Electronic Supplementary Material (ESI) for Nanoscale.

A new Dirac Cone material: A graphene-like Be_3C_2 Monolayer

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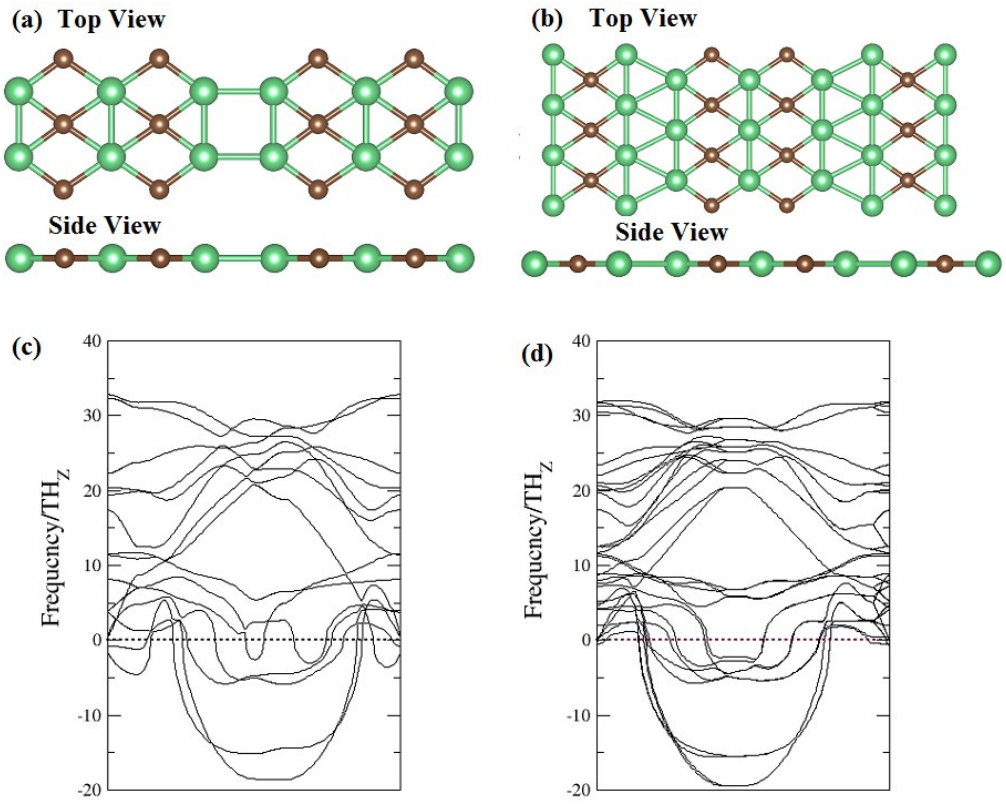

Figure S1. Optimized structures of Be_3C_2-I (2×2 supercell) (a) and Be_3C_2-II (2×1 supercell) (b) monolayer. Phonon dispersion spectrum of the Be_3C_2-I (c) and Be_3C_2-II (d) monolayer.

