Supplementary Information

Na_2C monolayer: a novel 2p Dirac half-metal with multiple symmetry-protected Dirac cones

Wei-xiao Ji,[*a] Bao-min Zhang,[a] Shu-feng Zhang,[a] Chang-wen Zhang,[a] Meng Ding,[a] Pei-ji Wang,[a] and Ruiqin Zhang[†b,c]

[a] *School of Physics and Technology, University of Jinan, Jinan 250022, China*
[b] *Department of Physics, City University of Hong Kong, Hong Kong SAR*
[c] *Beijing Computational Science Research Center, Beijing 100193, China*
[*] Corresponding author. E-mail: hellojiweixiao@163.com
[†] Corresponding author. E-mail: aprqz@cityu.edu.hk

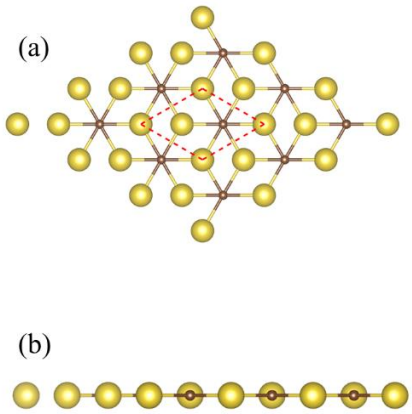

Figure S1 The (a) top and (b) side view of planar Na_2C monolayer structure. The yellow and brown balls represent Na and C atoms respectively.

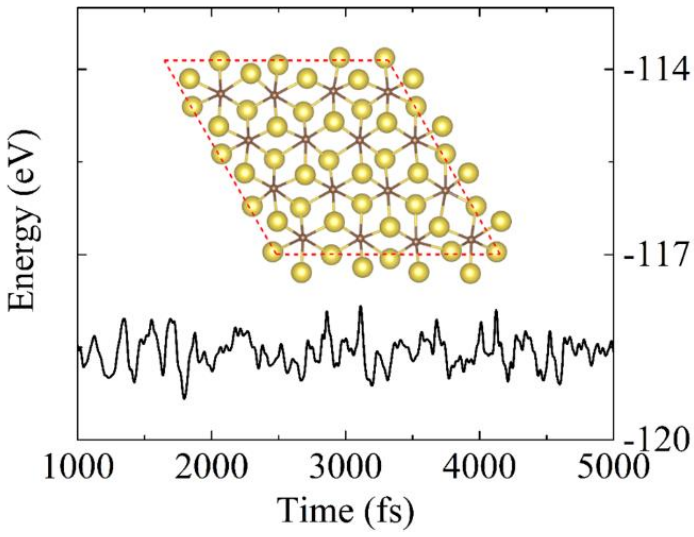

Figure S2 The energy evolutions of MD at 300 K for 5 ps, with the final geometric structure of Na_2C monolayer after 5ps MD simulations.

