Supplementary Information

Oxygen vacancy engineering in MXene for sustainable electrochemical energy conversion and storage applications

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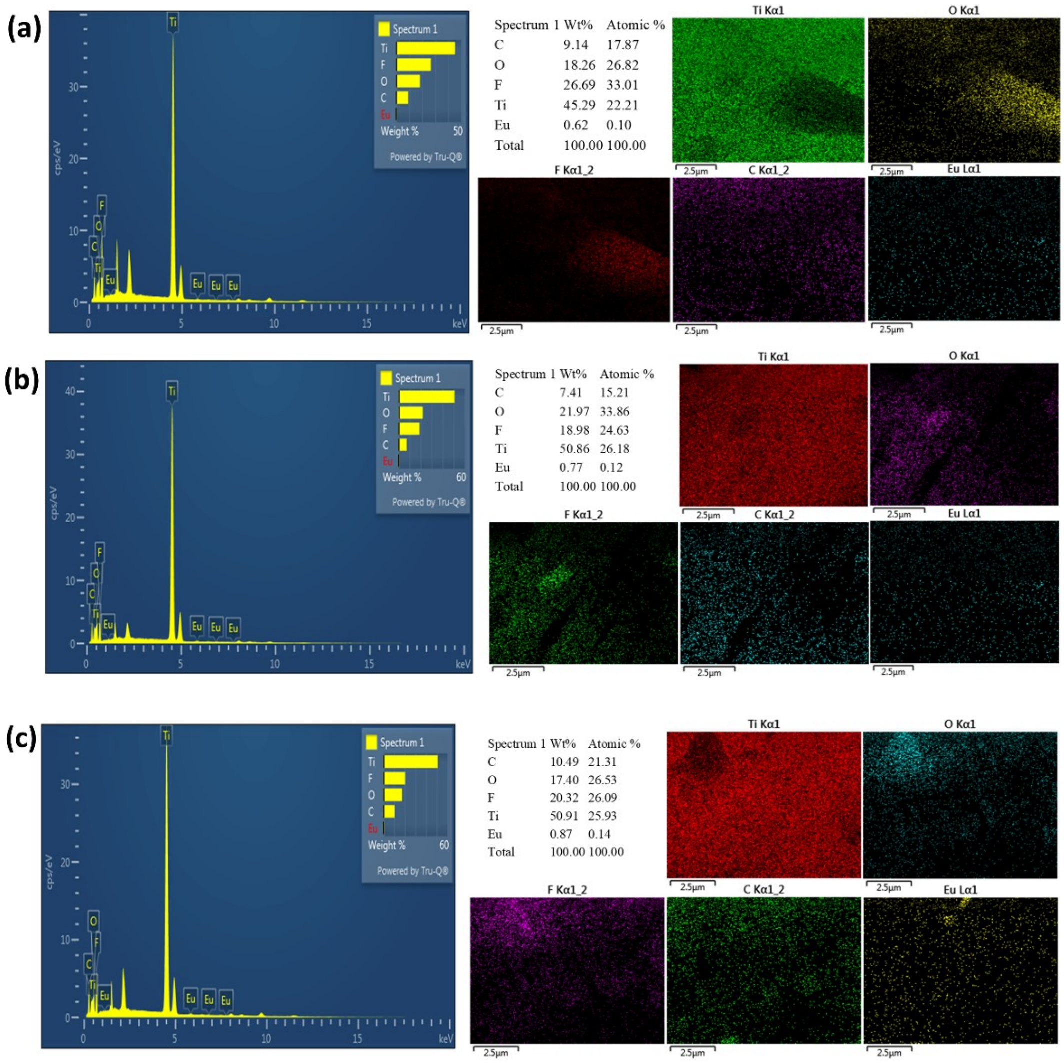

Figure S1. EDS spectra and elemental mapping for **(a)** 3-EuM, **(b)** 5-EuM, and **(c)** 7-EuM samples.