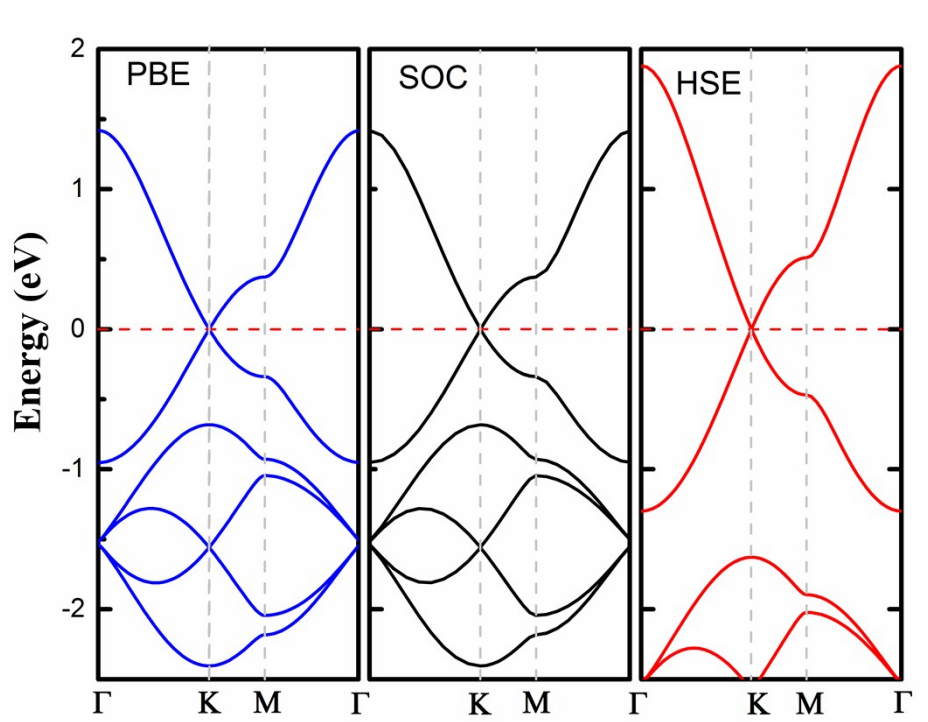

Figure S2. Band structure of Be_3C_2 monolayer calculated by PBE functional without and with SOC effect and by HSE06 method.

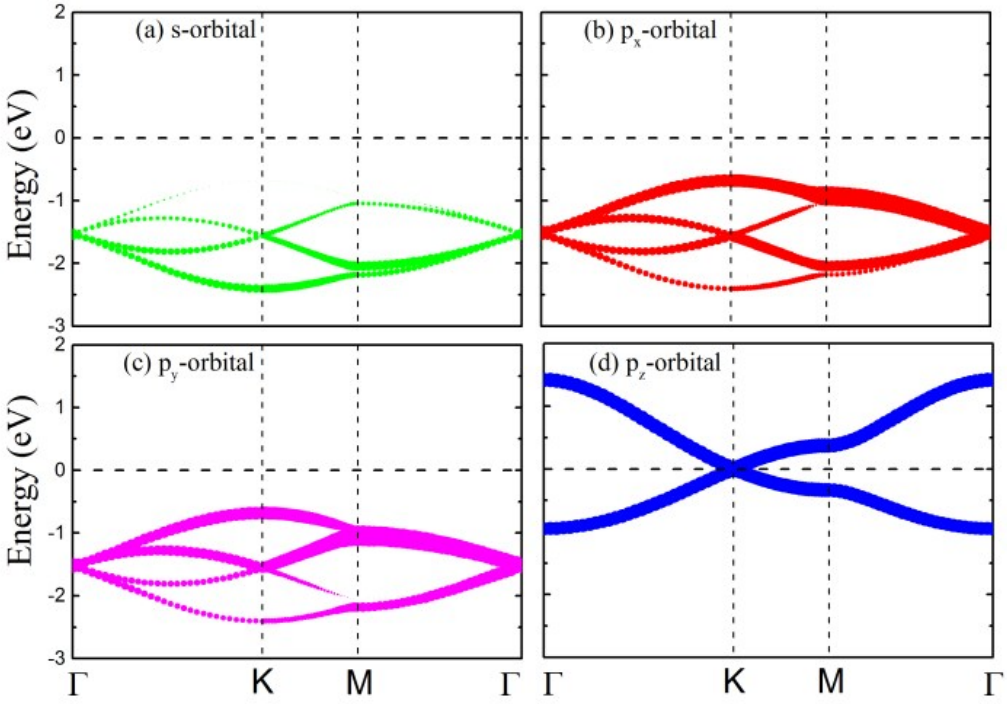

Figure S3. Orbitally resolved band structures of Be_3C_2 monolayer calculated by PBE method.