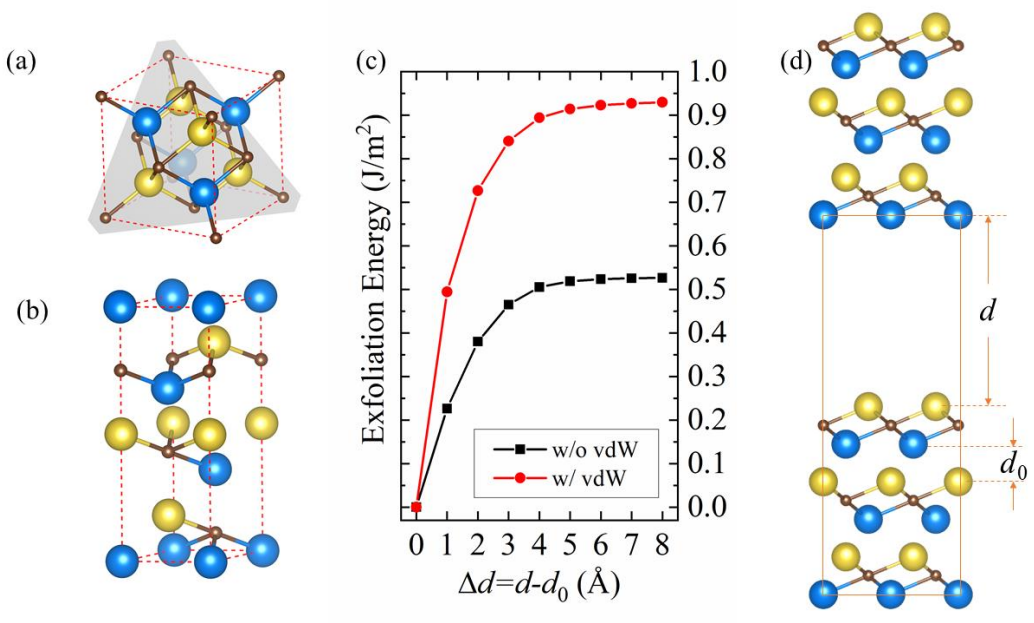

Figure S3 (a) The geometric structure of Na_2C_2. (b) The bulk model of layered Na_2C. (c) The exfoliation energy calculated as a function of the separation(Δd) between two fractured parts. (d) The definition of d and d_0 in (c). The yellow and blue balls represent Na atoms in different sublayers, and brown balls for C atoms.

