

Supplementary Material

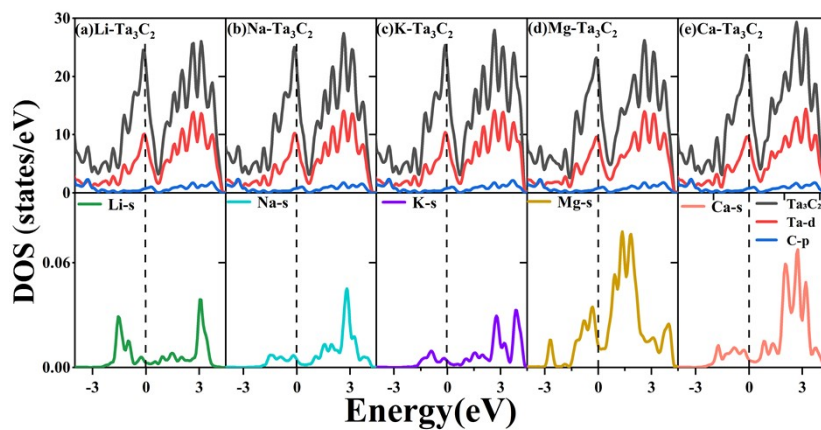


Figure S1. DOS of Ta₃C₂M (M = Li, Na, K, Mg, and Ca).

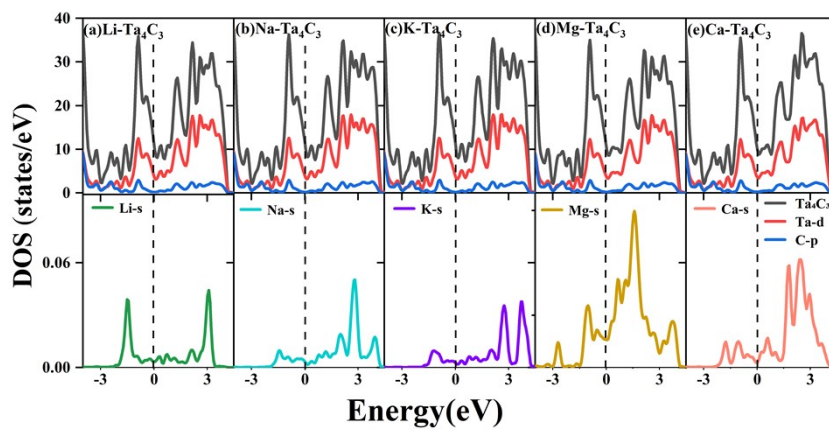


Figure S2. DOS of Ta₄C₃M (M = Li, Na, K, Mg, and Ca).

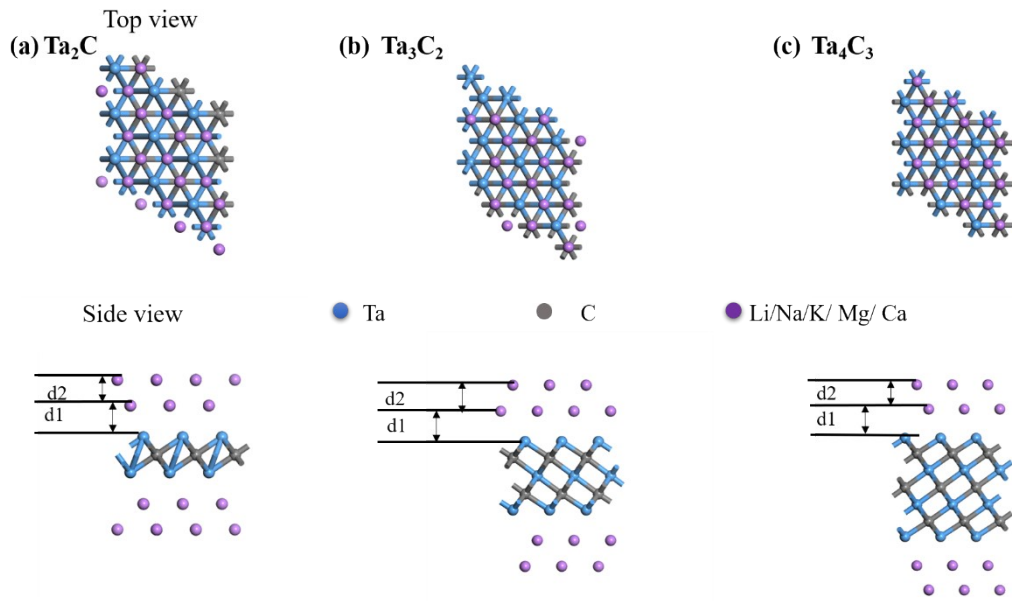


Figure S3. Vertical distance between the metal atoms and the surface of $Ta_{n+1}C_n$ MXenes.