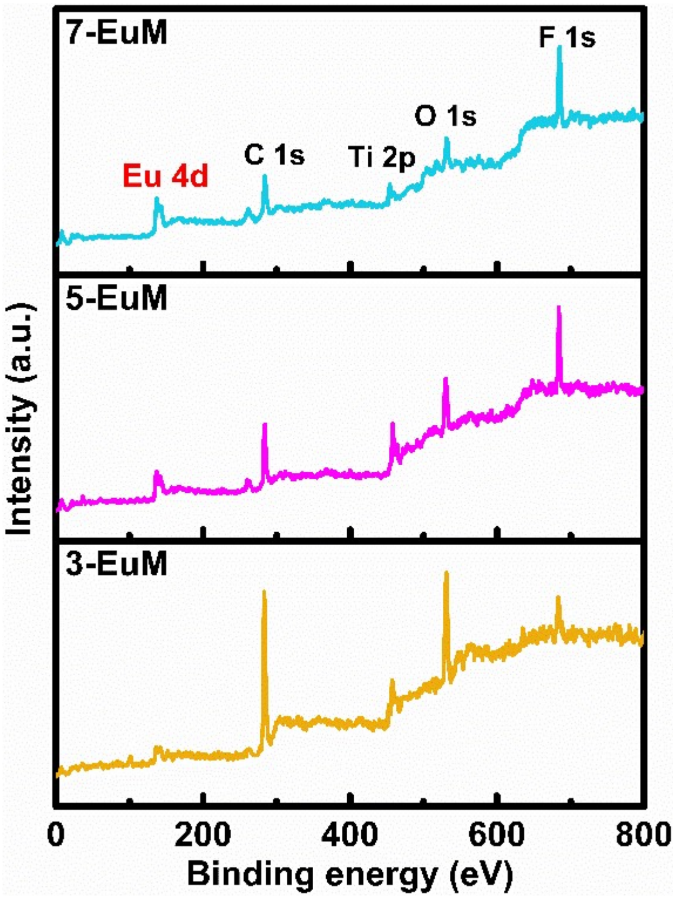

Figure S2. XPS survey scan spectra for 3-EuM, 5-EuM, and 7-EuM samples.

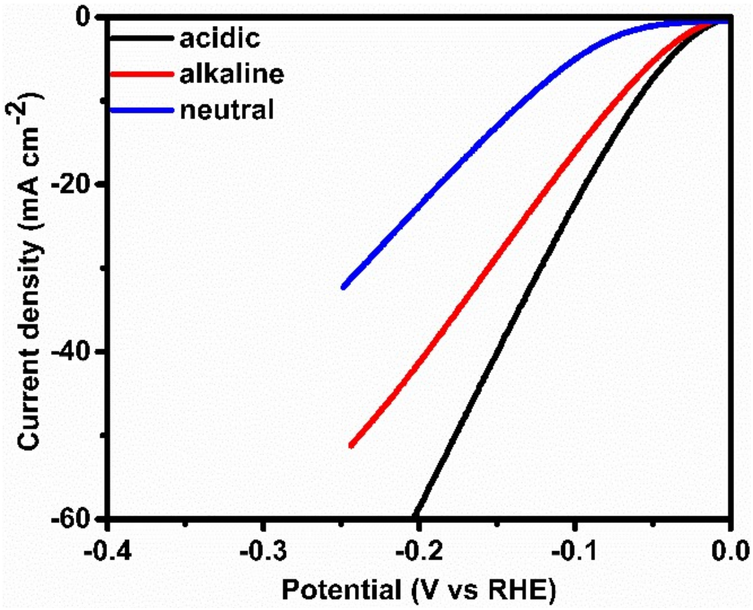

Figure S3. Comparison of LSV polarization curves of 5-EuM sample in acidic, alkaline, and neutral mediums.