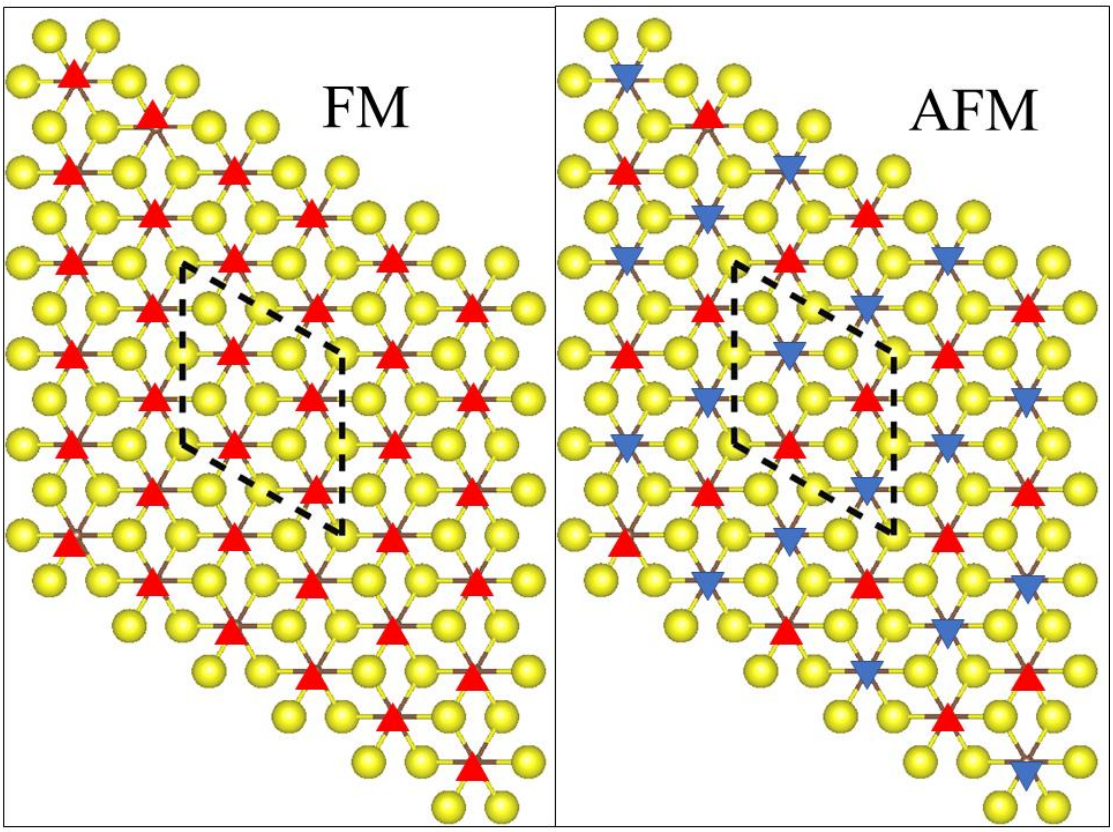

Figure S4 Spin configurations of ferromagnetism (FM) and anti-ferromagnetism (AFM), used to calculate the Curie temperature. The red (blue) triangles represent the up (down) spin.

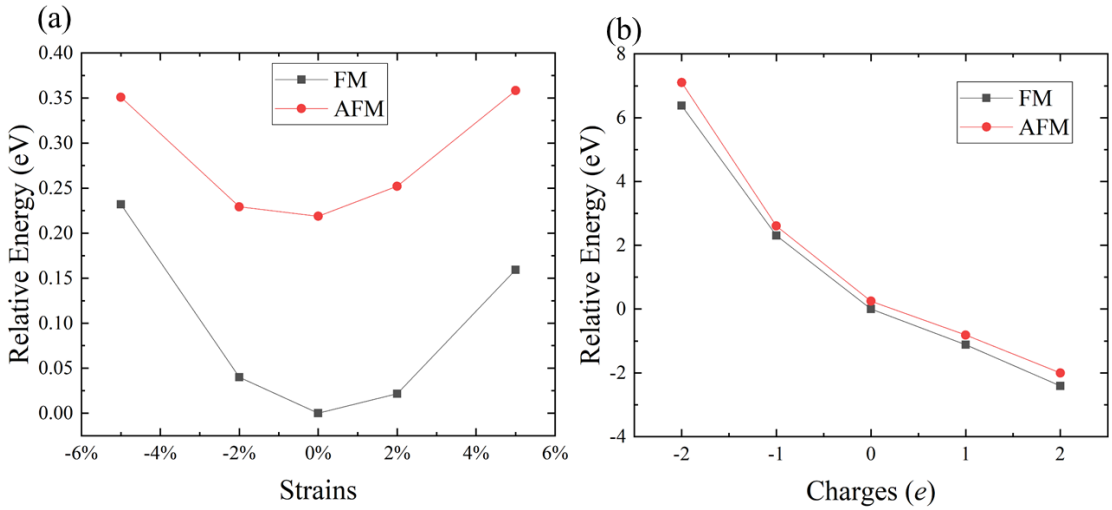

Figure S5 The comparison of relative energy between ferromagnetic (FM) and anti-ferromagnetic (AFM) as a function of biaxial strains and extra charges.

