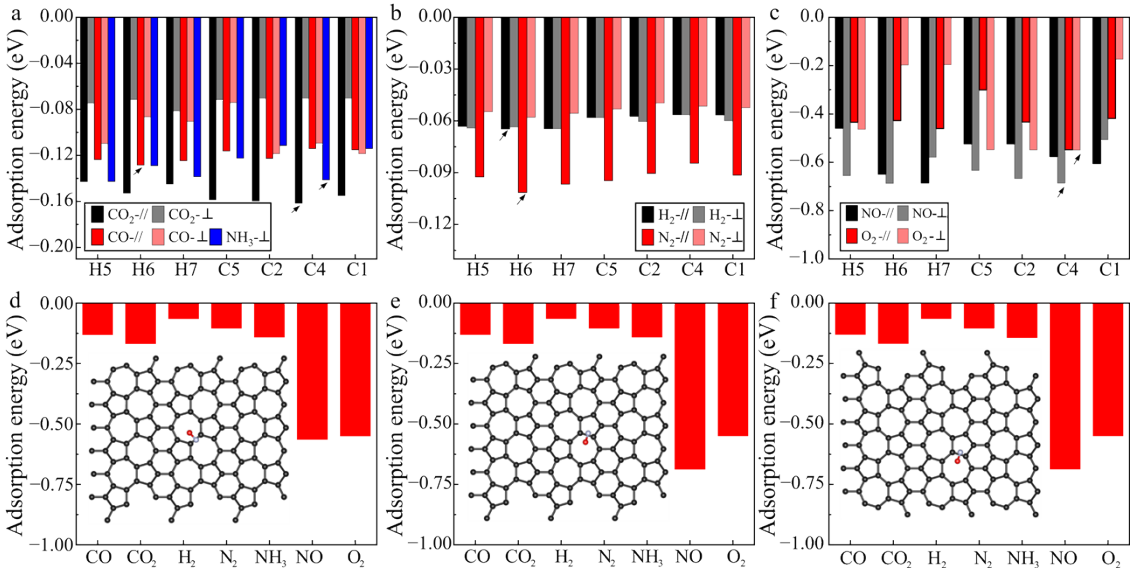

Fig. S3 (a-c) Adsorption energy at initial distance of 3.5 Å. (d-f) Adsorption energy for optimal sites as arrows pointing in (a-c) at the initial distances of 1, 1.3, and 1.5 Å.

