

Atomic-Level Design Principles for Hydrogen Evolution Reaction on High-Entropy MXene Catalysts

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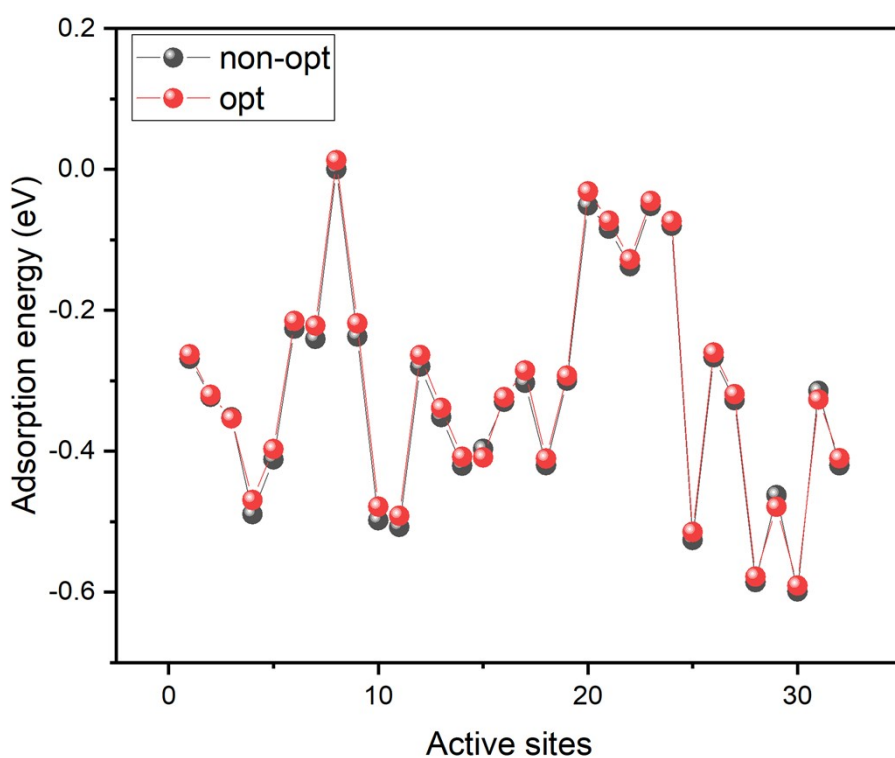


Figure S1. Comparison of hydrogen adsorption energies across 32 distinct active sites on the high-entropy MXene $\text{Ti}_{12}\text{Nb}_{17}\text{V}_{24}\text{Mo}_{11}$, evaluated using two different lattice constants: an optimized lattice ($a = b = 12.11 \text{ \AA}$, red) and a fixed lattice ($a = b = 12.16 \text{ \AA}$, black). Each data point represents the adsorption energy at a specific site. The close alignment between the two datasets indicates minimal sensitivity of hydrogen adsorption energy to lattice relaxation, validating the use of fixed-lattice approximations for high-throughput screening.

Table S1. Lattice constants and H adsorption free energies of selected MXenes and Pt.

	Lattice constant (Å)	ΔG (eV)
Ti ₄ C ₃ O ₂	3.04	-0.257
V ₄ C ₃ O ₂	2.92	-0.457
Nb ₄ C ₃ O ₂	3.15	0.363
Mo ₄ C ₃ O ₂	3.05	-0.387
Pt		-0.32

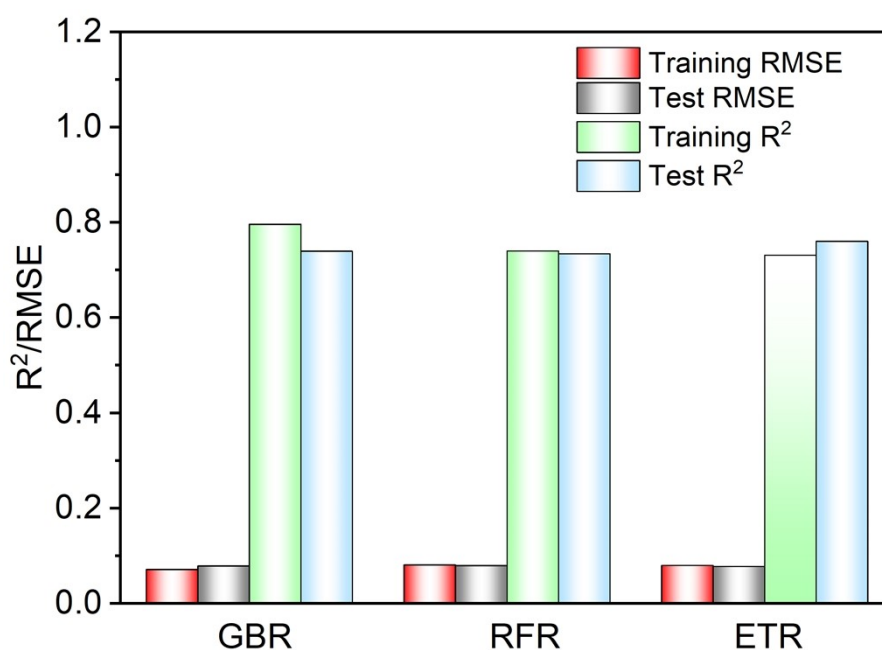


Figure S2. Comparison of predictive performance for three machine learning models: Gradient Boosting Regressor (GBR), Random Forest Regressor (RFR), and Extra Trees Regressor (ETR), evaluated using both training and test datasets. Bars represent four key performance metrics: Root Mean Square Error (RMSE) for training (red) and test sets (gray), and R² scores for training (green) and test sets (blue). A lower RMSE and higher R² indicate better model accuracy and generalizability.