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

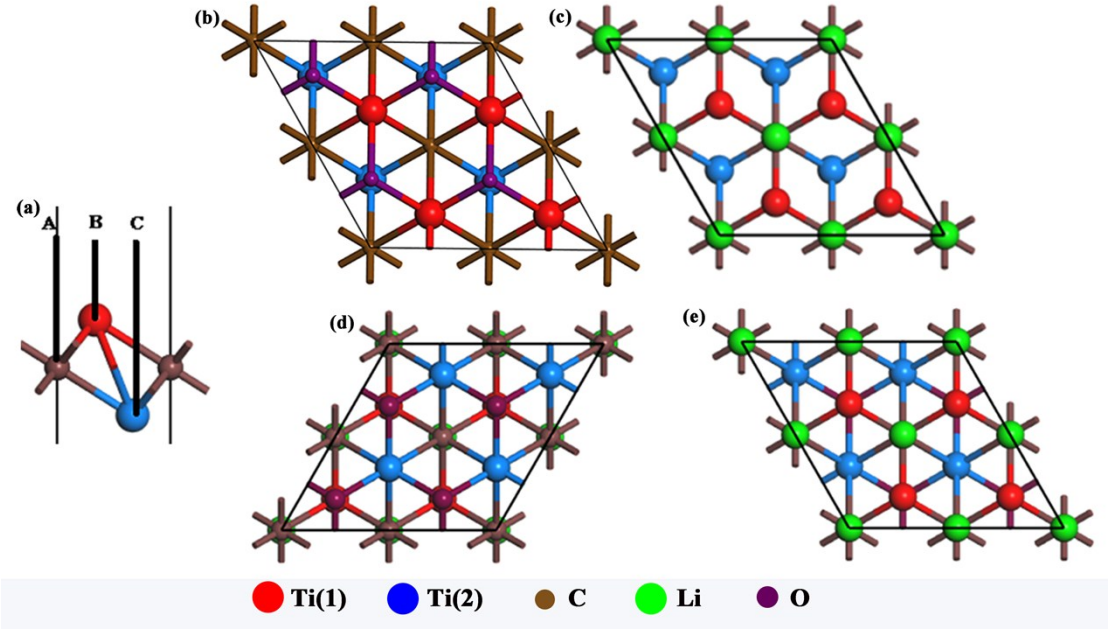

Fig. S1 The structure of pristine Ti_2C monolayer and functional Ti_2C monolayer. (a) side view of the unitcell of Ti_2C monolayer, where A, B, C represent the possible adsorption site of functional groups; (b) (c) the top view of 2×2 supercell of Ti_2C-O and Ti_2C-Li monolayer; (d) (e) the bottom and top viewer of Ti_2C-LiO monolayer.

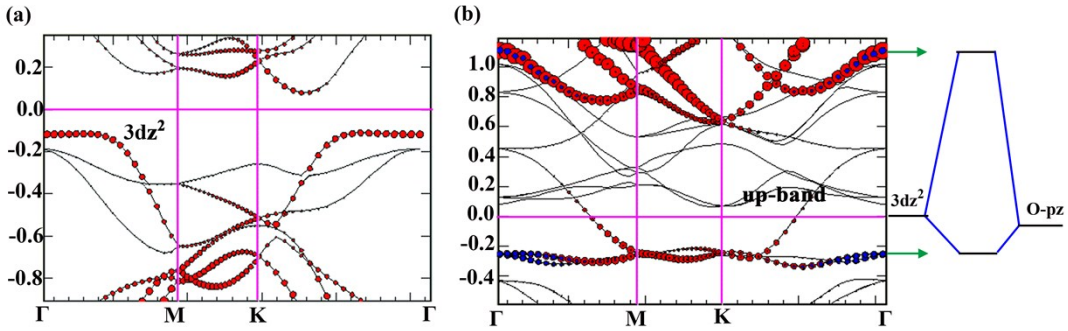

Fig. S2 The orbital energy level diagram of (a)Ti_2C monolayer, (b) the spin-up channel of Ti_2C-O monolayer, where the red circle represents the contribution of $3d_z^2$ orbitals of Ti atoms and the blue circle represents the contribution from p_z orbitals of O atoms.

