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 PBE_{sol}+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 PBE_{sol}+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.

Structural parameters	U=0.25 eV	U=0.5 eV	U=1 eV	U=2 eV	PBE	Experiment[7]
a (Å)	7.21	7.22	7.22	7.23	7.24	7.20
b (Å)	3.85	3.86	3.86	3.87	3.87	3.87
c (Å)	10.44	10.43	10.41	10.38	10.36	10.40
β	93.64	93.67	93.73	93.78	93.83	93.70

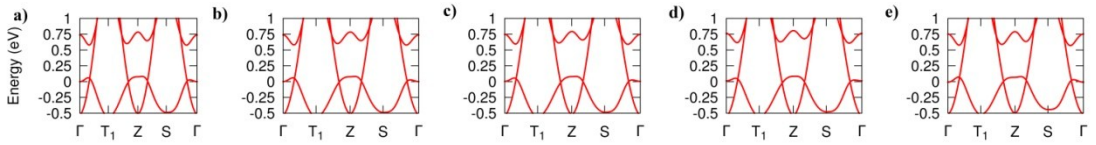

Figure S1. The band structure without SOC of $Y_2C_2I_2$ calculated with PBEsol+U with U values of a) 0.25 eV, b) 0.5 eV, c) 1 eV, d) 2 eV and e) calculated with the PBE functional.

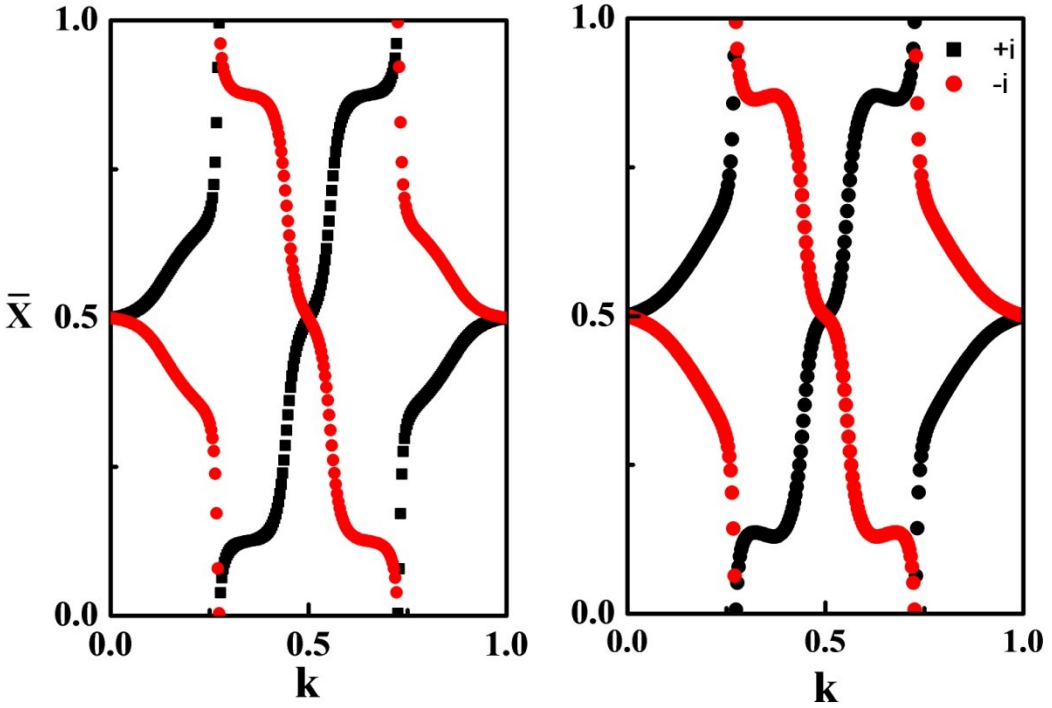

Figure S2. Evolution of the Wannier charge center associated with the k_z = 0 (left) and k_z = 0.5 (right) mirror planes for the eigenvalues +i and –i.

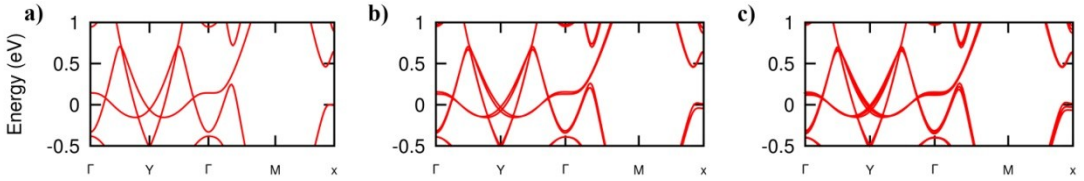

Figure S3. The band structure without SOC of a) 1 layer $Y_2C_2I_2$, b) 2 layers $Y_2C_2I_2$, and c) 3 layers $Y_2C_2I_2$.

Figure S4. Crystal structure of the (010) edge in the monolayer $Y_2C_2I_2$

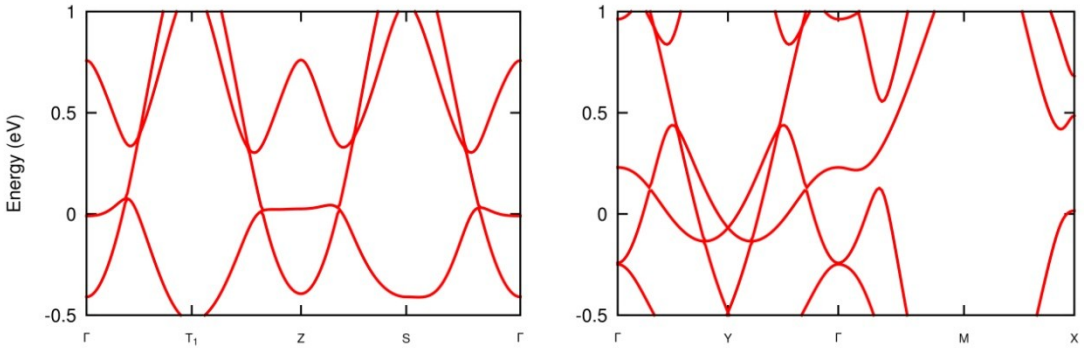

Figure S5. The band structure without SOC of a) 3D double nodal lines $La_2C_2I_2$, and b) 2D nodal line in a single layer $La_2C_2I_2$.

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