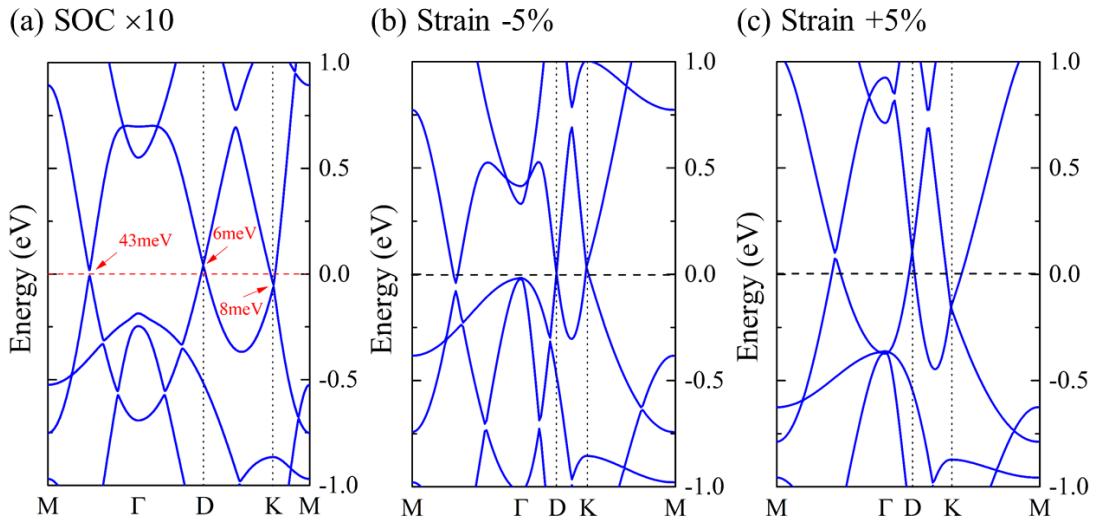

Figure S6 The band structures of Na_2C with (a) the SOC strength artificially increased by ten times, and under biaxial strains of (b) -5% and (c) +5%.

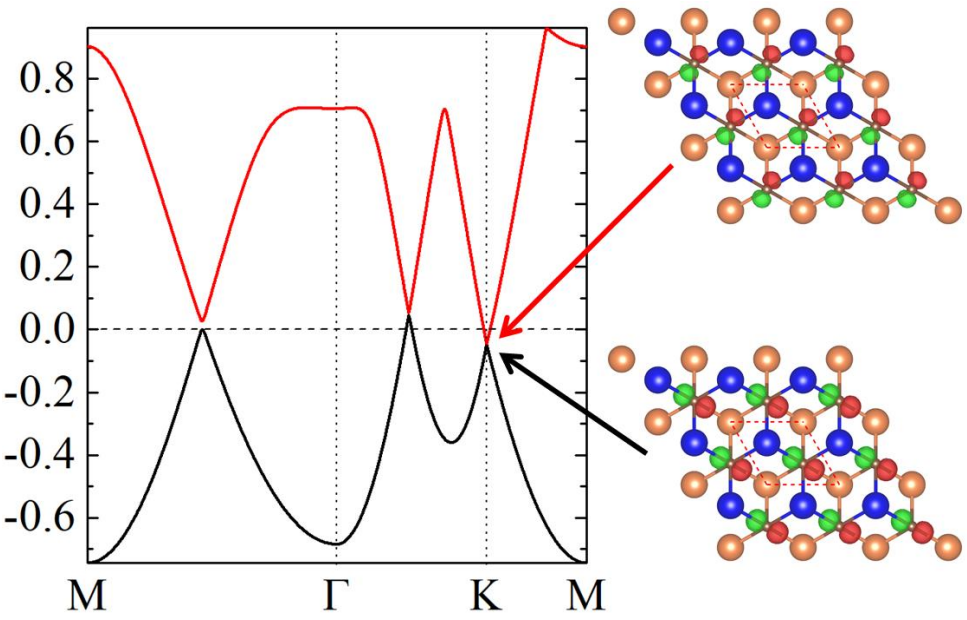

Figure S7 The real space wave function at Dirac point K. The blue (orange) balls represent Na atoms in different layers, and brown balls are C atoms. The red (green) area shows the wave function with positive (negative) sign.

