Supplementary Information

March 28, 2024

Computational Study Based Prediction of New Photocatalysts for water splitting by systematic manipulation of MXene surfaces.

Swati Shaw*[a] and Subhradip Ghosh*[b]

[a] *Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India.*
E-mail: swatishaw@iitg.ac.in
[b] *Department of Physics, Indian Institute of Technology Guwahati, Guwahati-781039, Assam, India.*
E-mail: subhra@iitg.ac.in

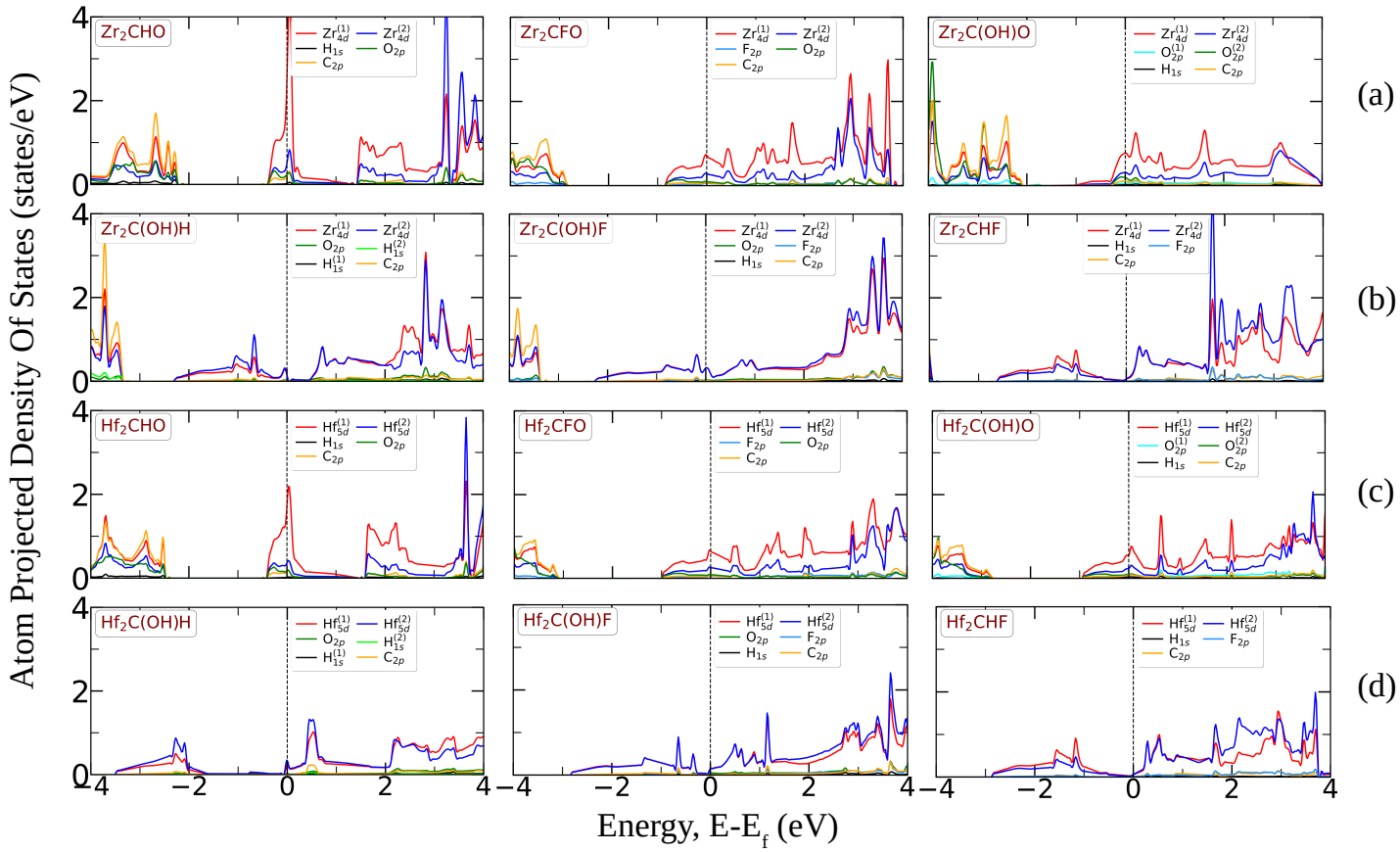

Fig. S1 Atom-projected densities of states of (a) Zr_2CTO, T = H, F, OH; (b) Zr_2CTT', T,T′ = H, F, OH; (c) Hf_2CTO, T = H, F, OH ; (d) Hf_2CTT', T,T′ = H, F, OH. Fermi level is set at 0 eV.

