https://doi.org/10.1038/s41565-022-01238-6

The pull of the MXene vortex

First synthesized in 2011, MXenes are two-dimensional materials currently generating a whirlpool of interest.

The term MXenes (pronounced 'maxenes') was first introduced in 2011[1] by Naguib et al. to indicate the exfoliated material obtained from a MAX bulk phase. A MAX phase (general formula $M_{x+1}AX_n$, with $n = 1–4$) is a ternary carbide or nitride (X = C, N), with M an early transition metal and A an element from groups 13 or 14 of the periodic table. An important MAX phase material is Ti_3AlC_2. To make the corresponding MXenes, Naguib et al. treated it with HF, which extracts the Al layer from the crystal structure, exposing the Ti atoms to possible chemical functionalization. In the first report, functionalization consisted of either F atoms or OH groups (after reacting with water). A sonication step then led to exfoliation into nanometer-thick crystal layers of the corresponding Ti_3C_2 MXene (general formula $M_{x+1}X_n$).

Since then, the MXene family has increased to more than 30 members, with compositions predicted computationally now reaching over a hundred. According to Web of Science, the number of papers with 'MXene' in the abstract has been steadily increasing in the past 10 years (Fig. 1). A prominent figure in the field, and probably one of the reasons behind the success of this family of 2D materials, is Yury Gogotsi, a Ukrainian-born scientist working at Drexel University in Philadelphia. His group, in collaboration with Michel W. Barsoum, and collaborators from Linkoping University in Sweden, reported the first MXene in 2011[1]. Gogotsi recalls the enthusiasm in his group after the successful exfoliation and characterization of the new nanomaterial: "We understood right away that 2D Ti_3C_2 was just the beginning of something very promising. Although we didn't have any funding for it at the time, everyone in my and Barsoum's lab wanted to work on MXenes – we called it, the MXene vortex". This centripetal excitement seemed justified for a number of reasons that became clearer as experimental evidence piled up in the following months and years.

First and foremost, Ti_3AlC_2 was just one of the more than 60 layered MAX phases known at the time that seemed to be just waiting to be transformed into the corresponding 2D MXene. Second, the possibility to chemically functionalize the end group added a whole new layer of possibilities; so much so that now the general formula has become $M_{n+1}X_nT_x$ ($n = 1–4$), where T_x identifies surface termination. Third, the fact they are water soluble made it easy to work with using colloidal chemistry techniques. Fourth, the surface functionalization did not seem to disrupt their electronic properties; on the contrary, many MXenes are metals or semimetals for which the Fermi level could be tuned through the composition of the surface termination group. Gogotsi wanted to take the 'MXene vortex' out of his lab and into the world. So, he started to share samples and expertise with many collaborators domestic and abroad. And indeed, he seems to have succeeded. "With each new paper, it felt like a small community formed" he says.

The large versatility of MXenes, both in composition and functionalization, is what differentiates them from other exfoliated nanomaterials, like graphene, hexagonal BN and transition metal dichalcogenides. However, this versatility is both an advantage and a curse, because it becomes hard to identify the best composition and functionalization to maximize properties for a targeted application. Gogotsi believes this is a solvable problem. He and his collaborators have pulled resources to run sophisticated density functional theory, ab-initio and multiscale calculations to find the best MXene, or at least narrow down the choice, for a desired property[2].

Speaking of applications, most MXenes papers currently target energy storage and catalysis applications. Gogotsi however feels that optoelectronics is where the most promising applications are lurking, owing to their high electronic conductivity and tunable work function. In a paper in 2016[3], Gogotsi and Chong Min Koo, from the Korea Institute of Science and Technology, showed that a 45-μm-thick $Ti_3C_2T_x$ film could block 99.99999994% (or ~92dB) of an incident electromagnetic wave between ~8–12 GHz. Materials for electromagnetic interference (EMI) shielding in that frequency range are hotly researched by the telecommunication industry as the adoption of 5G networks and the deployment of the Internet of Things widen.

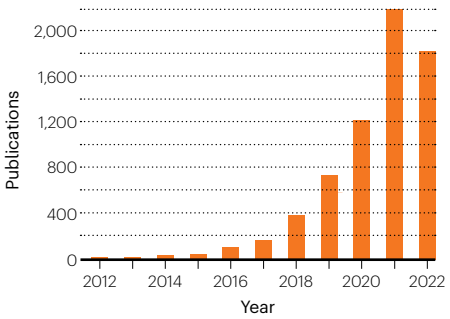

Fig. 1 | Number of publications with 'MXene' in the abstract. Source: Web of Science.

Additionally, because of their high electrical conductivity and possibility to form stable colloidal solutions in water, MXenes are also set to play a role in printable inks for flexible electronic devices and transparent electrodes.

The remarkable growth of research interest in MXenes risks creating a hype. An issue the community is currently grappling with is the need to better control the synthesis of the material, in terms of the composition, size and thickness of the flakes, develop more robust termination methodologies, and ultimately scale-up production moving away from HF. The proliferation of results without a clear protocol for the synthesis and characterization of MXenes is an issue the community could face in light of the increasing number of researchers embracing these materials. To protect the field from this happening, Gogotsi has created online courses and published several educational-type articles with what he believes are the best practices in the field[4,5].

MXenes are but the latest of a number of materials that nanoscience has fashioned with the unique, enticing feature of precision control; that is, the idea that by working at the atomic or molecular level, it will be possible to create a material with tailored properties sporting fine control of the structure-function relationship from the bottom-up.

Published online: 11 October 2022

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