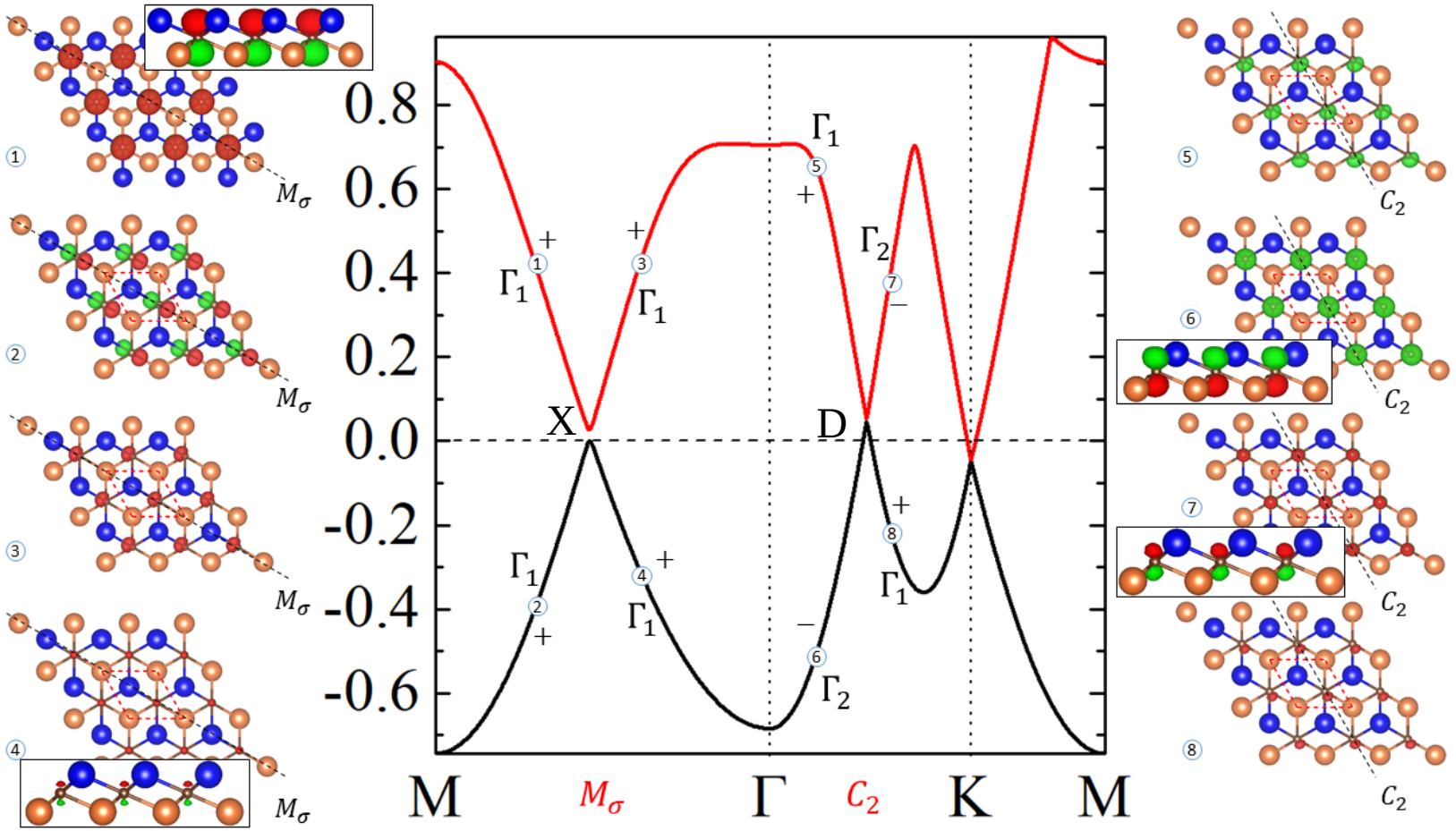

Figure S8 The real space wave function along M-Γ and Γ-K. The blue (orange) balls represent Na atoms in different layers, and brown balls are C atoms. The red (green) area shows the wave function with positive (negative) sign.

