MXenes: the largest family of 2D materials

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Two-dimensional (2D) materials have attracted huge attention in nanotechnology thanks to the enhanced low-dimensional quantum effects resulting in outstanding electronic, optical, and magnetic properties. Among these 2D systems, the emerging family of 2D transition metal carbides and nitrides, known as MXenes, stands out because of the wide chemical diversity allowing for materials property tuning. In contrast to graphite-like layered materials which can be mechanically exfoliated to obtain 2D flakes, MXenes are obtained from the chemical treatment of the three-dimensional MAX phases, represented in **Figure 1** [1,2]. MAX phases are layered ceramics with the general formula $M_{n+1}AX_n$, where M represents an early transition metal, A an element from groups 13 to 16, X either a carbon or a nitrogen atom, and n varies from 1 to 3 [3]. Since the discovery of the first MXene, $Ti_3C_2T_z$, at Drexel University in 2011, more than 30 MXenes have been synthesized, and the stability and properties of dozens more have been investigated using *ab initio* calculations [4]. The exploration of new MAX phases and derivative MXenes is of great interest to further control materials properties and highlight potential applications, such as catalysis, energy storage, and related electrochemical applications. In this talk, the different classes of MAX phases will be introduced and their potential exfoliation into their 2D counterparts, MXenes, will be discussed (**Figure 2**) [5]. Additionally, their respective structural, electronic, and elastic properties predicted by *ab initio* calculations and characterized by various experimental techniques will be discussed.

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FIGURES

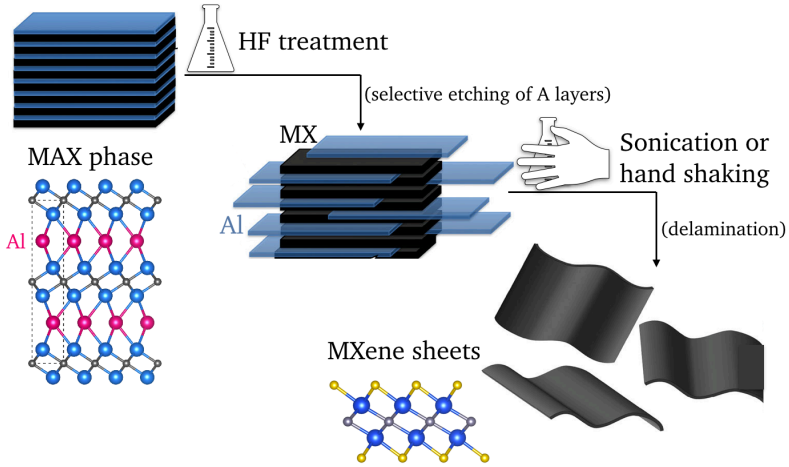

Figure 1: Schematic representation of the synthesis process of 2D MXenes, obtained from the selective etching of the Al planes from the parent 3D MAX phases when immersed in HF solution. Adapted from [2].

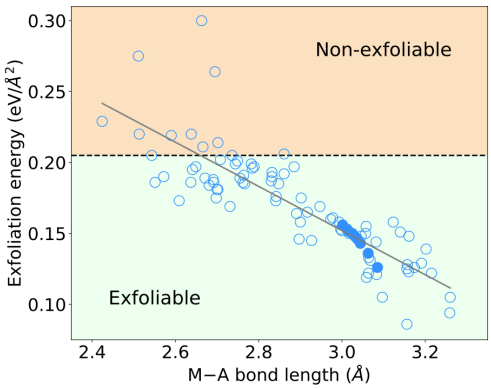

Figure 2: Computed static exfoliation energy as a function of the bond length for a series of ~90 MAX phases. Data from [6] are also presented (empty circle). Adapted from [4].