

Electronic supplementary information

MXene: A promising photocatalyst for water splitting

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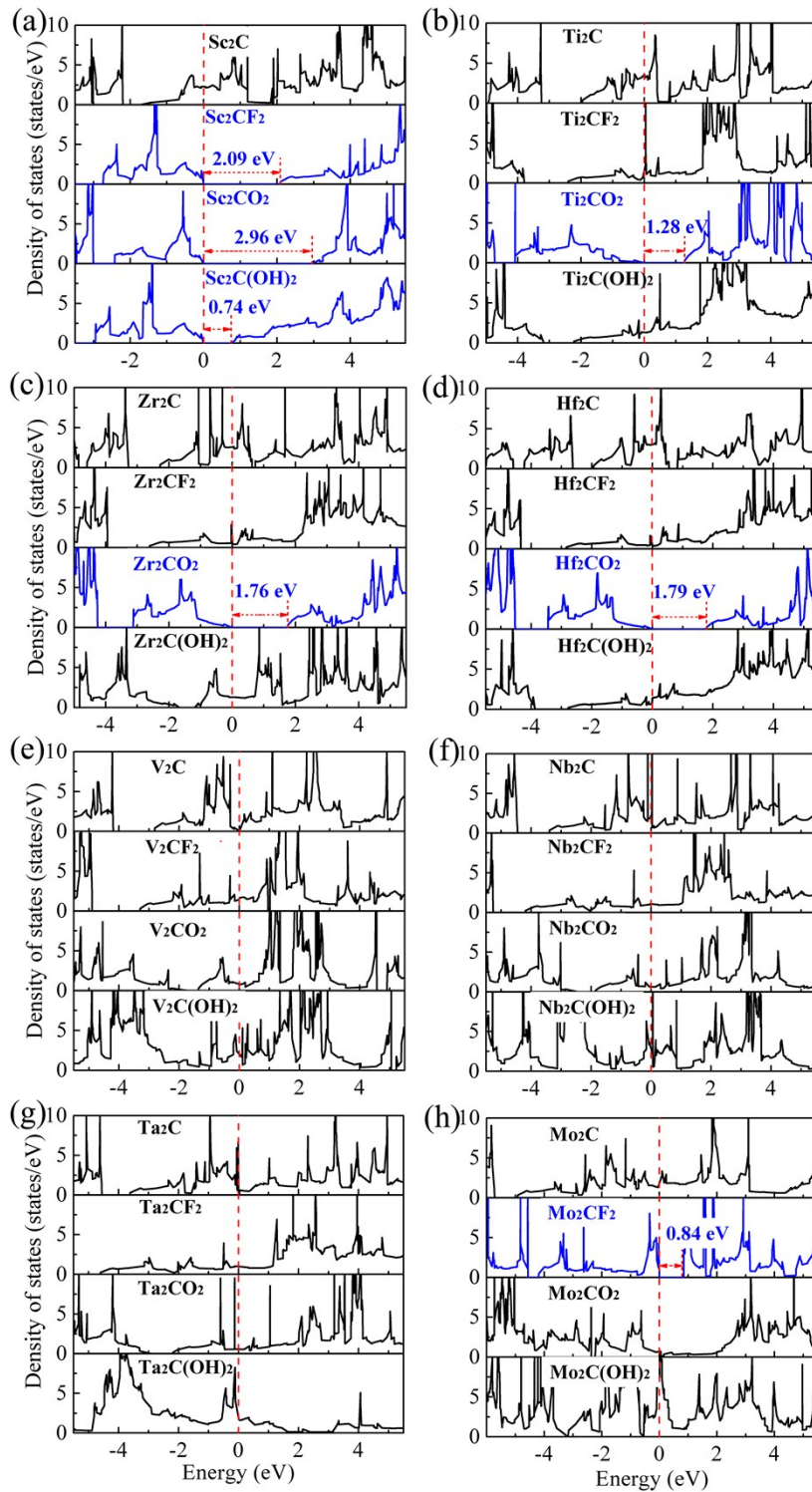


Fig. S1. Calculated (using HSE06) density of states (DOS) of pristine and functionalized 2D (a) Sc₂C, (b) Ti₂C, (c) Zr₂C, (d) Hf₂C, (e) V₂C, (f) Nb₂C, (g) Ta₂C and (h) Mo₂C. The Fermi energy is set to 0 eV and indicated by vertical dashed line.

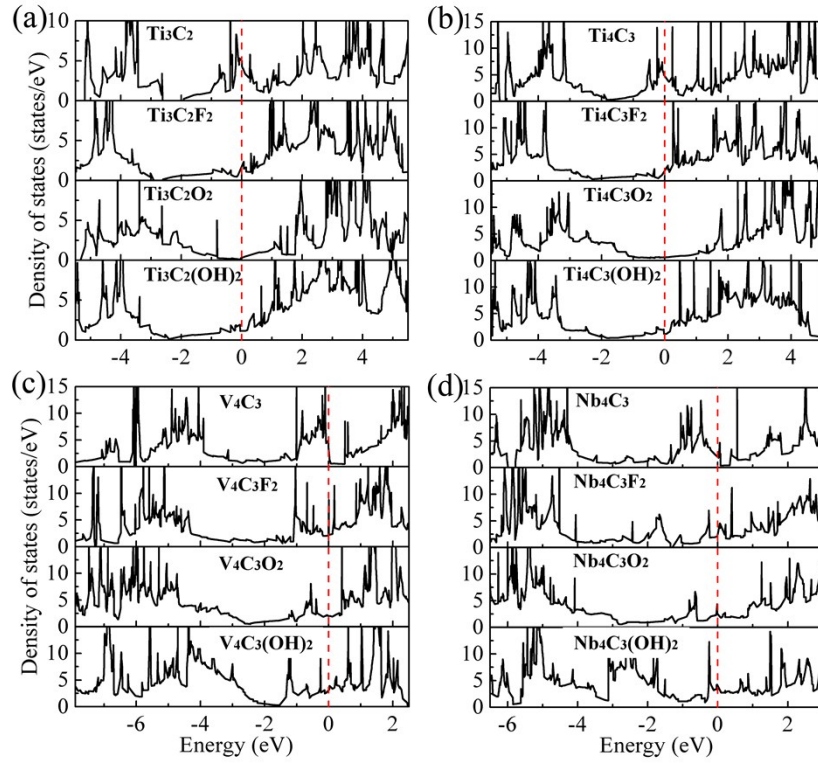


Fig. S2. Calculated (using HSE06) density of states (DOS) of pristine and functionalized 2D (a) Ti_3C_2 , (b) Ti_4C_3 , (c) V_4C_3 and (d) Nb_4C_3 . The Fermi energy is set to 0 eV and indicated by vertical dashed line.