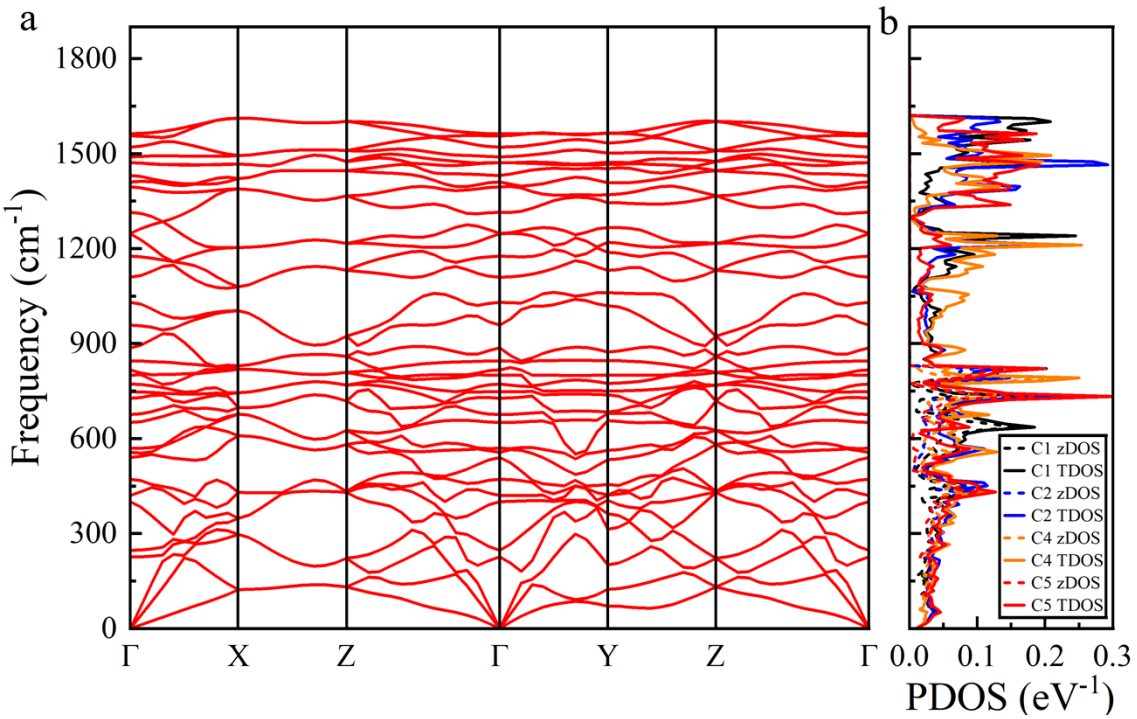

Fig. S4 (a) Phonon dispersion and (b) PDOS.

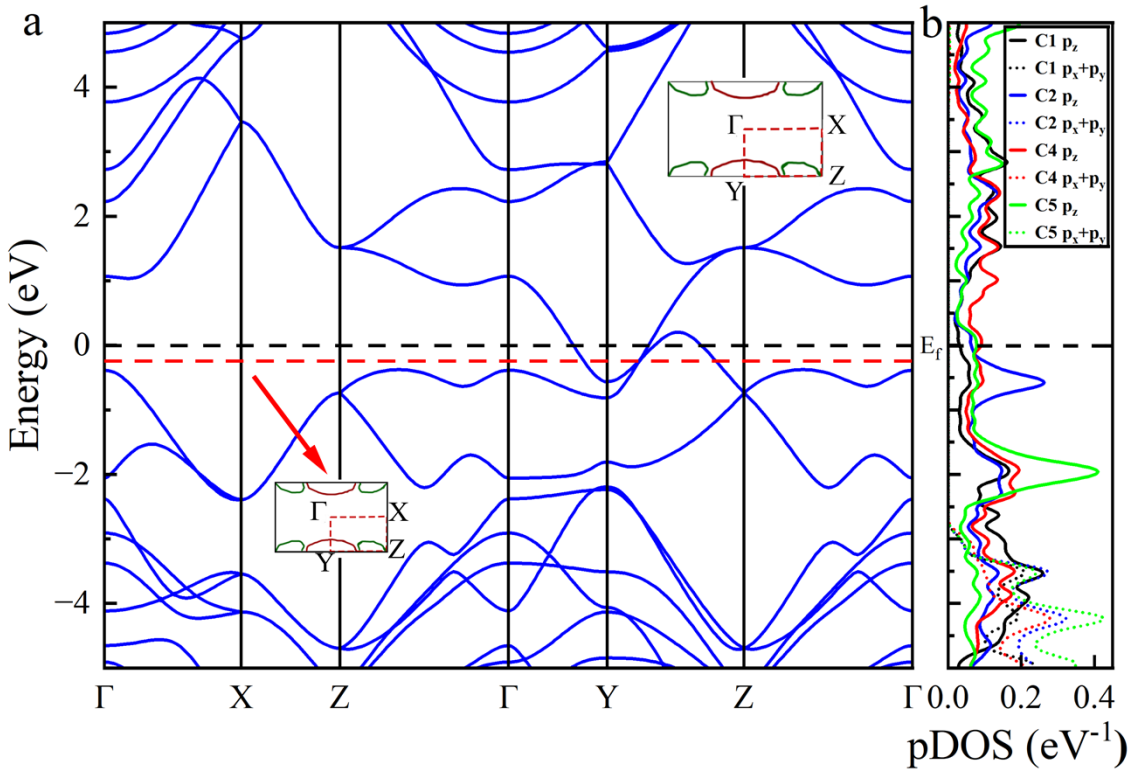

Fig. S5 (a) Band structure and (b) pDOS. The inset on the left shows Fermi surface (up). The inset graph (down) of (a) is the isoenergy surface at the band-crossing point.