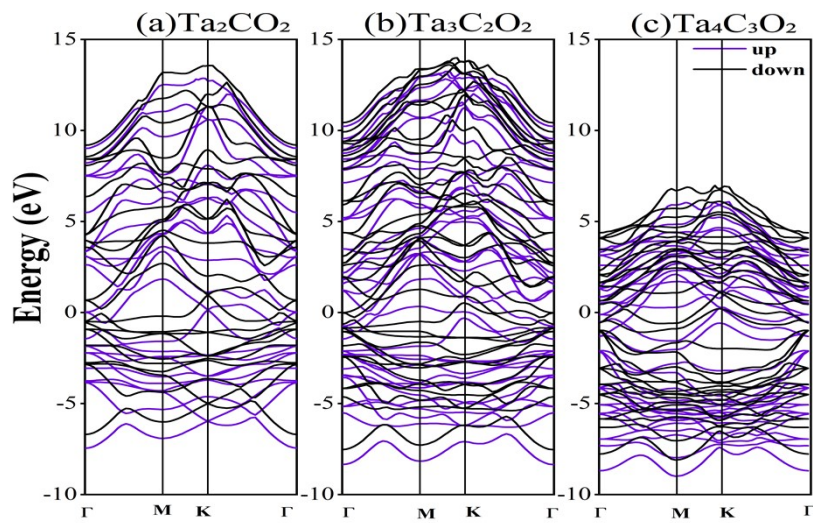


Figure S4. Band structures of $Ta_{n+1}C_nO_2$ MXenes.

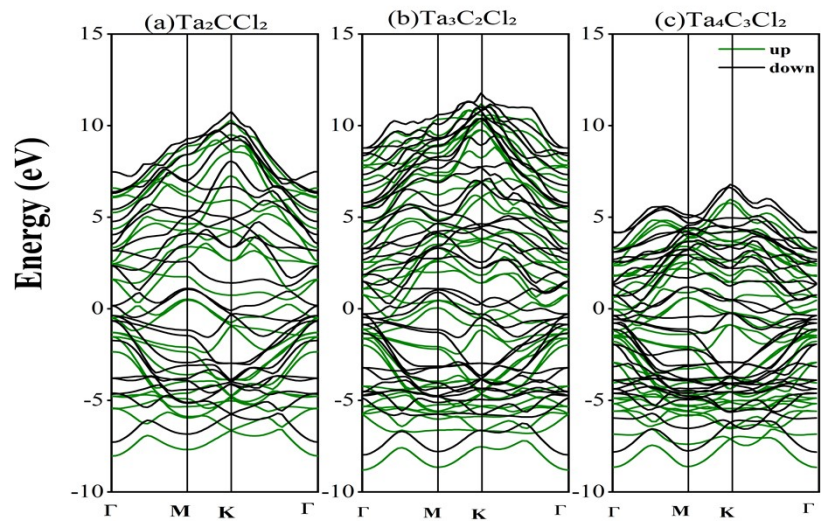


Figure S5. Band structures of $Ta_{n+1}C_nCl_2$ MXenes.