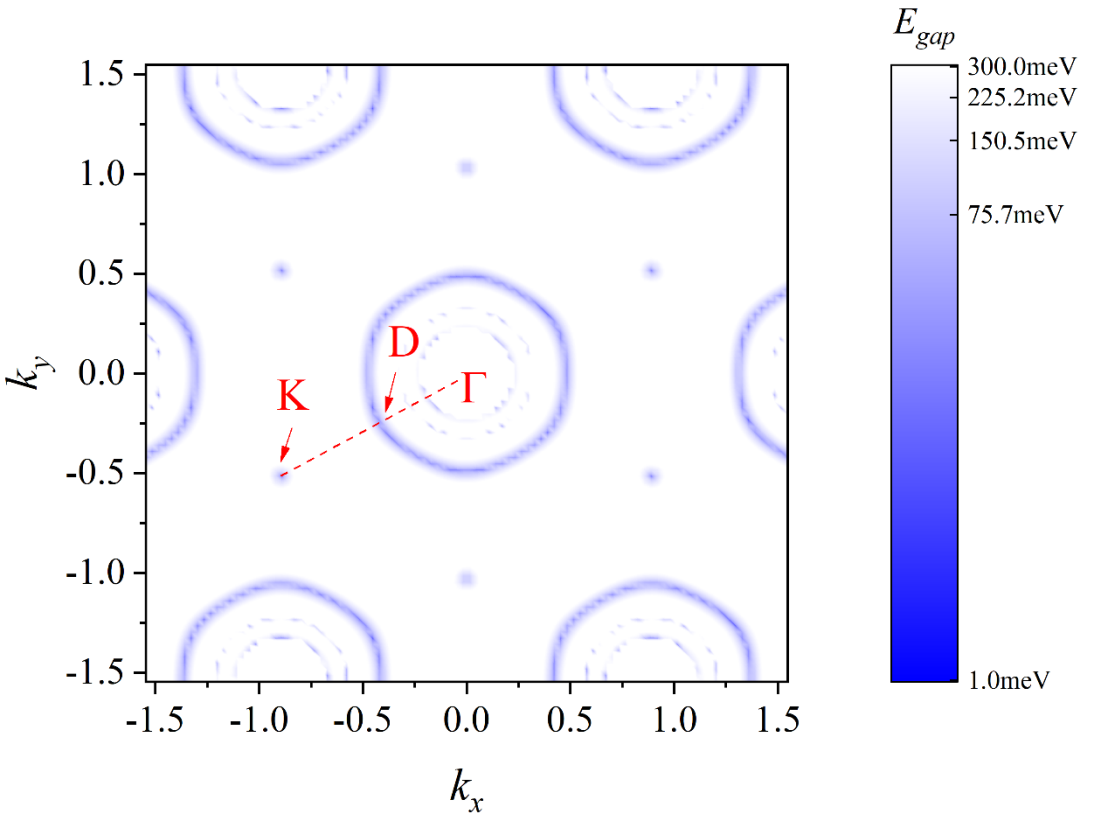

Figure S9 The contour of energy difference between the two bands that are closest to the Fermi level.