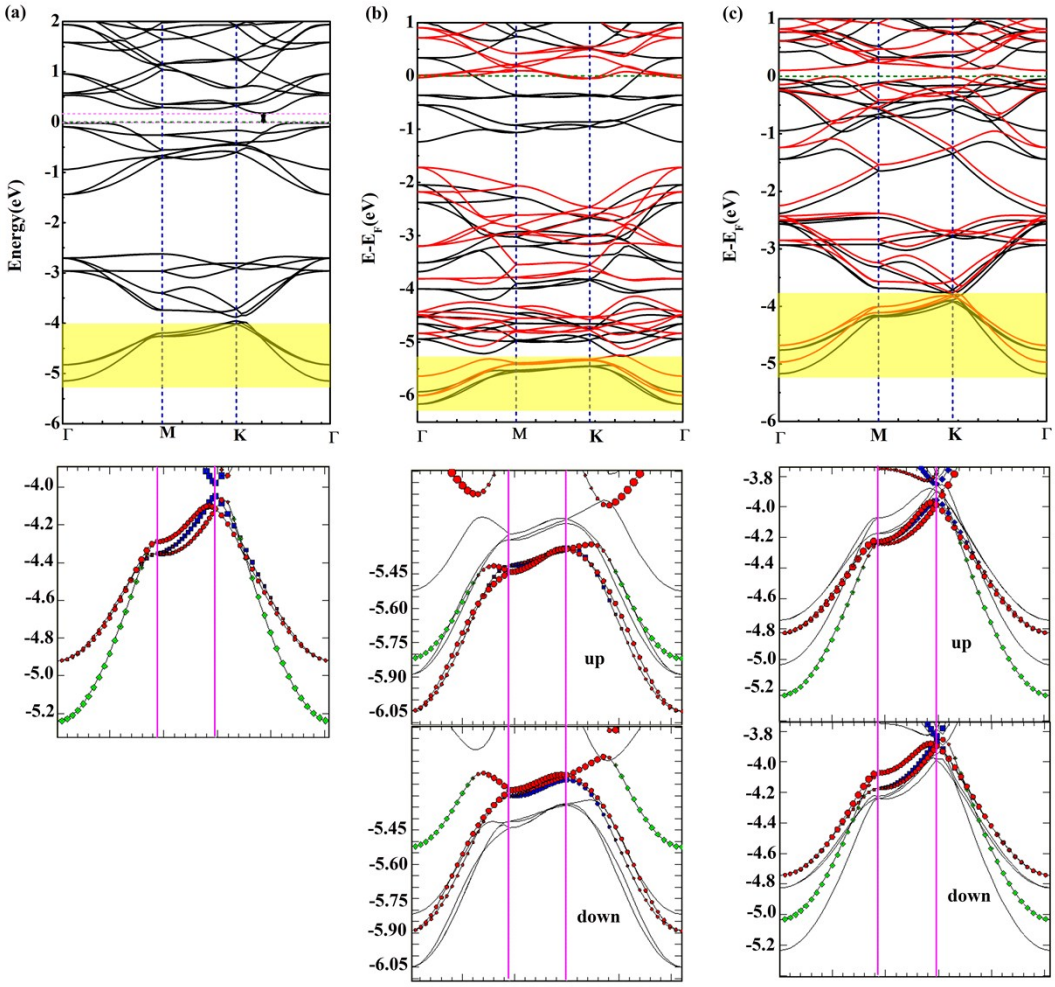

Fig. S3 The band structure for Ti_2C(a), Ti_2CO(b), Ti_2CLi(c), where the red, blue and green circle represent the band composed of $3d_{xy}$, $3d_{x^2-y^2}$; $3d_{xz}$, $3d_{yz}$ and $3d_{z^2}$.

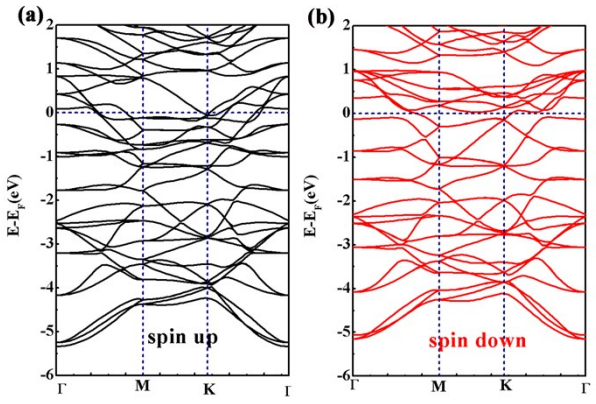

Fig. S4 The band-structure of Ti_2C-P monolayer. (a) spin up; (b) spin down.

