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Structural design of large area two-dimensional transition metal carbides, MXenes

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MXenes (M=transition metal, X=C) are two-dimensional (2D) materials which have attracted extensive attention due to excellent properties for e.g. energy storage. Recently, theoretical calculations were reported where selected MXenes, depending on transition metal, are predicted to be direct bandgap semiconductors. Of particular interest is Mo_2C MXene, predicted to be a promising candidate for hosting topological states. Until now, the understanding of the electronic properties of this family of 2D materials is still in its infancy due to challenges associated with theoretical modelling as well as controlled synthesis of large area high quality samples allowing detailed transport studies. Here, we present high quality single layer Mo_2C MXene, obtained from thin film as well as bulk synthesis of parent 3D materials which have been subject to chemical etching. The materials are characterized by X-ray diffraction and transmission electron microscopy, showing a lateral sheet size exceeding 5 µm. We also present a novel approach for tailoring the structure as well as the chemistry of the MXene through alloying. Through first-principles calculations we predict that depending on choice of alloying element and its concentration, a MXene with in-plane chemical order can be stabilized. Furthermore, depending on choice of etching procedure, selective etching is suggested to induce a MXene with ordered vacancies. This has been experimentally verified for Mo_2C, and large area Mo_2C with ordered vacancy formation is presented. The obtained 2D material may be of importance for enhanced density of electrochemically active sites and improved ionic transport.

Keywords
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