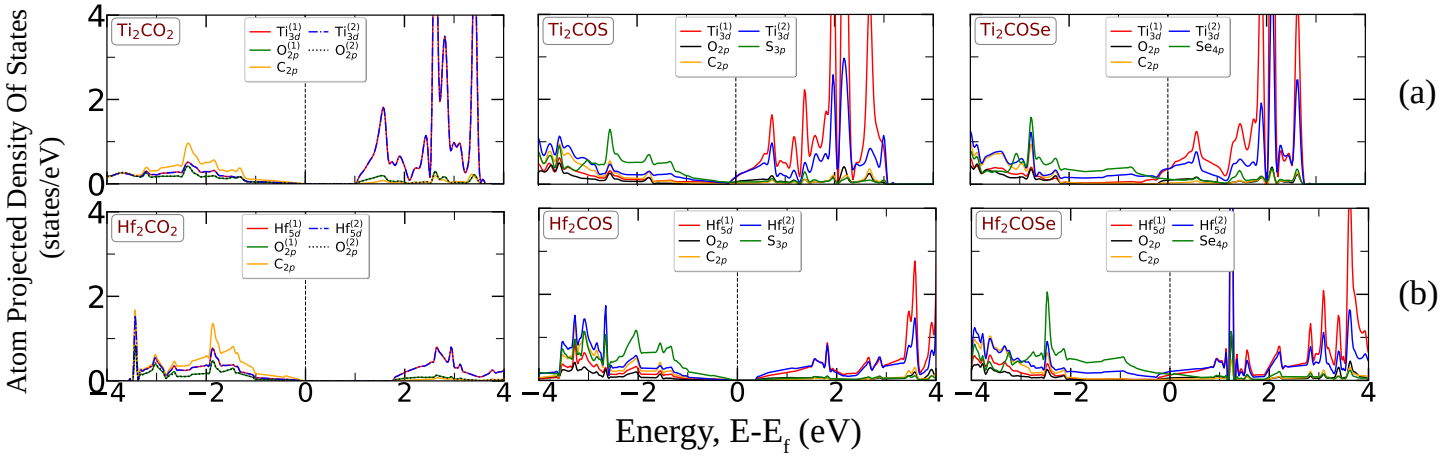

Fig. S2 Atom-projected densities of states of of (a) Ti_2COT, T= O, S, Se; (b) Hf_2COT, T= O, S, Se. Fermi level is set to 0 eV.

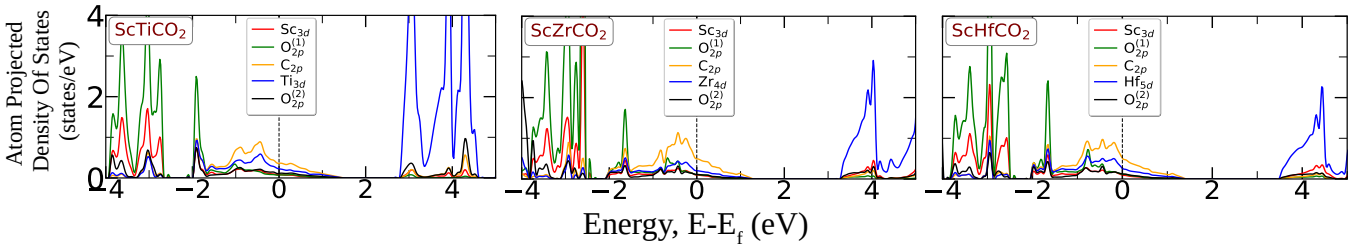

Fig. S3 Atom-projected densities of states of $ScM'CO_2$, M′ = Ti, Zr & Hf. Fermi level is set to 0 eV.