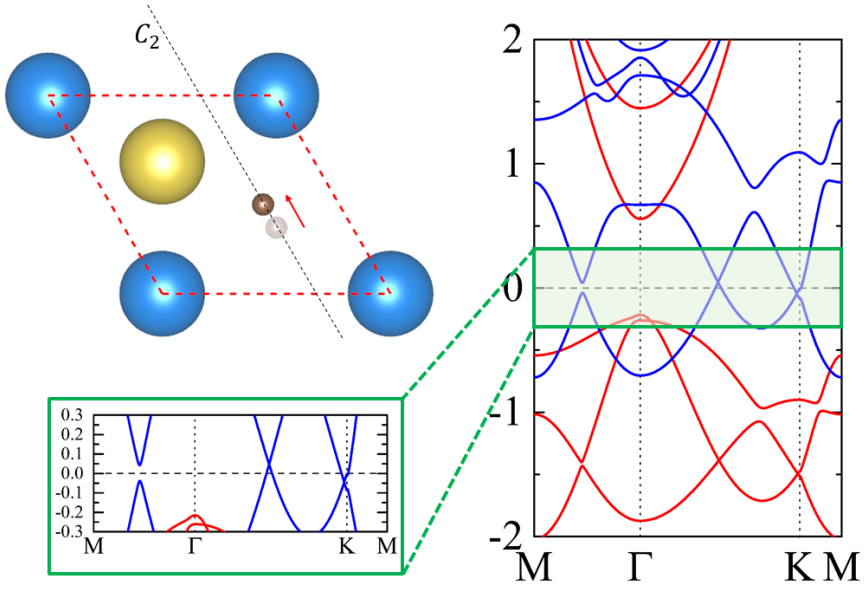

Figure S10 The band structures of Na_2C under symmetry reductions by moving carbon atom along the C_2 axis. The yellow and blue balls represent the Na atoms in different sublayers.

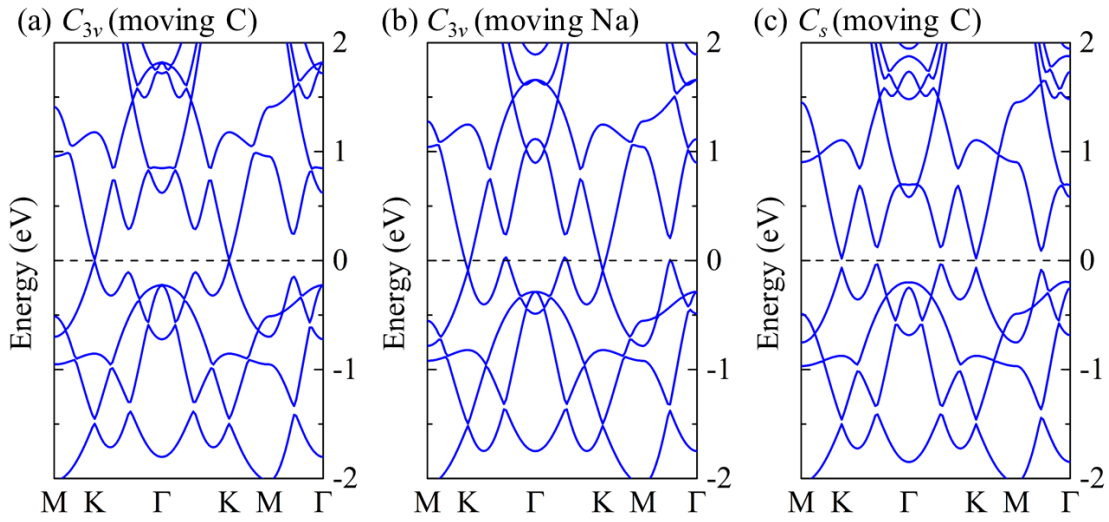

Figure S11 The band structures of Na_2C under symmetry reductions by (a) moving C along the z axis, (b) moving Na along the z axis, and (c) moving C along the long diagonal in the lattice plane.

The CIF file of the Na_2C monolayer:

```
data_Na2C


_chemical_name_common                  “Na2C”                                '
_cell_length_a                         4.06252
_cell_length_b                         4.06252
_cell_length_c                         20.00000
_cell_angle_alpha                      90
_cell_angle_beta                       90
_cell_angle_gamma                        120
_space_group_name_H-M_alt                “P 1”
_space_group_IT_number                   1

loop_
_space_group_symop_operation_xyz
   “x, y, z”

loop_
   _atom_site_label
   _atom_site_occupancy
   _atom_site_fract_x
   _atom_site_fract_y
   _atom_site_fract_z
   _atom_site_adp_type
   _atom_site_B_iso_or_equiv
   _atom_site_type_symbol
   C1      1.0     0.666667     0.333333     0.287109     Biso    1.000000 C
   Na1     1.0     0.000000     0.000000     0.235792     Biso    1.000000 Na
   Na2     1.0     0.333333     0.666667     0.338425     Biso    1.000000 Na
```