Atomistic Design and Engineering of Two-dimensional MXenes for Electrocatalysis

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MXenes, with their $M_{n+1}X_nT_x$ chemical formula, have one of the most diverse chemical compositions and structures among the family of two-dimensional (2D) materials. This notable compositional diversity, spanning across the transition metal carbides, nitrides, and carbonitrides, positions MXenes as potential material candidates for applications ranging from energy conversion and storage to biomedicine[1]. The rapid growth of the 2D MXenes family is driven by their tailorable surface chemistry, diverse compositions, structures, and architectures, including the transition metal and surface functional groups, non-metal X sublattice, and atomic-layer configurations [2]. This compositional diversity controls MXenes' structure-property relationships, which tailor their functional performance in various application domains [3,4]. In this talk, we will explore how variations in compositional diversity, atomic arrangement, atomistic design, and material engineering strategies enable the systematic fine-tuning of the properties of 2D MXenes and their applications in clean energy [2,4]. The discussion will center around the six key factors that play a critical role in tunability and controlling MXenes' performance for electrocatalysis, including composition (M, X, and T_x), the thickness of the 2D flake (number of atomic layers), lateral flake dimensions, surface adatoms, intercalating ions, atomic defects (e.g., vacancies), and heteroatom doping [2,4,5]. The discussion will highlight recent advances in the growing research on MXenes and offer forward-looking perspectives on leveraging MXene chemistry to develop high-performance 2D catalysts critical for achieving a carbon-neutral economy.

References

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Figures

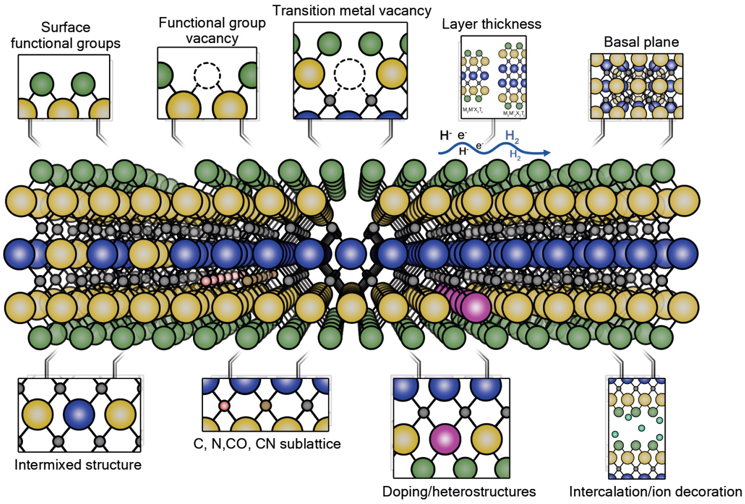

Figure 1: Strategies to tune two-dimensional MXenes for electrocatalytic and energy applications [2].