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Machine Learning and DFT - Driven Design of MXene Compositions for Enhanced Hydrogen Evolution Reaction Performance

MXenes ($M_{n+1}X_nT_x$) are rapidly emerging class of 2D transition metal carbides/nitrides. With their enormous surface area, high electrical conductivity, and tunable surface terminations, MXenes are promising electrocatalysts for the Hydrogen Evolution Reaction (HER). The composition of MXenes with their chemical formula (Mn+1XnTx) and surface terminations, significantly influences their properties and subsequent applications. In this work, we integrate machine learning (ML) and density functional theory (DFT) to accelerate the discovery of HER-optimized MXene compositions. A curated dataset reported in the literature and DFT-calculated HER descriptions (ΔG_H*, overpotential, Tafel slope) was combined with elemental and structural features to train predictive ML models. The optimized models identified several promising candidates, including $Ti_3C_2O_2$, Nb_2CO_2, and $Ta_4C_3O_2$, with near-thermoneutral hydrogen adsorption free energies, overpotentials and tafel slopes. Stability screening based on formation energy and energy above hull suggests these materials maintain structural integrity under electrochemical conditions. This ML-guided approach significantly reduces the search space for high-performance HER catalysts and offers a framework for the design of MXenes for sustainable hydrogen production. The methodology and predicted compositions will be experimentally validated, bridging computational predictions with practical electrocatalyst development.

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