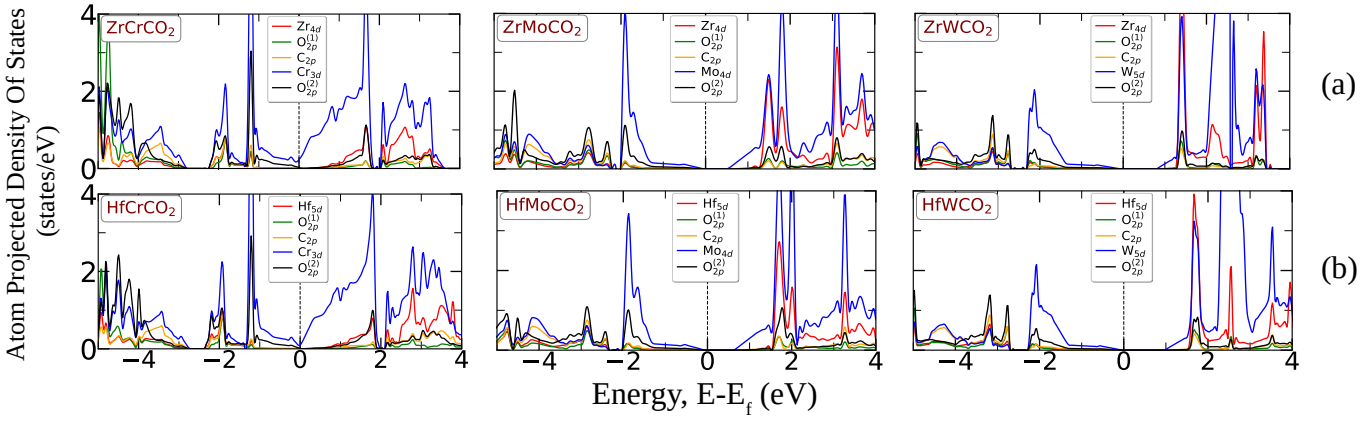

Fig. S4 Atom-projected densities of states of (a) $ZrM'CO_2$, M′ = Cr, Mo & W; (b) $HfM'CO_2$, M′ = Cr, Mo & W. Fermi level is at 0 eV