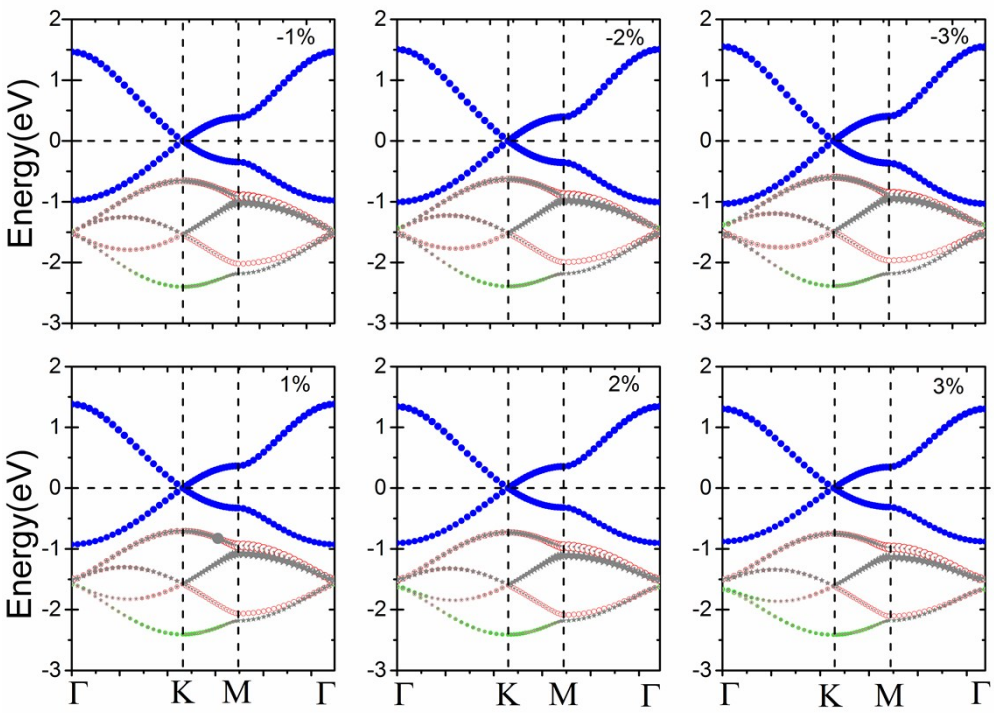

Figure S4. Orbital-resolved band structures of Be_3C_2 monolayer under mild tensile or compressional strains (-3%∽3%), under which the evident maintenance of Dirac cone persist. The green, red, magenta and blue dots represent the contributions from the *s*, p_x, p_y and p_z atomic orbitals, respectively.

Tight-binding model.

In our tight-binding (TB) model we consider only the p_z orbitals of Be and C atoms, and include hopping terms up to 5-th nearest neighbor in the summation of equation:

$$H_{ij}(\vec{k}) = \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \left\langle \vec{0}, i \middle| \hat{H} \middle| \vec{R}, j \right\rangle .$$

As a result, the Hamiltonian is a 5×5 matrix. Below we list the up-triangle part of the matrix while the other elements can be determined as the complex conjugate of their counterparts.

$$\begin{aligned}
H_{11} &= \varepsilon_1 \\
H_{12} &= t_2 + t_2 e^{-2\pi i k_a} + t_5 e^{-2\pi i k_b} + t_5 e^{-2\pi i (k_a + k_b)} \\
H_{13} &= t_2 e^{-2\pi i k_b} + t_2 e^{-2\pi i k_a} + t_5 e^{-2\pi i (k_a + k_b)} + t_5 \\
H_{14} &= t_1 + t_4 e^{-2\pi i (-k_a - k_b)} + t_4 e^{-2\pi i k_a} \\
H_{15} &= t_1 e^{-2\pi i k_a} + t_4 e^{2\pi i k_b} + t_4 \\
H_{22} &= \varepsilon_1 \\
H_{23} &= t_2 e^{2\pi i k_b} + t_2 + t_5 e^{2\pi i (k_a + k_b)} + t_5 e^{-2\pi i k_a} \\
H_{24} &= t_1 + t_4 e^{2\pi i k_a} + t_4 e^{-2\pi i k_b} \\
H_{25} &= t_1 + t_4 e^{2\pi i k_b} + t_4 e^{-2\pi i k_a} \\
H_{33} &= \varepsilon_1 \\
H_{34} &= t_1 e^{-2\pi i k_b} + t_4 e^{2\pi i k_a} + t_4 \\
H_{35} &= t_1 + t_4 e^{-2\pi i (k_a + k_b)} + t_4 e^{-2\pi i k_b} \\
H_{44} &= \varepsilon_2 \\
H_{45} &= t_3 e^{2\pi i k_b} + t_3 + t_3 e^{-2\pi i k_a} \\
H_{55} &= \varepsilon_2
\end{aligned}$$

