2D MXenes – Control of Properties through Surface Chemistry and Atomistic Design

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MXenes are a family of two-dimensional (2D) transition metal carbides and nitrides, with a general formula of $M_{n+1}X_nT_x$, where M is a transition metal, X is carbon and/or nitrogen, T represents the surface terminations (O, OH, halogen, chalcogen, etc.), and n = 2—5 [1]. More than 50 MXene compositions have already been reported, but the number of possible compositions is infinite, if one considers solid solutions and combinations of surface terminations. MXenes open an era of computationally driven atomistic design of 2D materials.

MXenes have shown electronic, optical, mechanical, and electrochemical properties that clearly differentiate them from other materials. Moreover, those properties are tunable by design and can be modulated using an ionotronic approach [2], leading to breakthroughs in fields from optoelectronics, electromagnetic interference shielding, and communication to energy storage, catalysis, sensing, and medicine. In several applications, such as electromagnetic shielding, MXenes have outperformed all other materials. In this talk, I'll discuss the synthesis and structure of MXenes, their optoelectronic and electrochemical properties, as well as coupling between electrochemical redox processes in MXenes and their optical properties, which can be monitored *in situ* using spectroelectrochemistry techniques [3].

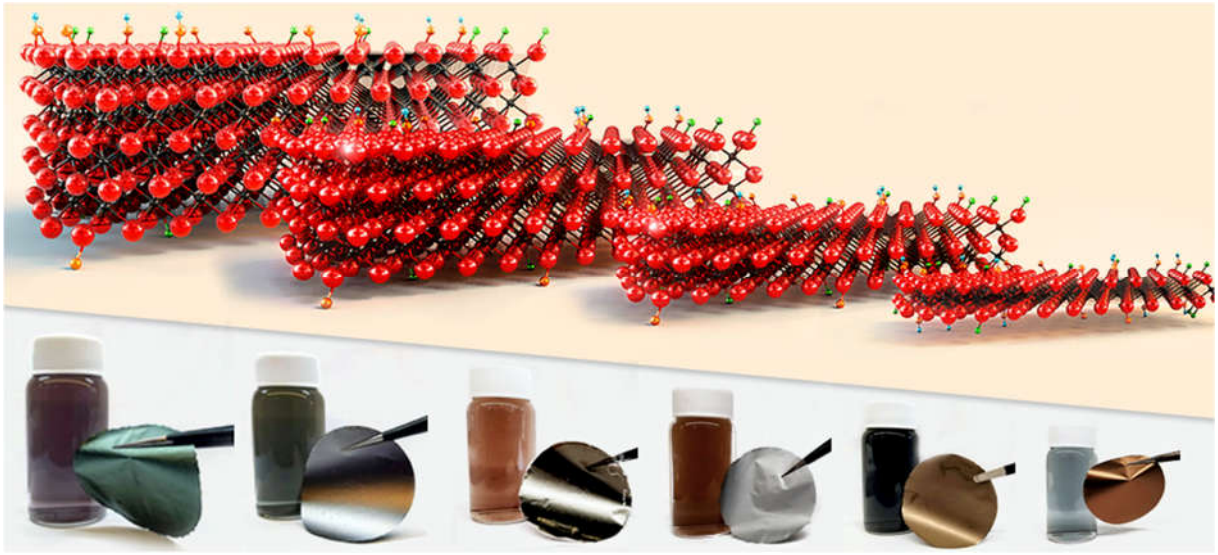

Fig. 1. Representative structures of MXenes (M – red, X – black) and samples of MXene films and colloidal solutions of 2D flakes showing a variety of colors, which originate from differences in optical absorption.

[1] A. VahidMohammadi, J. Rosen, Y. Gogotsi, The World of Two-Dimensional Carbides and Nitrides (MXenes), *Science,* **372**, eabf1581 (2021)

[3] M. Han, D. Zhang, C. E. Shuck, B. McBride, T. Zhang, R. (John) Wang, K. Shevchuk, Y. Gogotsi, Electrochemically Modulated Interaction of MXenes with Microwaves, *Nature Nanotechnology,* **18**, 373–379 (2023)

[2] D. Zhang, R. (John) Wang, X. Wang, Y. Gogotsi, *In situ* monitoring redox processes in energy storage using UV-Vis spectroscopy, *Nature Energy*, **8**, 567–576 (2023)