Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Monolayer Ti_2C MXene: Manipulating Magnetic Property and Electronic Structures by Electric Field

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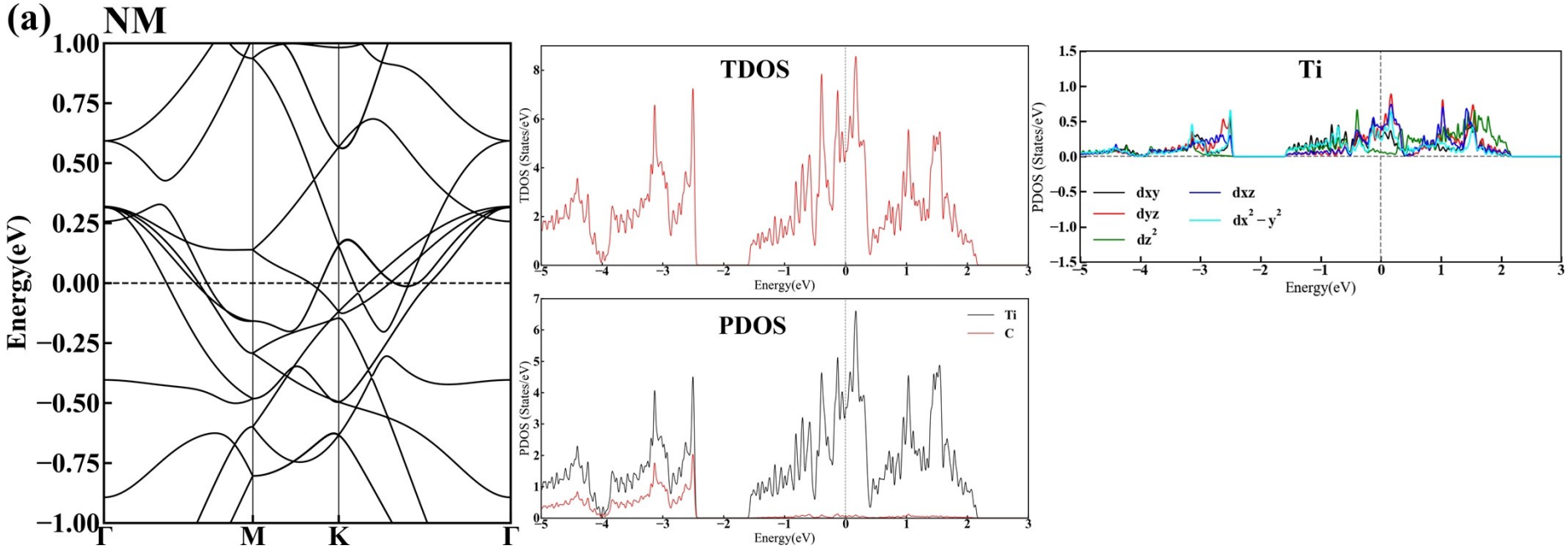
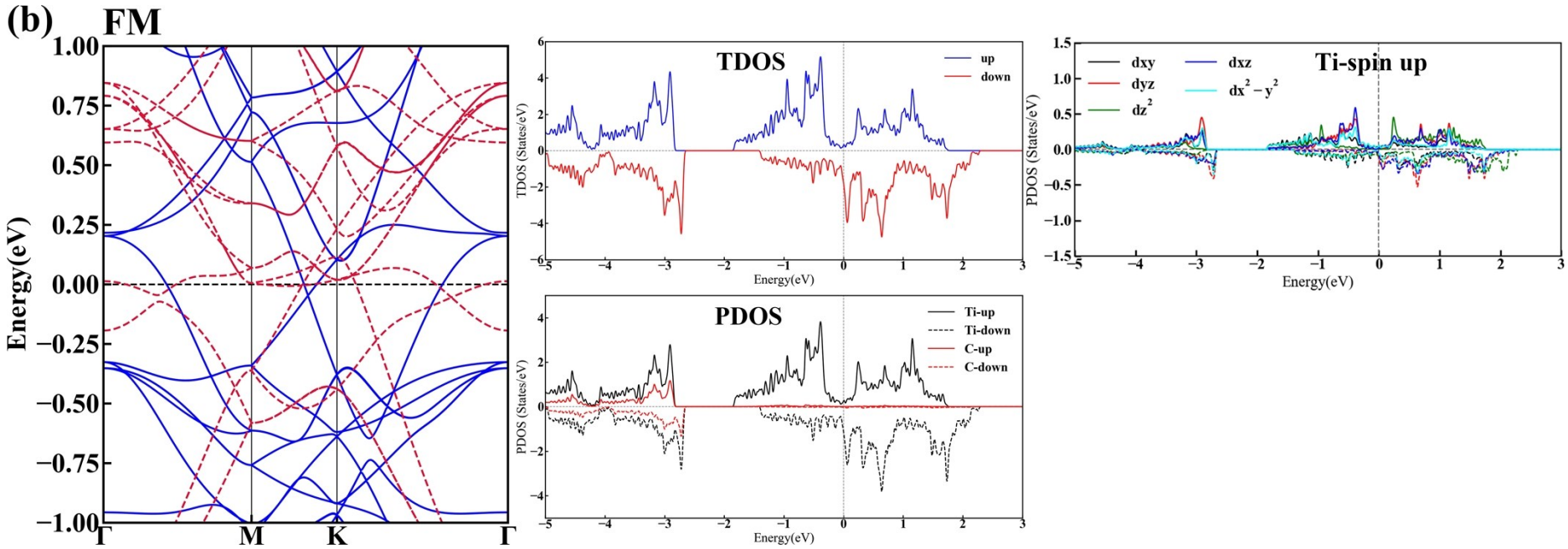
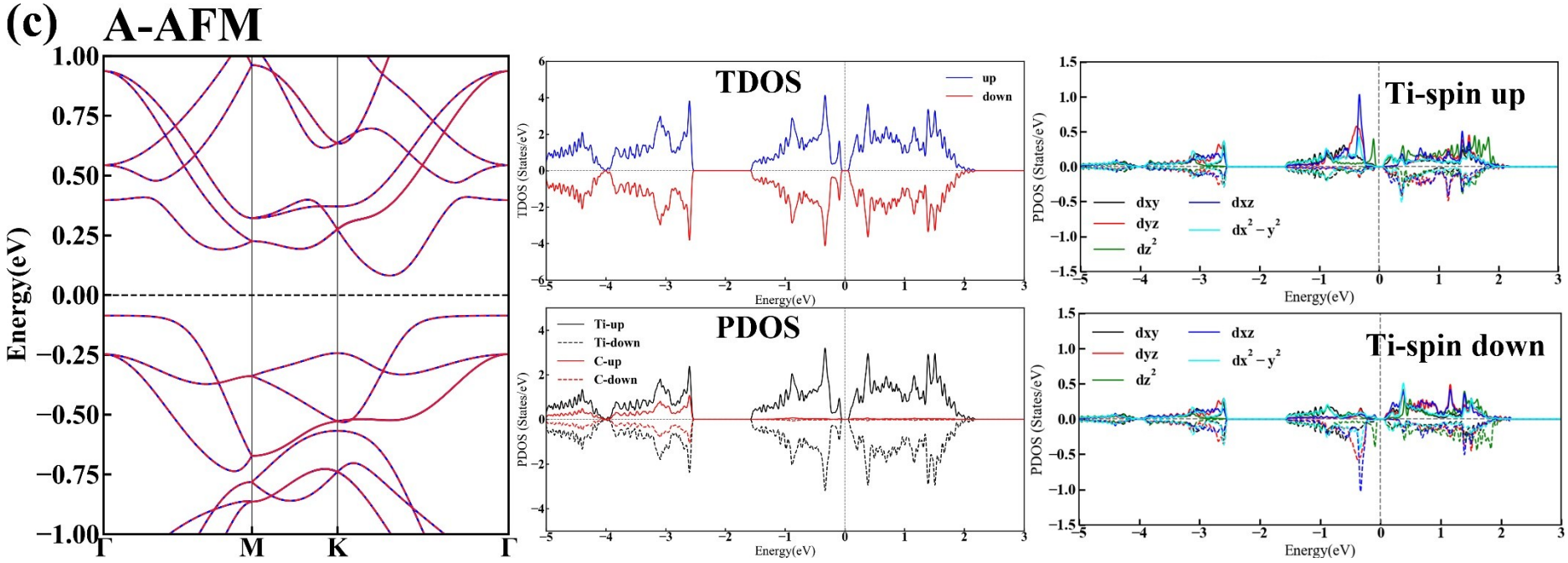
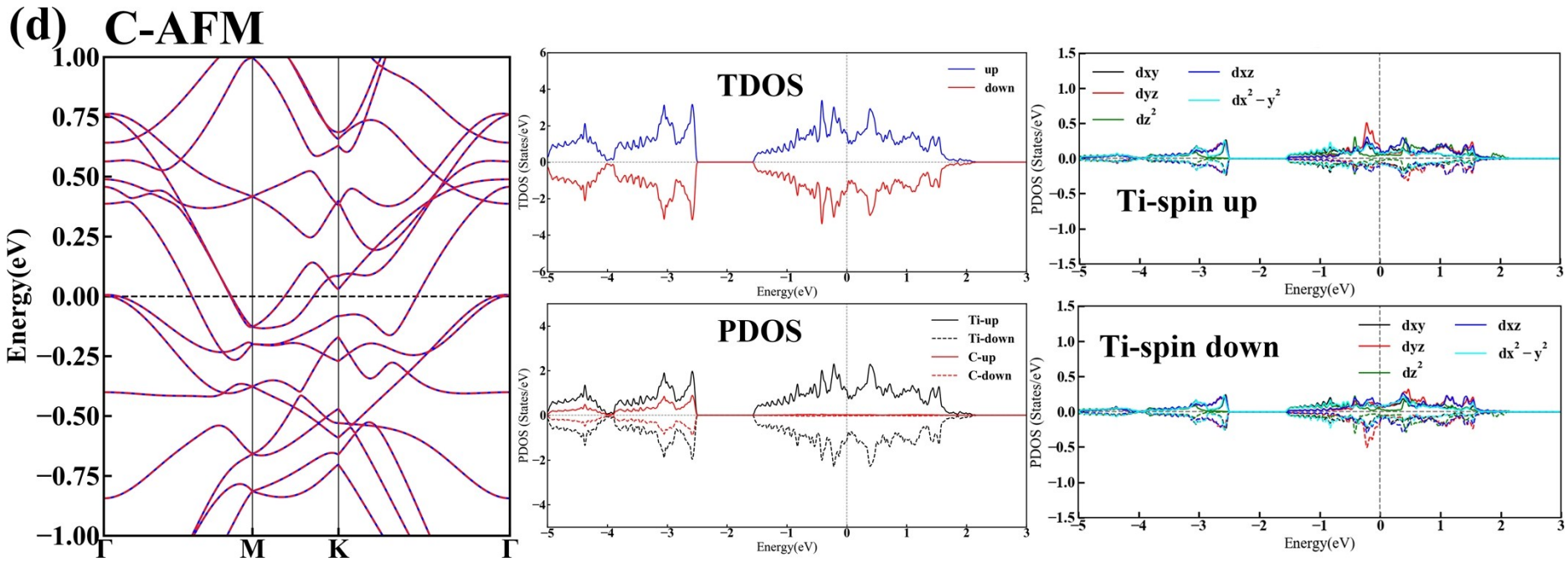
Figure S1: The band structures, total density of states (TDOS) and PDOS of Ti atoms, C atoms and 3*d*-orbitals of Ti atoms in (a) NM, (b) FM, (c) A-AFM, (d) C-AFM and (e) G-AFM states.




