A new Dirac Cone material: A graphene-like Be$_3$C$_2$ Monolayer

Bing Wang, Shijun Yuan, Yunhai Li, Li shi and Jinlan Wang*

School of Physics, Southeast University, Nanjing 211189, P. R. China

Corresponding Author

*To whom correspondence should be addressed: J. W. (E-mail: jlwang@seu.edu.cn)

Figure S1. Optimized structures of Be$_3$C$_2$-I (2×2 supercell) (a) and Be$_3$C$_2$-II (2×1 supercell) (b) monolayer. Phonon dispersion spectrum of the Be$_3$C$_2$-I (c) and Be$_3$C$_2$-II (d) monolayer.
Figure S2. Band structure of Be$_3$C$_2$ monolayer calculated by PBE functional without and with SOC effect and by HSE06 method.

Figure S3. Orbitally resolved band structures of Be$_3$C$_2$ monolayer calculated by PBE method.
Figure S4. Orbital-resolved band structures of Be$_2$C$_2$ 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:

$$H_{ij} = \sum_k e^{i \frac{\pi}{k} R_i} \langle 0, i | \hat{H} | 1, j \rangle.$$ 

As a result, the Hamiltonian is a $5 \times 5$ 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.

$$H_{11} = \epsilon_1$$
$$H_{12} = t_2 + t_2 e^{-2\pi i k_a} + t_3 e^{-2\pi i k_b} + t_5 e^{-2\pi i (k_a+k_b)}$$
$$H_{13} = t_2 e^{-2\pi i k_b} + t_2 e^{-2\pi i k_a} + t_5 e^{-2\pi i (k_a+k_b)} + t_5$$
$$H_{14} = t_1 + t_4 e^{-2\pi i (-k_a-k_b)} + t_4 e^{-2\pi i k_a}$$
$$H_{15} = t_4 e^{-2\pi i k_a} + t_4 e^{2\pi i k_b} + t_4$$
$$H_{22} = \epsilon_1$$
$$H_{23} = t_2 e^{2\pi i k_b} + t_2 + t_3 e^{2\pi i (k_a+k_b)} + t_5 e^{-2\pi i k_a}$$
$$H_{24} = t_1 + t_4 e^{2\pi i k_a} + t_4 e^{-2\pi i k_b}$$
$$H_{25} = t_1 + t_4 e^{2\pi i k_a} + t_4 e^{-2\pi i k_a}$$
$$H_{33} = \epsilon_1$$
$$H_{34} = t_1 e^{-2\pi i k_b} + t_4 e^{2\pi i k_a} + t_4$$
$$H_{35} = t_1 + t_4 e^{-2\pi i (k_a+k_b)} + t_4 e^{-2\pi i k_b}$$
$$H_{44} = \epsilon_2$$
$$H_{45} = t_3 e^{2\pi i k_b} + t_3 + t_3 e^{-2\pi i k_a}$$
$$H_{55} = \epsilon_2$$

Here $\epsilon_1$ and $\epsilon_2$ 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 $\mathbf{k}$, and $t_1$-$t_5$ 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$_3$C$_2$. All quantities are in eV.

<table>
<thead>
<tr>
<th>( \varepsilon_1 )</th>
<th>( \varepsilon_2 )</th>
<th>( t_1 )</th>
<th>( t_2 )</th>
<th>( t_3 )</th>
<th>( t_4 )</th>
<th>( t_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.5700</td>
<td>-3.7005</td>
<td>-1.3029</td>
<td>-0.2283</td>
<td>-0.1752</td>
<td>0.1243</td>
<td>-0.1722</td>
</tr>
</tbody>
</table>

Figure S5. Demonstration of hopping integrals \( t_1 \)-\( t_5 \) in a 3×3 super cell of Be$_3$C$_2$. Green and dark brown spheres denote Be and C atoms, respectively.