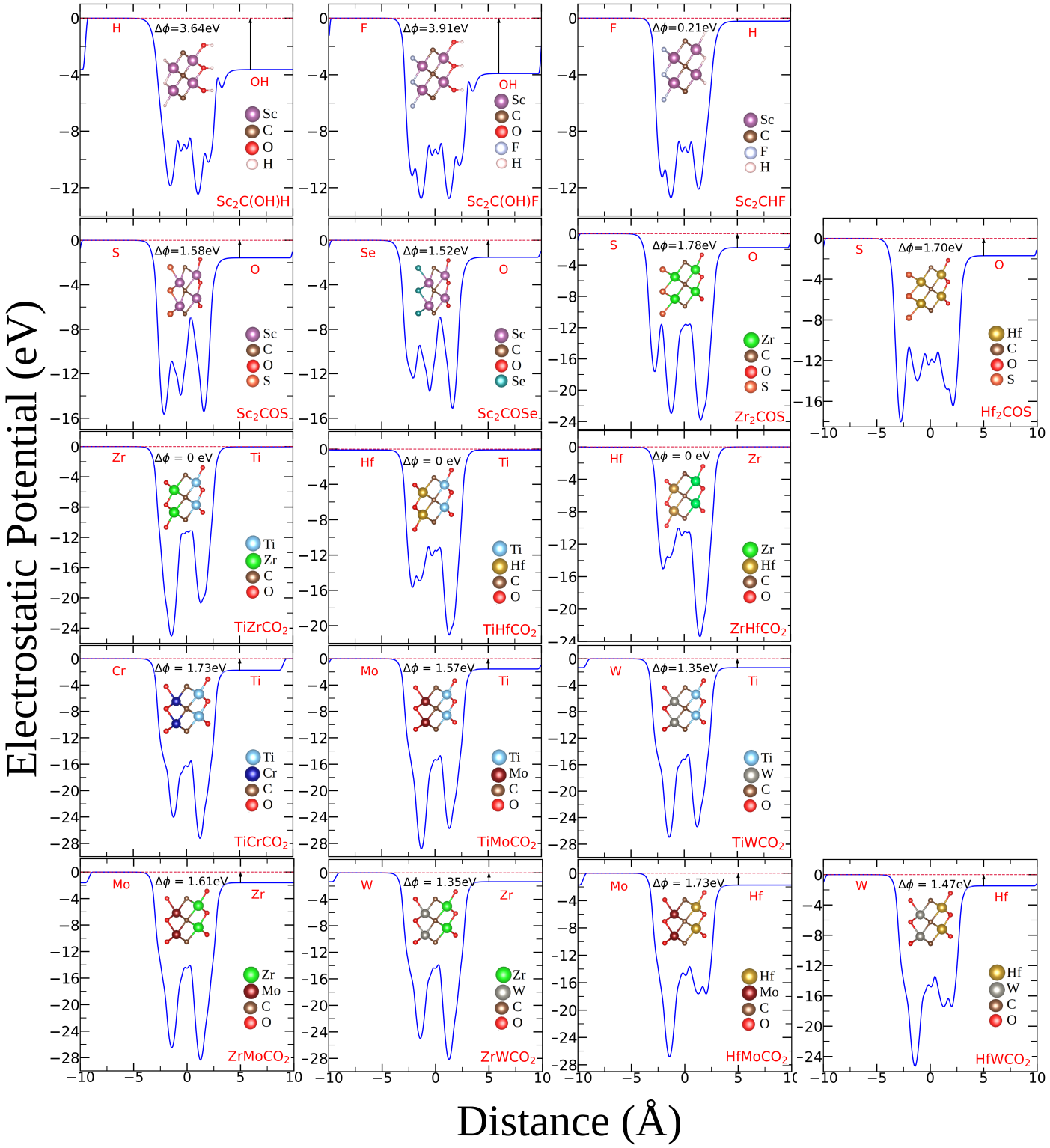

Fig. S5 Electrostatic potential profile of 17 Janus MXenes along z-direction. Potential profiles are calculated by setting vacuum level of the surface at (00-1) to zero eV.

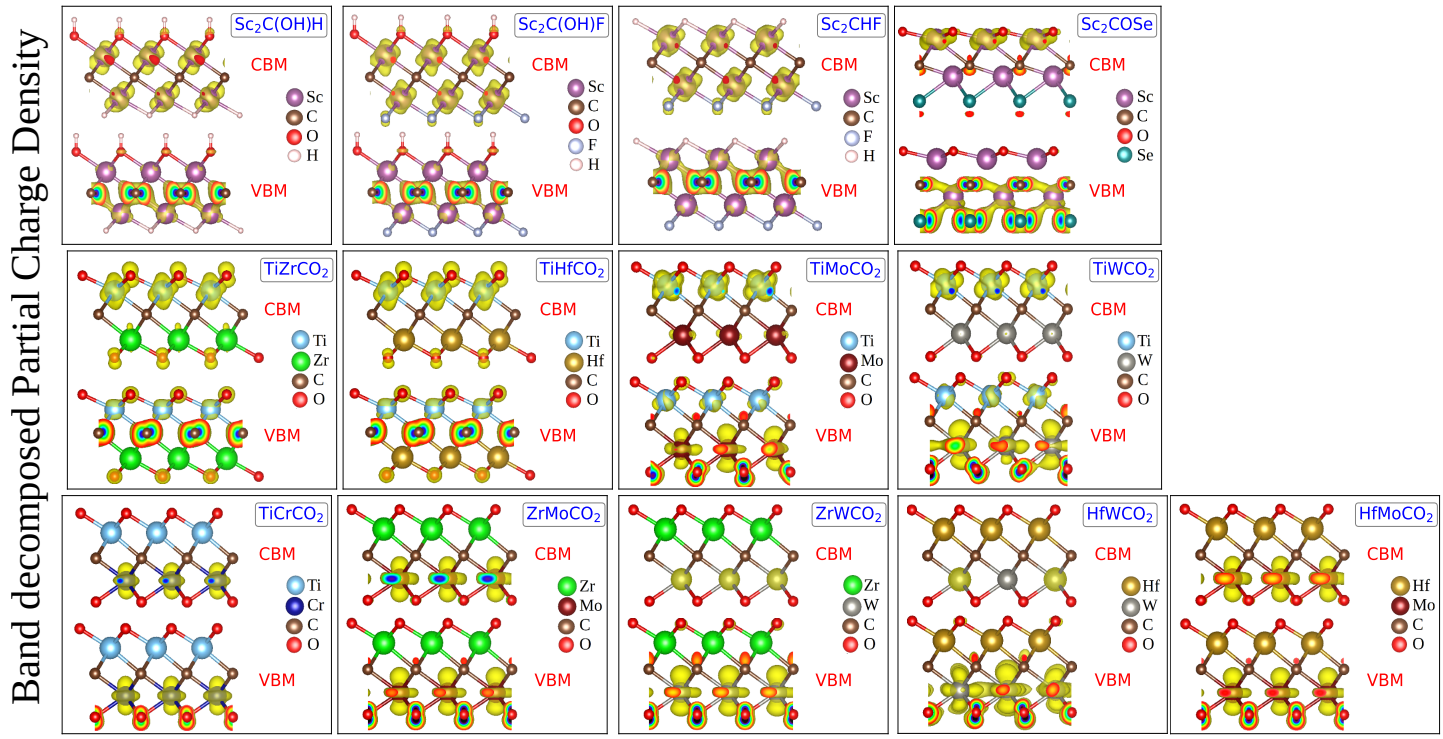

Fig. S6 Charge density contributions of constituents towards VBM and CBM for the Janus MXenes where appropriate band alignments with respect to OER and HER energies are not found.