

## SUPPLEMENTARY INFORMATION

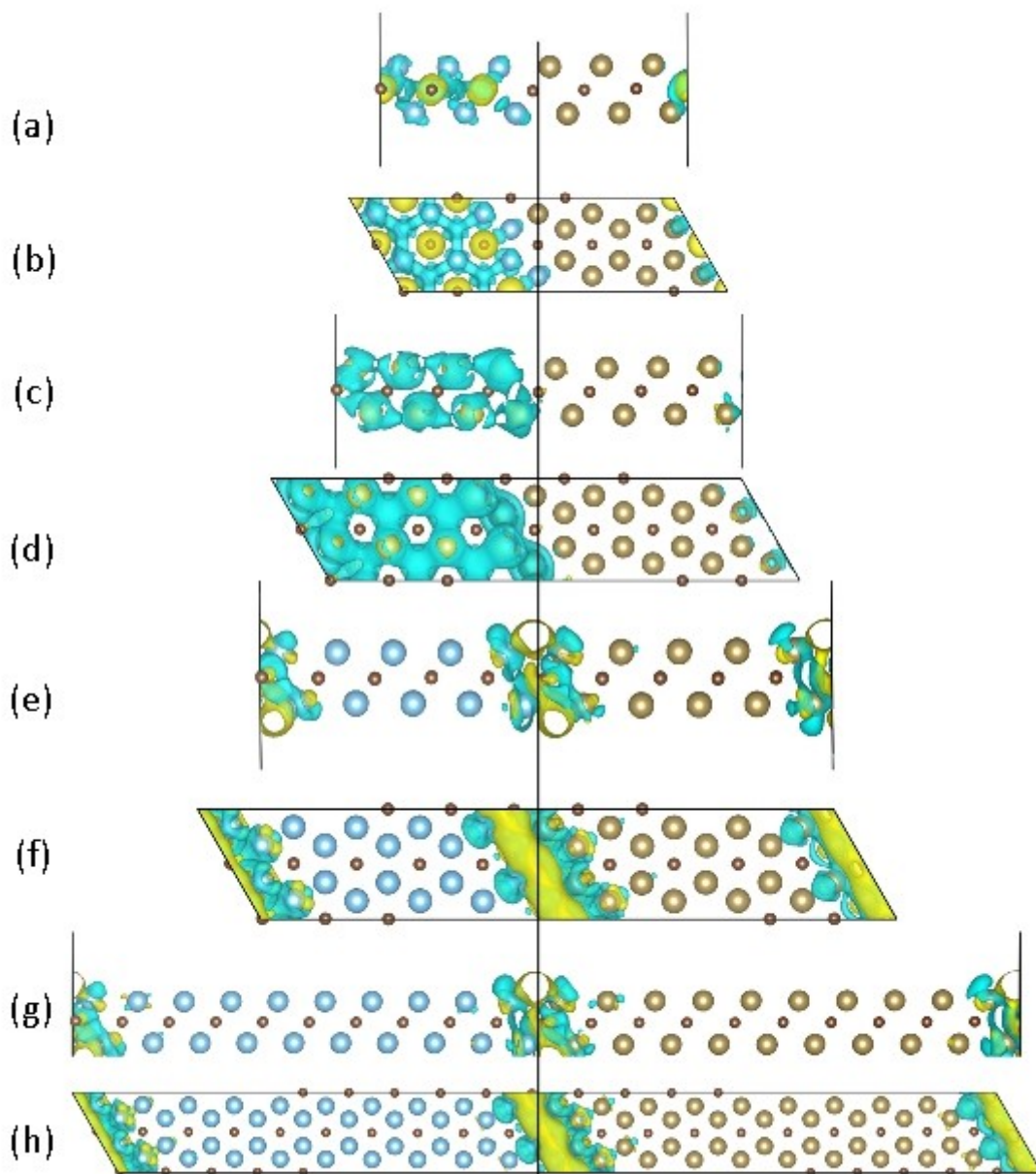


Fig. S1. (a-c-e-g) Side and (b-d-f-h) top views of the charge density difference for the  $(\text{Ti}_2\text{C})_p/(\text{Ta}_2\text{C})_q$   $p=q = 3,4,5,10$ , respectively.

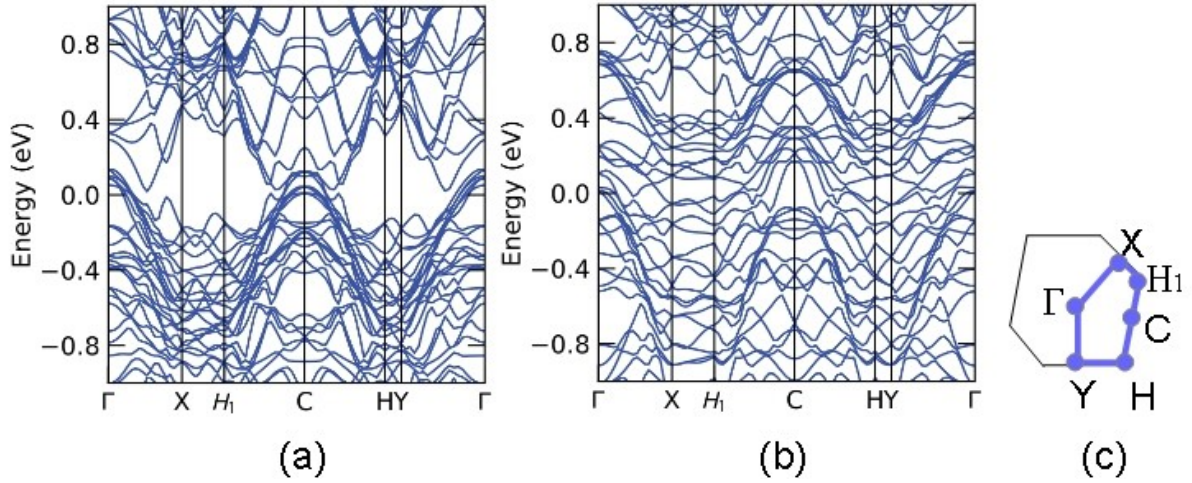


Fig. S2. (a) Spin up, and (b) spin down band structures of  $(\text{Ti}_2\text{C})_3/(\text{Ta}_2\text{C})_3$ . The Fermi level is set at 0 eV. (c) High symmetry points in the Brillouin zone of  $(\text{Ti}_2\text{C})_3/(\text{Ta}_2\text{C})_3$ .

Table S1. The total energy values determining the energy cutoff for  $(\text{Ti}_2\text{C})_3/(\text{Ta}_2\text{C})_3$ .

Encut (eV)	Energy (eV)
450	-279.36617
550	-279,33973
650	-279,36160
750	-279,37616
850	-279,37900

In this paper, the chosen 450 eV plane wave cutoff energy is based on the energy difference becoming of the order of  $1 \times 10^{-2}$  eV. The total energies reported in the table are calculated for the  $(\text{Ti}_2\text{C})_3/(\text{Ta}_2\text{C})_3$ , using spin-polarized calculation.