From MAX phases to MXenes: A First-Principles Exploration

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Two-dimensional materials made from transition metals have garnered significant attention in recent years because of their extensive electronic, magnetic, and catalytic characteristics. Among these materials, MXenes stand out as a forefront area of materials research, opening up new scientific and technological possibilities. MXenes are produced through the chemical exfoliation of MAX phases, which are a class of layered ceramics characterized by the general formula $M_{n+1}AX_n$, where M represents an early transition metal, A denotes a group 13 or 14 element, and X signifies carbon and/or nitrogen. The selective removal of the A-layer from MAX phases by using weak acid solutins, leads to the creation of two-dimensional transition metal carbides and nitrides ($M_{n+1}X_n$), known as MXenes. These materials typically exhibit a range of electronic properties that vary based on the specific transition metal and the surface chemical ligands involved.[1-3]

Given the extensive range of compositional options available for MAX phase compounds, it is anticipated that a variety of MAX phases and MXenes with unique properties will be developed in the future, tailored for applications in electronics, optoelectronics, energy storage, catalysis, environmental remediation, and more. In this regard, first-principles calculations have provided significant insights into the structural stability, electronic properties, superconductivity, and the potential for synthesizing new MAX phases, as well as their exfoliation into MXenes. In this presentation, I will highlight the exceptional characteristics of MAX phases and MXenes from a firstprinciples perspective.

References

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