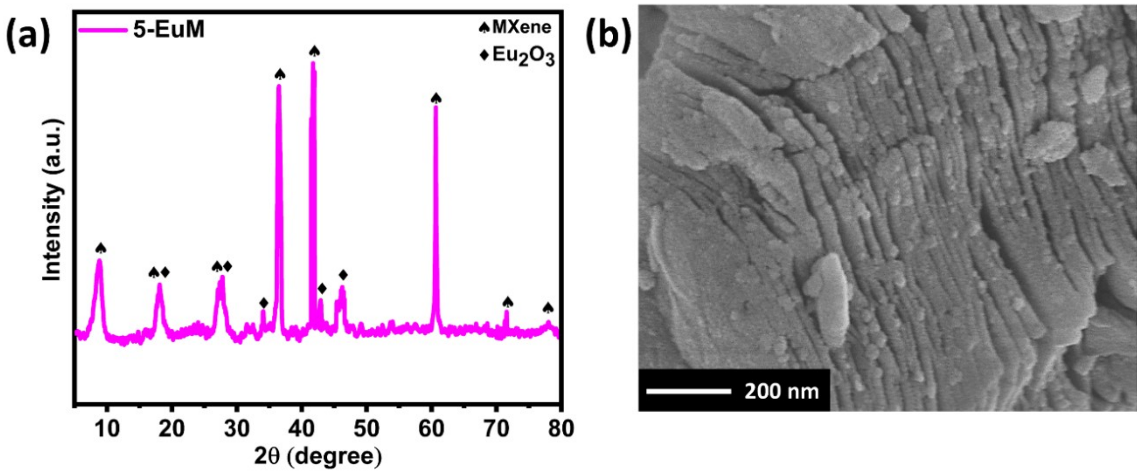

Figure S4. Post catalytic **(a)** XRD and **(b)** SEM image of 5-EuM sample.

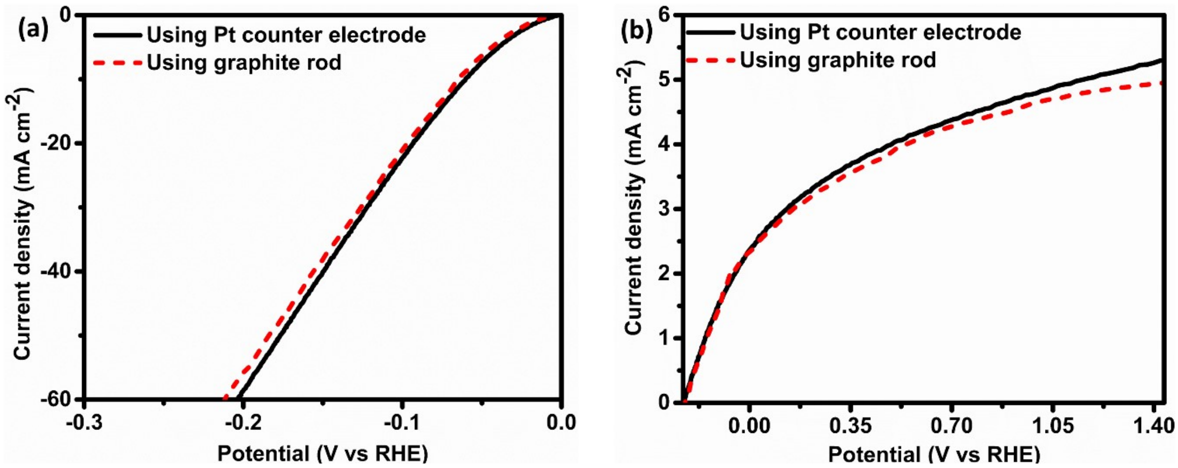

Figure S5. Comparison of LSV polarization curves **(a)** electrocatalytic, **(b)** photocatalytic using Pt and graphite rod counter electrodes.

