Structural and chemical tailoring of 2D MXenes

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MXenes constitute a family of two-dimensional transition metal carbides, carbonitrides and nitrides. MXenes are rapidly emerging as breakthrough materials in applications such as energy storage [1], water filtering, electromagnetic shielding[2], as catalysts for H2 evolution from water[3] and as astonishingly effective materials for capturing CO2. [4] Discovered in 2011, [5] the number of MXenes has expanded significantly and more than 20 different MXenes have been synthesized, with many more predicted from theoretical calculations. MXenes constitute an exceptional family of materials based on their availability for elemental alloying [1,6,7] and control of surface terminations, [4] which enables synthesis of a range of structures and chemistries. Consequently, the MXenes exhibit an unparalleled potential for tuning of the materials properties for a wide range of applications.

Using first principles calculations, theory guided synthesis, and characterization and tailoring by aberration corrected scanning transmission electron microscopy (STEM) in combination with X-ray photoelectron spectroscopy, we have explored some the range of structural and chemical modifications available in the MXene family.

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