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A Panoramic View of MXenes via an Atomic Coordination-Based Design Strategy

Two-dimensional (2D) transition metal carbides and nitrides, known as MXenes, possess unique physical and chemical properties, enabling diverse applications in fields ranging from energy storage to communication, catalysis, sensing, healthcare, and beyond. Despite extensive research and notable advancements, a fundamental understanding of MXenes' phase diversity and its connection to their hierarchical precursors, including the intermediate MAX phases and the ancestral bulk phases, remains limited. Here, we hypothesize that the atomic coordination environments adopted by transition metal and nonmetallic atoms in their 3D bulk precursors may persist in 2D MXenes to govern their phase diversity. Using high-throughput modeling based on first-principles density functional theory, we unveil a wide range of MXene phases and comprehensively evaluate their relative stabilities across a large chemical space. The key to our approach lies in considering various atomic coordination environments drawn from four types of ancestral bulk phases. Through this comprehensive structural library of MXenes, we uncover general guiding principles, such as a close alignment between the phase stability of MXenes and that of their 3D precursors. We further observe that variations in atomic coordination also influence mechanical properties such as stiffness and elasticity, highlighting the broader impact of coordination environments on MXene functionalities. These findings introduce a new design strategy in which the atomic coordination environments in bulk phases can serve as reliable predictors for accessing a broadened landscape of MXenes.

Topical Area

Hard matter: quantum, electronic, semiconducting materials

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