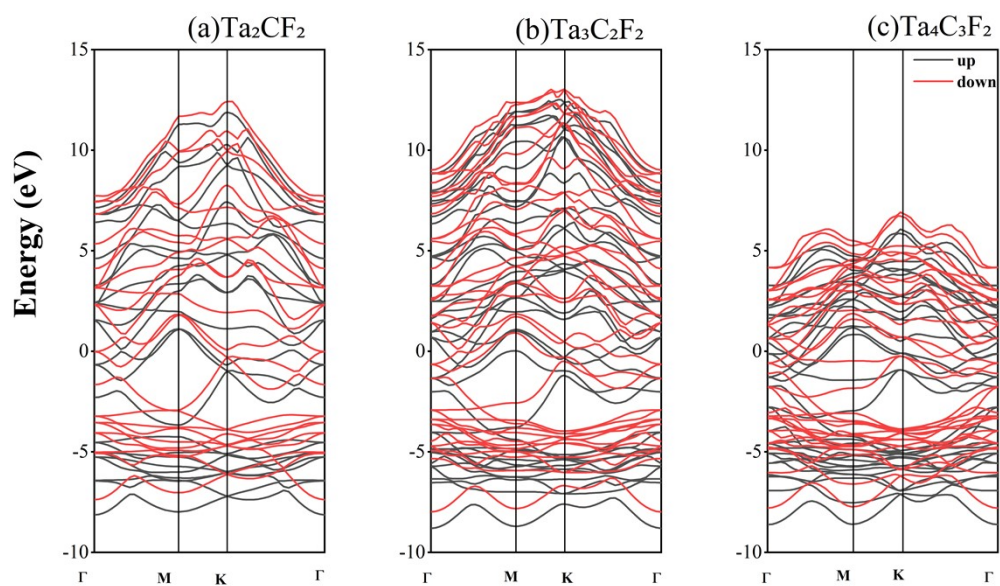


Figure S6. Band structures of $Ta_{n+1}C_nCl_2$ MXenes.

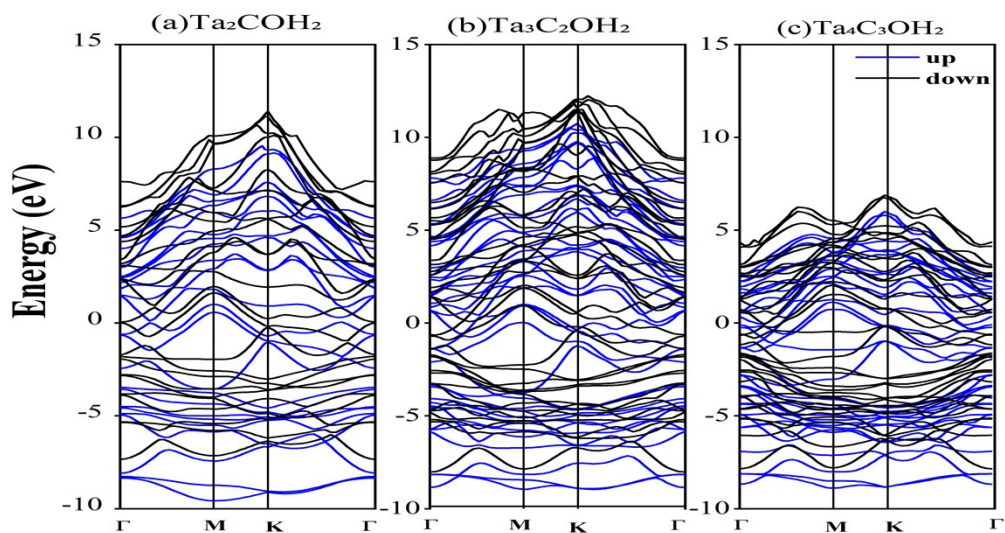


Figure S7. Band structures of $Ta_{n+1}C_nCl_2$ MXenes.