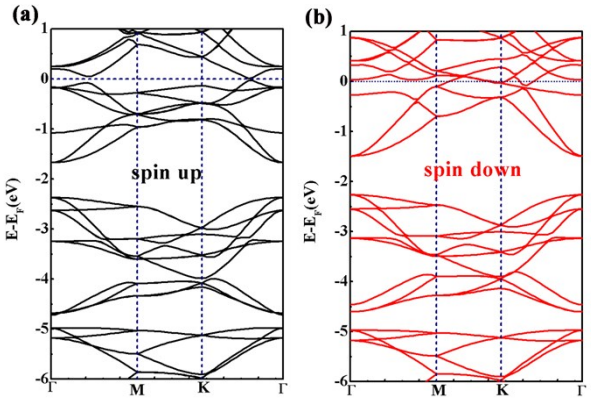

Fig. S5 The band-structure of Ti_2C-OH monolayer. (a) spin up; (b) spin down.

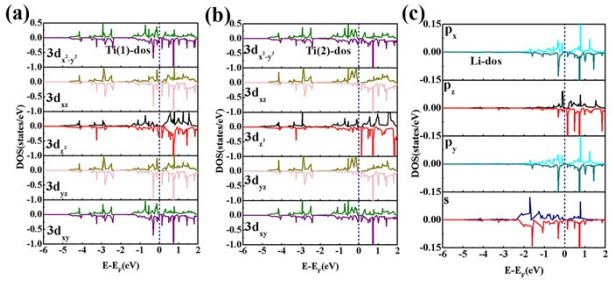

Fig. S6 The projected density of states of Ti(1) atoms, Ti(2) atoms, Li atoms in ferrimagnetic Ti_2C-Li monolayer, respectively.

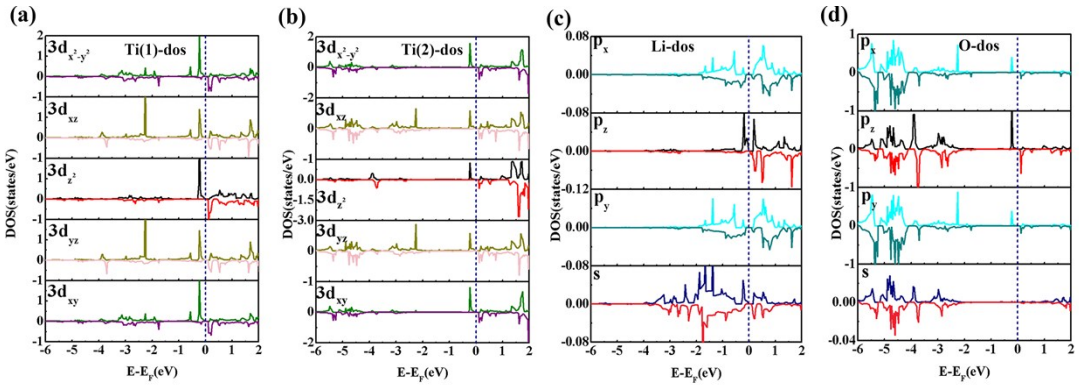

Fig. S7 the projected density of states of Ti(1) atoms, Ti(2) atoms, O atoms, Li atoms in ferromagnetic Li-Ti_2C-O monolayer, respectively.

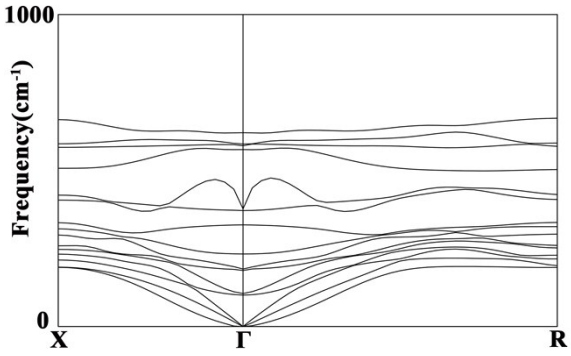

Fig. S8 Phonon dispersion curves of the asymmetrically Li-Ti_2C-O monolayer.