Here ε_1 and ε_2 are on site energies for Be and C atoms, respectively. k_a and k_b are components of the fractional coordinate of the wave vector $\vec{k}$, and $t_1 \backsim t_5$ are

hopping integrals as demonstrated in Figure S5. Note that we have already used the symmetry of the crystal and Slater-Koster relation to reduce the number of hopping integrals, so only 5 integrals are essential. We find it mandatory to include hopping terms beyond the first nearest neighbor to accurately describe the band structure near the Dirac cone. The on-site energies and hopping integrals are obtained using the Wannier90 software package, which are summarized in Table 1.

Table 1. On-site energies and hopping integrals up to 5-th nearest neighbor for Be_3C_2. All quantities are in eV.

ε_1	ε_2	t_1	t_2	t_3	t_4	t_5
0.5700	**-3.7005**	**-1.3029**	**-0.2283**	**-0.1752**	**0.1243**	**-0.1722**

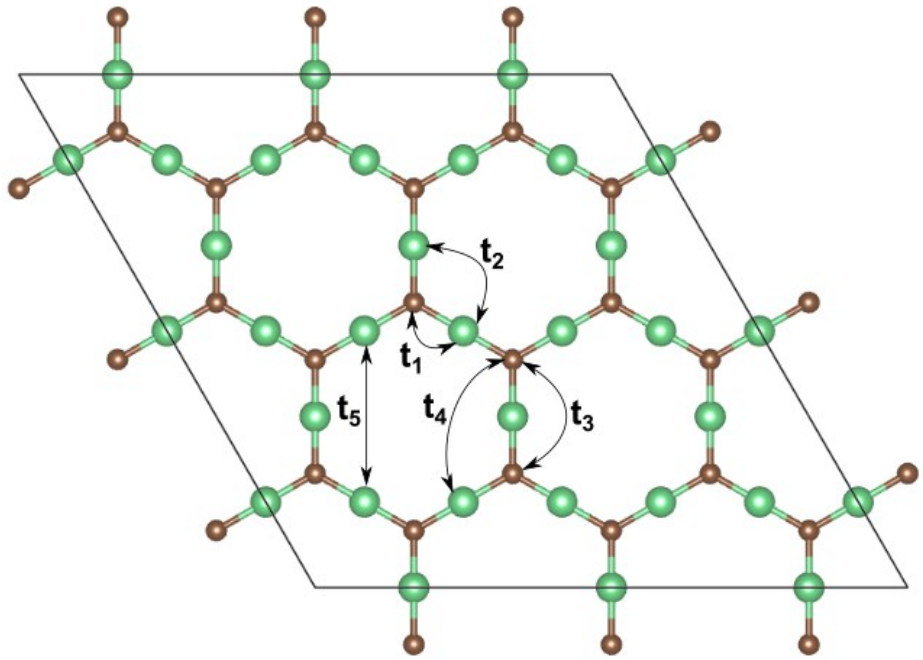

Figure S5. Demonstration of hopping integrals t_1-t_5 in a 3×3 super cell of Be_3C_2. Green and dark brown spheres denote Be and C atoms, respectively.