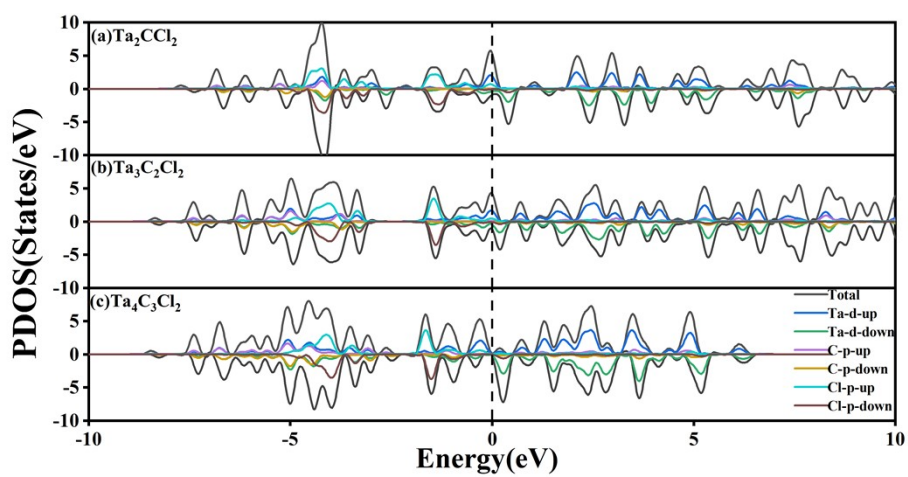


Figure S8. DOS structures of $Ta_{n+1}C_nCl_2$ MXenes

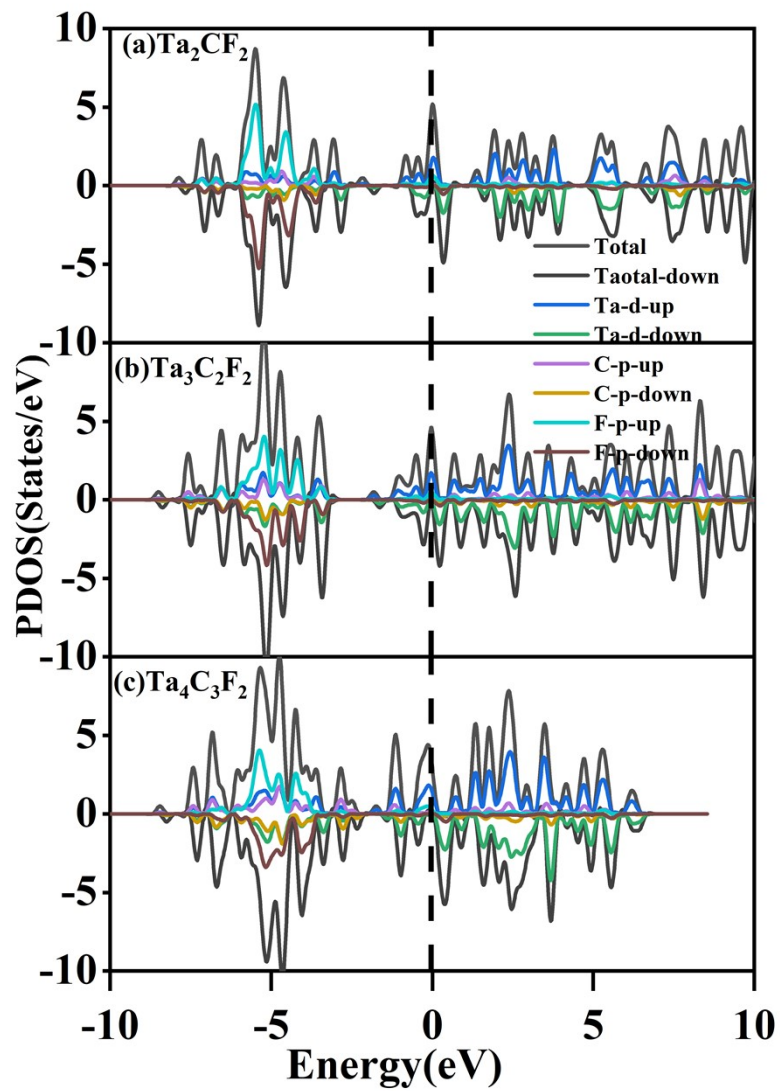


Figure S9. DOS of $\text{Ta}_{n+1}\text{C}_n\text{Cl}_2$ MXenes