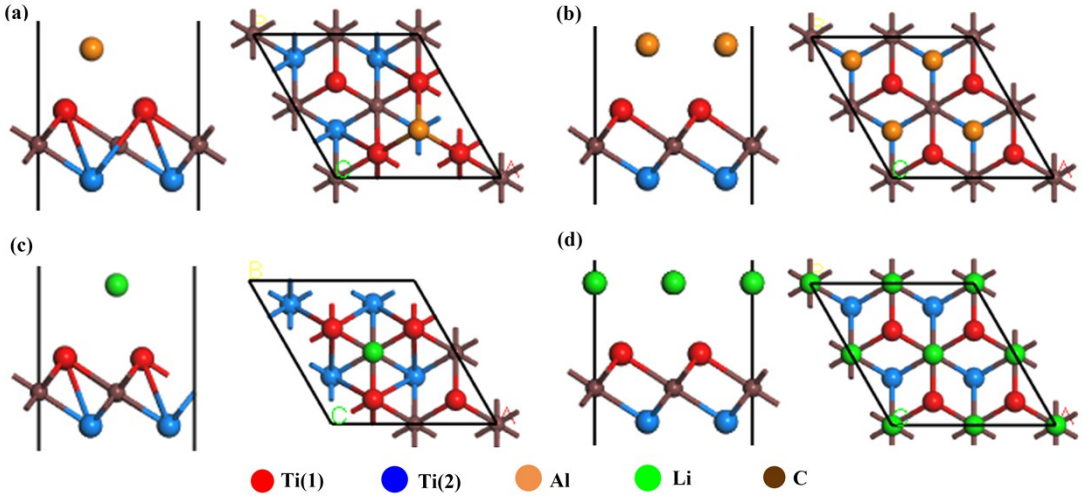

Fig. S9 The structure of a single atom or a layer of atoms adsorbed on the surface of Ti_2C surface.

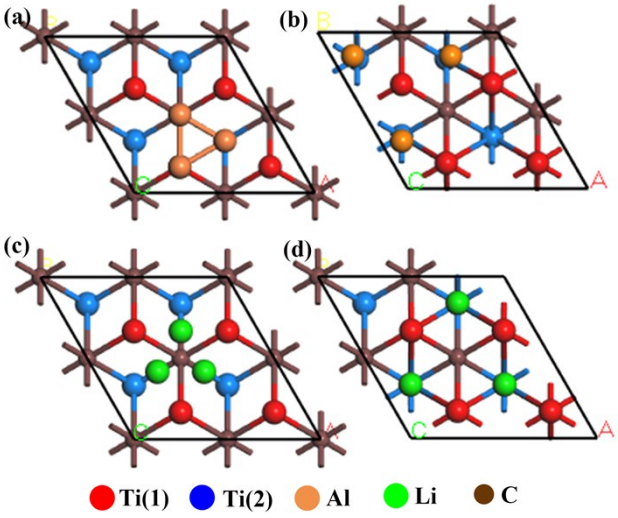

Fig. S10 The structures before and after optimization of the metal clusters on the surface of Ti_2C monolayer. (a)unrelaxed (b)relaxed structures of Ti_2C-Al clusters; (c)unrelaxed (d)relaxed structures of Ti_2C-Li clusters.

The calculation of adsorption energy

In order to verify the stability, we calculated the absorption energy, which can be calculated in the formula: $\Delta E = E_{Ti_2CT} - E_{Ti_2C} - E_T$, where E_{Ti_2CT} and $E_{T_{i2}C}$ are the total energies of adsorbed and pristine Ti_2C , respectively. And E_T is the energy of surface functional groups. For the configuration of O adsorbed Ti2C monolayer, the E_T is equal to half of the energy of oxygen. For the adsorption of metal atoms, the energy of Li atoms refers to the bulk energy of face-centred cubic structure. And the negative value indicates the stable configuration.

Table S1 The total energy and adsorption energy of all possible configurations of Ti_2C-O monolayer in unit cell

	A	B	C
Total energy(eV)	-31.14583	-28.69305	-31.51384
Adsorption energy(eV)	-4.68792	-2.23514	-5.05593

Table S2 The total energy of five different configurations of Ti_2C-O monolayer.

	AFM1	AFM2	AFM3	FM	NM
PBE	-125.61886	-125.61363	-125.61325	-126.06208	-125.61361
HSE06	-159.88158	-159.84498	-159.84492	-160.66769	-159.66813

Table S3 The total energy and adsorption energy of all possible configurations of Ti_2C-Li monolayer in unit cell

	A	B	C
Total energy(eV)	-24.35434	-24.16877	-24.31739
Adsorption energy(eV)	-0.37580	-0.19023	-0.33885

Table S4 The total energy of five different configurations of Ti_2C-Li monolayer.

	AFM1	AFM2	AFM3	FM	NM
PBE	-97.39419	-97.22306	-97.22093	-97.41781	-97.17737
HSE06	-116.58665	-116.16276	-116.16280	-116.58735	-115.63574

Table S5 The total energy of all possible configurations of Ti_2C-LiO monolayer in unit cell

Li \ O	A	B	C
A	-33.329946	-33.727598	-30.950590
B	-33.146451	-33.567881	-30.677700
C	-33.309885	-33.717606	----

The minimal adsorption energy is -5.3548eV.

Table S6 The total energy of five different configurations of Ti_2C-LiO monolayer.

	AFM1	AFM2	AFM3	FM	NM
PBE	-134.90354	-134.69800	-134.69789	-134.90402	-134.68152
HSE06	-169.36794	-169.36797	-168.95870	-169.36807	-168.67608