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Supplementary Information

Surface Modifications of 2D-$Ti_3C_2O_2$ by Nonmetal Doping for Obtaining High Hydrogen Evolution Reaction Activity: A Computational Approach

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Table S1. Formation Energy (E_f) of 2D-$Ti_3C_2O_2$ before and after doped with X (X = S, Se, Te) in the 3 × 3 supercell. Bond Length (B_{NM}-Ti) of Ti-X, charge transfer (Bader) of X. Positive values denude the obtained electron and the corresponding lattice constant (a).

3 × 3 supercell	E_f (eV)	$B_{NM\text{-}Ti}$ (Å)	Bader (eV)	a (Å)
$Ti_{27}C_{18}O_{18}$	−7.454	1.969	1.109	9.059
$Ti_{27}C_{18}O_{17}S_1$	−7.4204	2.394	0.836	9.065
$Ti_{27}C_{18}O_{17}S_3$	−7.349	2.390	0.824	9.107
$Ti_{27}C_{18}O_{17}Se_1$	−7.409	2.532	0.705	9.067
$Ti_{27}C_{18}O_{17}Se_3$	−7.315	2.532	0.700	9.109
$Ti_{27}C_{18}O_{17}Te_1$	−7.393	2.756	0.496	9.082
$Ti_{27}C_{18}O_{17}Te_3$	−7.268	2.770	0.490	9.121

Table S2. Structure optimization results of 2D-$Ti_3C_2O_2$.

$Ti_3C_2O_2$	a (Å)	O-Ti1 bond (Å)	Ti1-C bond(Å)	C-Ti2 bond(Å)
This work	3.020	1.969	2.179	2.144
Reference	3.019	1.970	2.180	2.144

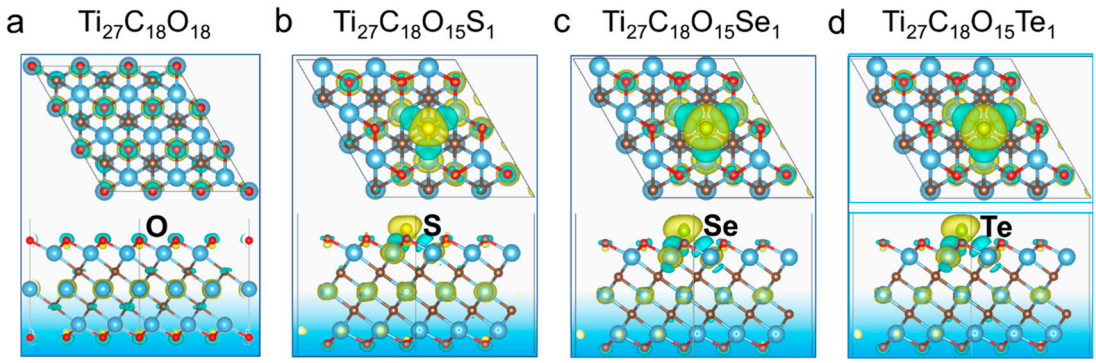

Figure S1. 3 × 3 supercell spin density of 2D-$Ti_3C_2O_2$ before and after doped with X. (a) $Ti_{27}C_{18}O_{18}$; (b) $Ti_{27}C_{18}O_{15}S_1$; (c) $Ti_{27}C_{18}O_{15}Se_1$; (d) $Ti_{27}C_{18}O_{15}Te_1$. Yellow: Spin up electrons, Blue: Spin down electrons.

Reference

1. Xiaoxu Wang, Changxin Wang, Shinan Ci, Yuan Ma, Tong Liu, Lei Gao, Ping Qian, Chunlin Ji and Yanjing Su. Accelerating 2D MXene catalyst discovery for the hydrogen evolution reaction by computer-driven workflow and an ensemble learning strategy. **J. Mater. Chem. A**, **2020**, *8*, 23488–23497.