Insight into MAX Phases and their 2D MXenes: A First-Principles Perspective on Structures and Electronic Properties

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A wide range of 2D materials composed of transition metals have been extensively researched in the literature. Among them, MXenes have become a major focus in materials research, offering new opportunities in science and technology. MXenes are created through the chemical exfoliation of MAX phases — $M_{n+1}AX_n$ systems, where n = 1, 2, or 3, “M” is an early transition metal, "A" is A group elements, mainly groups 13 and 14 elements, and "X" is carbon and/or nitrogen — which belong to a large family of layered ceramics. The resulting 2D-$M_{n+1}X_n$ transitional metal carbides and nitrides are known as MXenes. With vast elemental compositional possibilities for MAX phase compounds, many MXenes with exceptional properties could potentially be discovered in the future. MXenes are anticipated to be utilized in electronic, optoelectronic, and energy devices. My research has been focused on exploring the exceptional features of these promising advanced materials. In this presentation, I aim to provide a comprehensive overview of the synthesis and applications of MAX phases and MXenes, while also delving into their structural and electronic properties from a first-principles perspective.