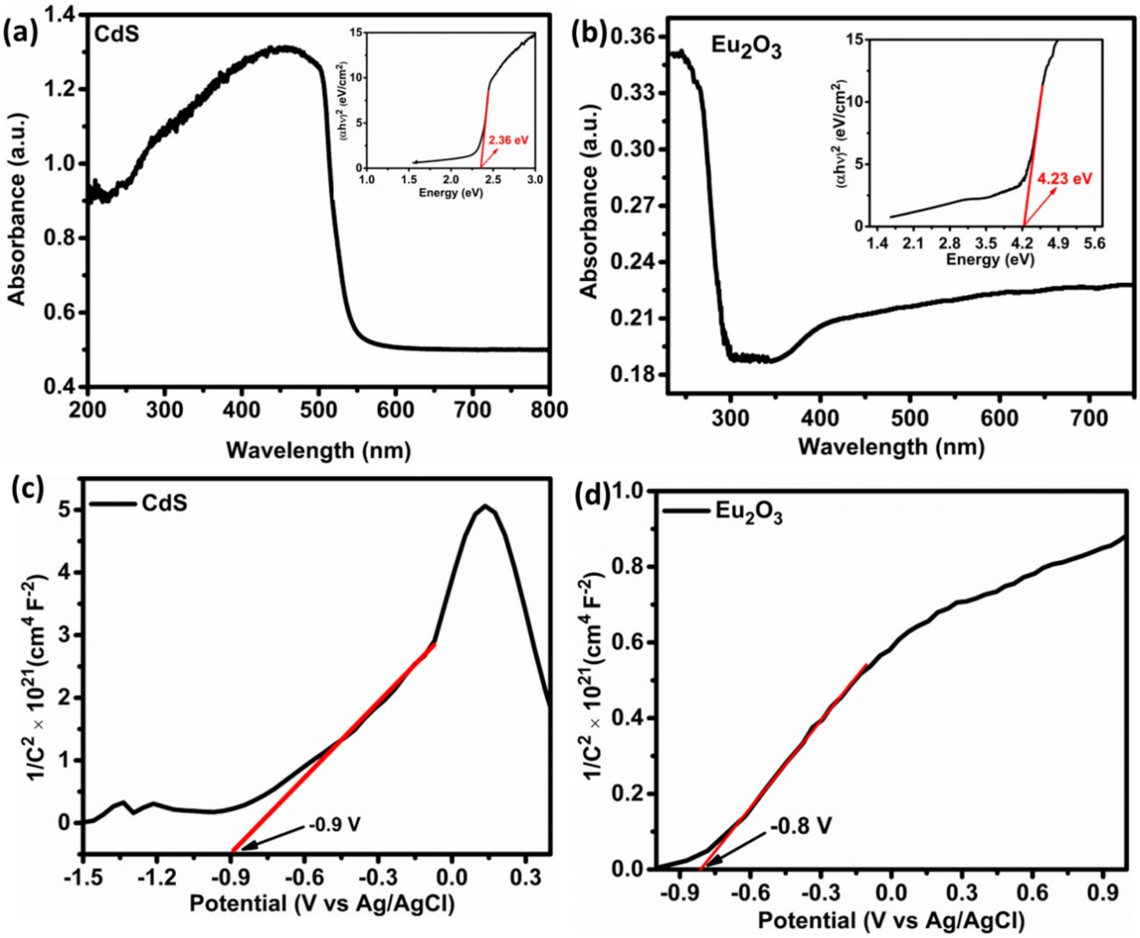

Figure S6. (a-b) UV-Vis absorption spectra of CdS and Eu_2O_3 and (inset) Tauc plot estimating the band gap values, (c-d) M-S plots for CdS and Eu_2O_3 estimating the flat-band potential (V_{fb}).