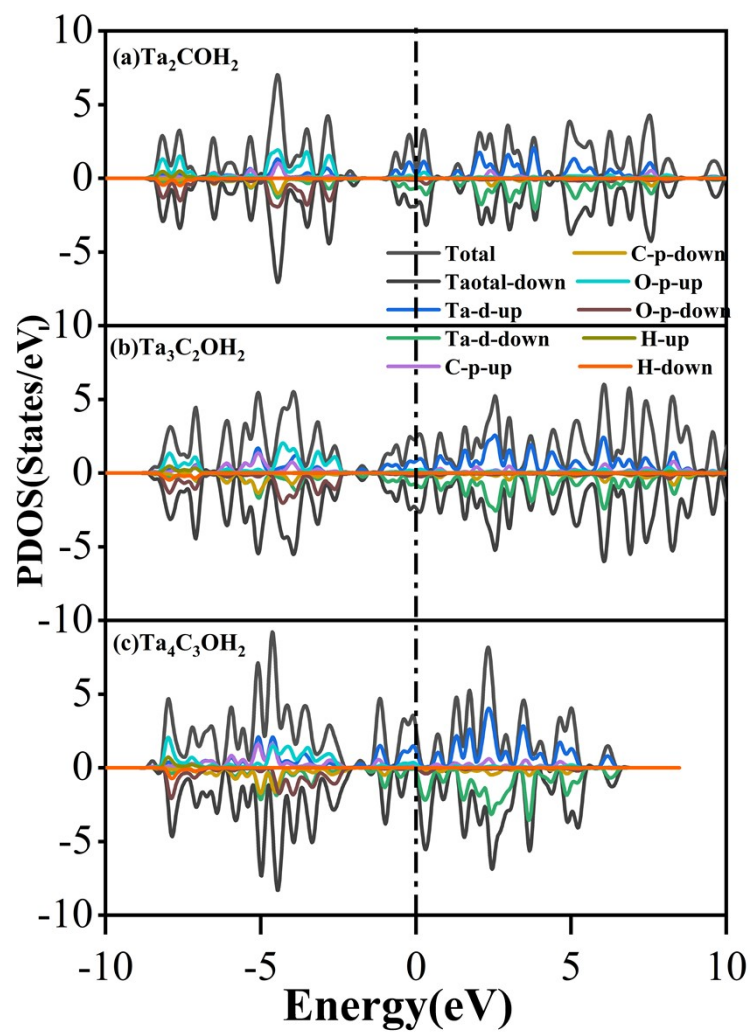


Figure S10. DOS of $\text{Ta}_{n+1}\text{C}_n\text{Cl}_2$ MXenes

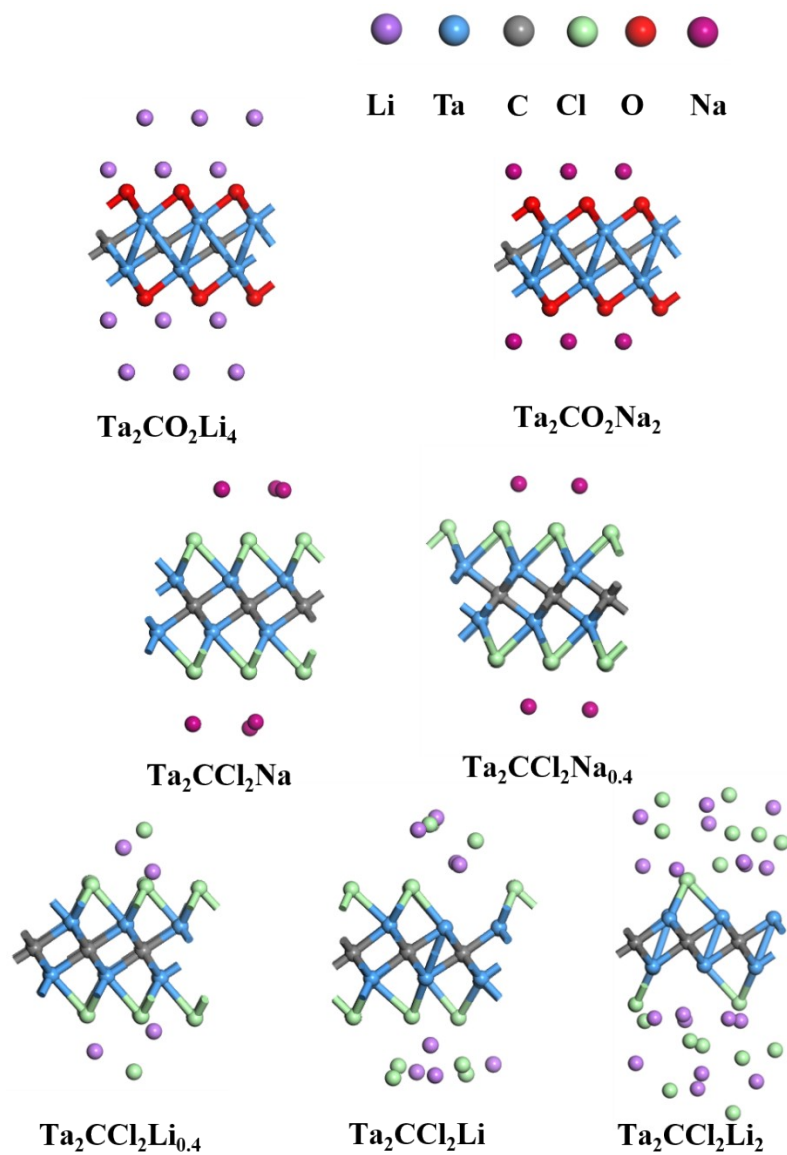


Figure S11. Side view structures of Ta₂CT₂M_x MXenes.