(b)
FM
Energy(eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ
TDOS
up
down
TDOS (States/eV)
Energy(eV)
PDOS
Ti-up
Ti-down
C-up
C-down
PDOS (States/eV)
Energy(eV)
Ti-spin up
dxy
dyz
dz²
dxz
dx² − y²
PDOS (States/eV)
Energy(eV)


(c) A-AFM
Energy(eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ
TDOS
up
down
TDOS (States/eV)
Energy(eV)
PDOS
Ti-up
Ti-down
C-up
C-down
PDOS (States/eV)
Energy(eV)
Ti-spin up
dxy
dxz
dyz
dx² − y²
dz²
PDOS (States/eV)
Energy(eV)
Ti-spin down
dxy
dxz
dyz
dx² − y²
dz²
PDOS (States/eV)
Energy(eV)


(d) C-AFM
Energy(eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ
TDOS
up
down
TDOS (States/eV)
Energy(eV)
PDOS
Ti-up
Ti-down
C-up
C-down
PDOS (States/eV)
Energy(eV)
Ti-spin up
dxy
dyz
dz²
dxz
dx²−y²
PDOS (States/eV)
Energy(eV)
Ti-spin down
dxy
dyz
dz²
dxz
dx²−y²
PDOS (States/eV)
Energy(eV)

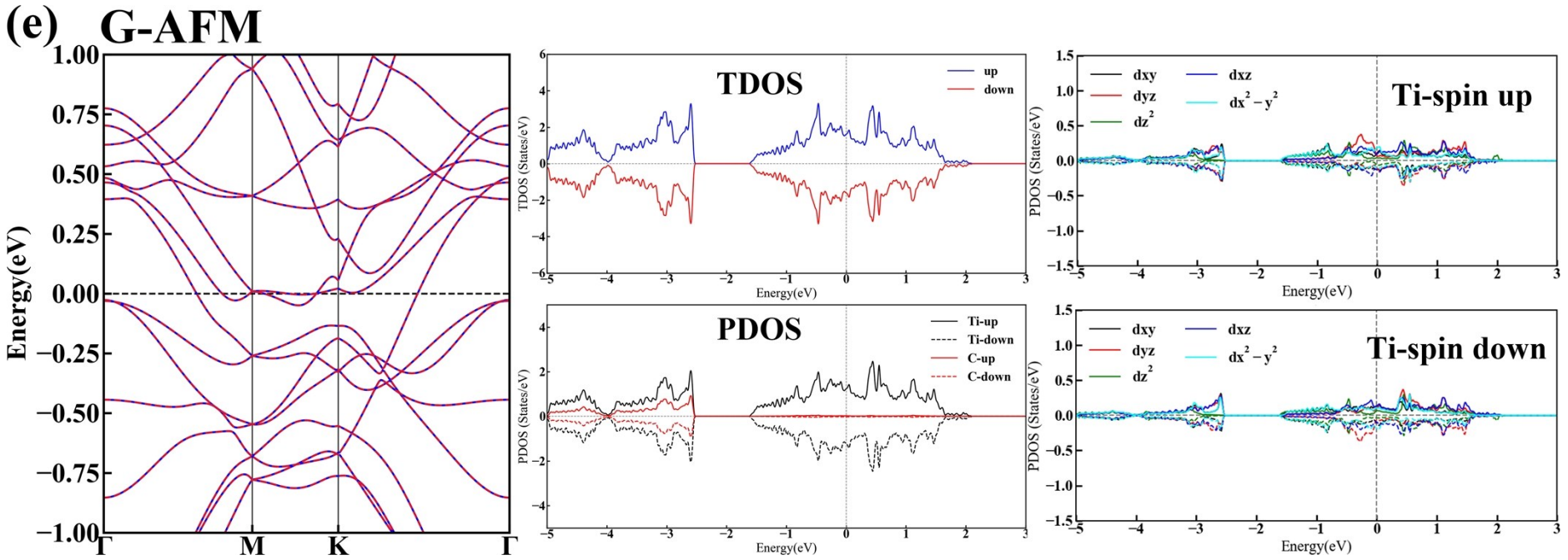

(e) G-AFM
Energy(eV)
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
Γ
M
K
Γ
TDOS
up
down
TDOS (States/eV)
Energy(eV)
PDOS
Ti-up
Ti-down
C-up
C-down
PDOS (States/eV)
Energy(eV)
Ti-spin up
dxy
dyz
dz²
dxz
dx²−y²
PDOS (States/eV)
Energy(eV)
Ti-spin down
dxy
dyz
dz²
dxz
dx²−y²
PDOS (States/eV)
Energy(eV)

Table S1. The exchange parameters (J_1, J_2 and J_3) under different electric field.

Electric field ($E_{\perp}$) (V/Å)	J_1 (meV)	J_2 (meV)	J_3 (meV)
0	− 2.35	5.95	− 0.35
0.06	− 1.95	5.65	− 0.5
0.1	− 1.65	4.65	− 0.4
0.12	− 1.55	3.75	− 0.35
0.14	− 1.35	2.6	− 0.4
0.16	− 0.75	1.25	− 0.2
0.18	− 0.6	0.7	− 0.2
0.2	− 0.15	0.15	0.05