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ABSTRACTS BOOK

MXenes - Atomistically Designed Materials for Future Technology

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2D carbides, nitrides, and related structures, known as MXenes, are the most structurally and chemically diverse family in the materials flatlands. They can be designed atom by atom into a variety of structures using over a dozen transition metals and rare-earth elements on the M site; carbon, nitrogen, and oxygen on the X site; and a dozen elements (halogens, chalcogens, and pnictogens) as surface terminations (T*x*).

The family can be broadened further by adding 2D borides, silicides, and MXeneoids. Such diversity and compositional/structural complexity were unknown in the inorganic materials world until recently.

Since the discovery of $Ti_3C_2T_x$ in 2011, more than 50 stoichiometric MX compositions and dozens of solid solutions have been reported. The number of MXenes is infinite when considering solid solutions, high-entropy compositions, in- and out-of-plane ordered structures, and combinations of surface terminations. MXenes can be synthesized directly from metal halides and carbon sources or by selectively etching layered ceramics in aqueous etchants, molten salts, or halogen-containing gases.

MXenes have ushered in an era of computationally driven atomistic design of 2D materials. MXenes complement graphene, transition metal dichalcogenides, and other 2D materials by offering high metallic conductivity, electrochemically active surfaces, and extreme strength. More importantly, the optical and electronic properties of MXenes can be tuned and modulated during use. Demonstrated properties include chemically tunable superconductivity, work function, electromagnetic interference
(EMI) shielding effectiveness, and electrical and optical properties. These properties can be modulated optically or via an ionotronic approach, enabling breakthroughs in fields ranging from optoelectronics and EMI shielding to communication, energy storage, catalysis, sensing, and healthcare.

In this keynote lecture, I'll discuss how structure and composition influence MXene properties. I'll also outline prospects for MXene applications in electronics, healthcare, thermal management, communications, and energy generation and storage.

Towards the sustainable synthesis of MXenes: self-propagated synthesis of MAX phases

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Today's price for a kilogram of MAX phase is more than tenfold the price of the starting powders – and MXene suspensions are about tenfold the price of MAX phases. Due to their energy intensive nature, the processes necessary to produce MAX phases are among the crucial points making MXenes expensive materials. During the first two decades of the 21st century, MAX phases have been produced through three powder metallurgy routes: sintering processes, mechanochemical synthesis and self-propagated synthesis. Sintering consists in heating the starting powders to activate diffusion which requires about an hour of heating and therefore a significant amount of energy especially for large scale production. Mechanochemical synthesis relies on the cold welding and mechanical to thermal energy conversion due to balls impact on the starting powder mix, necessitating a continuous movement of the mill for tens of hours which is energy consuming. While sintering is preferred to produce very pure MAX phases, mechanochemical synthesis induces contamination and the formation of secondary phases and is usually used in combination with the later. Recent development such as solid-state reaction/molten salts synthesis tend to reduce the reaction temperature and simplify it, however the reaction times remain long. Self-propagated high-temperature synthesis (SHS) consist of the initiation of the MAX phase formation reaction by a short but intense heating of the mix and the propagation of the self-sustaining reaction. Due to its nature, SHS is hard to control and usually suffers from quite low purities (85-90 %), however its low energy consumption and easy setup illustrated in figure 1A is a strong point in favour of their development.

The research we are developing at the Laboratoire des Sciences des Procédés et des Matériaux (Université Sorbonne Paris-Nord) focuses on the elaboration of large quantities of high-purity MAX phase powders by SHS reactions and the subsequent exfoliation by HF-free methods. So far, we worked on the synthesis of titanium aluminium carbide (Ti3AlC2/Ti2AlC) and titanium tin carbide (Ti2SnC), and now extending our scope to the synthesis of molybdenum- and chromium- based MAX phases. While purity is still a challenge, promising results were obtained through a single step reaction as showed by the nicely elongated grains in the SEM micrograph in figure 1B.

