Supporting Information:

Layered nodal lines in halide carbides

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In this Supporting Information, we first show the independence of the crystal structure and band structure with respect to the different value used in the mean field method PBEsol+U [1,2], to justify our calculation of using the results from the PBE functional [3]. All the calculations were done within the inclusion of the van-der-waals interaction within the DFT+D3 scheme [4]. Next, we show the show evolution of the Wannier charge centres for the two mirror eigenvalues corresponding with the two mirror planes k_z = 0 and k_z = 0.5 using the Wilson loop method [5, 6]. The band structure of different number of layers of Y_2C_2I_2 which demonstrates persistent 2D nodal line property protected by the k_z = 0 mirror plane. The crystal structure of the (010) edge state is shown Fig. S4. We also demonstrate that the 3D and 2D nodal line properties are also present in La_2C_2I_2 similar to Y_2C_2I_2 due to the existence of the k_z = 0 and k_z = 0.5 mirror planes.

Table 1. Relaxed structural parameters of Y_2C_2I_2 for different functionals. The values of PBEsol+U (U=2 eV) and the PBE functional are almost identical with the experimental lattice parameters, which justify our usage of the PBE functional in the main text.

<table>
<thead>
<tr>
<th>Structural parameters</th>
<th>U=0.25 eV</th>
<th>U=0.5 eV</th>
<th>U=1 eV</th>
<th>U=2 eV</th>
<th>PBE</th>
<th>Experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td>a (Å)</td>
<td>7.21</td>
<td>7.22</td>
<td>7.22</td>
<td>7.23</td>
<td>7.24</td>
<td>7.20</td>
</tr>
<tr>
<td>b (Å)</td>
<td>3.85</td>
<td>3.86</td>
<td>3.86</td>
<td>3.87</td>
<td>3.87</td>
<td>3.87</td>
</tr>
<tr>
<td>c (Å)</td>
<td>10.44</td>
<td>10.43</td>
<td>10.41</td>
<td>10.38</td>
<td>10.36</td>
<td>10.40</td>
</tr>
<tr>
<td>β</td>
<td>93.64</td>
<td>93.67</td>
<td>93.73</td>
<td>93.78</td>
<td>93.83</td>
<td>93.70</td>
</tr>
</tbody>
</table>

Figure S1. The band structure without SOC of Y_2C_2I_2 calculated with PBEsol+U with U values of a) 0.25 eV, b) 0.5 eV, c) 1 eV, d) 2 eV and e) calculated with the PBE functional.
Figure S2. Evolution of the Wannier charge center associated with the \( k_z = 0 \) (left) and \( k_z = 0.5 \) (right) mirror planes for the eigenvalues +i and −i.

Figure S3. The band structure without SOC of a) 1 layer Y\(_2\)C\(_2\)I\(_2\), b) 2 layers Y\(_2\)C\(_2\)I\(_2\), and c) 3 layers Y\(_2\)C\(_2\)I\(_2\).

Figure S4. Crystal structure of the (010) edge in the monolayer Y\(_2\)C\(_2\)I\(_2\).
**Figure S5.** The band structure without SOC of a) 3D double nodal lines La$_2$C$_2$I$_2$, and b) 2D nodal line in a single layer La$_2$C$_2$I$_2$.

**References**