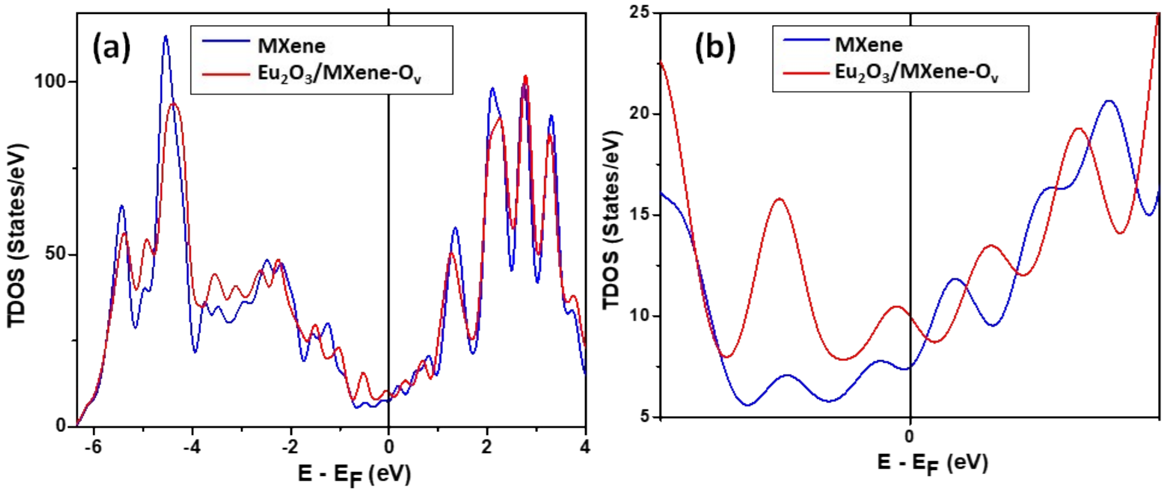

Figure S7 (a) Total density of states (TDOS) of MXene and Eu_2O_3/MXene-O_v, and **(b)** magnified view of the total density of states near the Fermi level.

Table S1. Comparison of water splitting and supercapacitor parameters for $Ti_3C_2T_x$ MXene-based catalyst.

Catalyst	Overpotential (mV)		Specific Capacitance	Current density	Reference
	HER	OER			
Ni_xCu_yMX–NF	111.0	185.2	380.86	0.5 mA/cm^2	1
WS_2/MC	-	307.0	305.45 F/g	10 mV s^{-1}	2
CTAB-rGO/MXene	179.0	360	544.5 F/g	0.5A/g	3
Na-MnO_{2-x}	439.7	381.2	395 F/g	5 mA/cm^2	4
$Ti_3C_2T_x$/NH_2-RGO/$MoSn_2Se_4$	-	-	120.2 F/g	1 A/g	5
$NiCo_2O_4$@$NiCo_2S_4$	59	201	1039 C/g	2A/g	6
MXene/MnO_2	-	-	242 F/g	1 A/g	7
Ni–NiO/$Ti_3C_2T_x$	72.0	248.0	-	-	8
Eu_2O_3/$Ti_3C_2T_X$ MXene	**63.0**	**169.0**	**374.98 F/g**	**0.6 A/g**	**This Work**

References

1 A. Raveendran, M. Chandran, M. R. Siddiqui, S. M. Wabaidur, S. Angaiah and R. Dhanusuraman, *Sustain. Energy Fuels*, 2024, **8**, 1509–1525.

2 M. Iqbal, N. G. Saykar, A. Singh, I. Ahmed, A. Arya, K. K. Haldar and S. K. Mahapatra, *Adv. Mater. Technol.*, 2024, **9**, 2301797.

3 A. Raveendran, M. Chandran, M. R. Siddiqui, S. M. Wabaidur, M. Eswaran and R. Dhanusuraman, *ACS Omega*, 2023, **8**, 34768–34786.

4 B. Thanigai Vetrikarasan, A. R. Nair, S. K. Shinde, D.-Y. Kim, J. M. Kim, R. N. Bulakhe, S. N. Sawant and A. D. Jagadale, *J. Energy Storage*, 2024, **94**, 112457.

5 S. De, S. Roy and G. C. Nayak, *Mater. Today Nano*, 2023, **22**, 100337.

6 Z. Sun, L. Sun, S. W. Koh, J. Ge, J. Fei, M. Yao, W. Hong, S. Liu, Y. Yamauchi and H. Li, *Carbon Energy*, 2022, **4**, 1262–1273.

7 Q. Wang, Z. Zhang, Z. Zhang, X. Zhou and G. Ma, *J. Solid State Electrochem.*, 2019, **23**, 361–365.

8 B. Zhang, Z. Du, R. Sun, X. Lai, J. Lan, X. Liu and L. Yan, *ACS Appl. Mater. Interfaces*, 2022, **14**, 47529–47541.