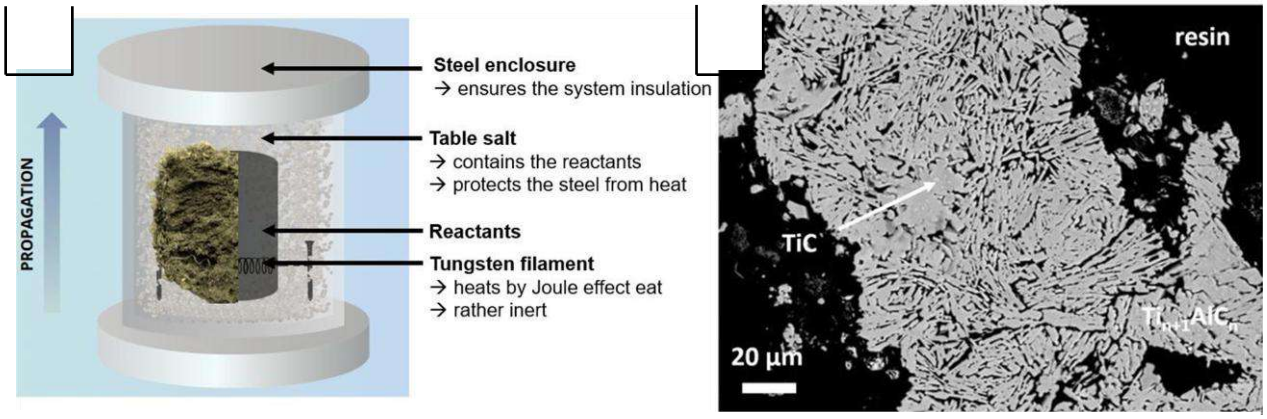

Figure 1: A) SHS reactor setup with sample image, B) SEM micrograph of titanium aluminium carbide by SHS (metallic route).

Ultrathin films of Ti3C2Tx MXene via interfacial assembly: effect of synthesis method on thickness and surface roughness

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MXene ultrathin films are promising for optoelectronic applications, as they have a high transmittance in the visible range and high conductivity. Furthermore, the hydrophilic nature of Ti3C2Tx MXene produced via wet etching has deemed it attractive for creating interfaces with biomolecules. An emerging application which warrants the above properties of MXene is its use in single-molecule biosensing [1], [2]. Such applications often require that both the roughness of the interface and the thickness of the film are low, so as to not interfere with the quality of the biointerface [3] and with the sensitivity of the sensing method, respectively. This requires nanometer-scale control over the morphology of films produced from these solution-processed materials, which exhibit polydispersity in 2D-flake size and thickness. Conventional top-down approaches for thin film deposition like spray coating and spin coating often result in poorly packed films of non-uniform thicknesses [1], [4]. To obtain compact, ultrathin films, we employ an interfacial film assembly (IFA) method which has been shown to produce large-area, defect-minimized films with single to few layer coverage [5], [6]. However, these works do not take into account the inherent heterogeneity of the MXene nanosheet inks used for film assembly, whose properties depend greatly on their synthesis route [7], [8].

In this work, a semi-automated IFA method at the liquid-liquid interface [9] was used to produce thin films of Ti3C2Tx MXene synthesized via three different methods: standard HF-based synthesis or “STAN” [10], soft delamination or “SOFT” [11] and minimally intensive layer delamination or “MILD” [12]. We chose inks which exhibit different degrees of variation in lateral flake size, which may affect the surface roughness (larger the flake size, lower the inter-flake overlapping regions in the film) and reported monolayer yield, which would impact the overall thickness of the film. Here we show that interfacial assembly is a reliable method to produce densely packed, sub-5 nm films from a range of colloidal flake dispersions of MXene. The thickness distribution of the nanosheets comprising the films and the surface roughness of the films, characterized via atomic force microscopy, show noticeable variation across the three types of films. Of those, films assembled with ink from the MILD synthesis route are observed to have the lowest thickness (50% monolayer coverage) as well as surface roughness (4.24 nm RMS over a 400 μm2 area). In contrast, films made with the SOFT ink have only 20% monolayer coverage and a high surface roughness (17.32 nm RMS). Films produced from the STAN route exhibit properties in

between the former inks with 24% monolayer coverage and a surface roughness of 9.2 nm. While the large lateral flake sizes of the SOFT ink make it ideal for single-flake electronics [11], its low monolayer yield results in films with large thickness variations. On the other hand, the presence of particles (approximately 30 nm mean thickness) in the STAN films results in a higher surface roughness. Hence, the MILD films make a suitable choice for applications requiring optical transparency and precise control of surface morphology. This study therefore establishes a foundation for engineering optimal MXene-based substrates, placing emphasis on selection and optimization of the source ink formulations for thin film development.

Surface Diffusion Liquid Metal Chemical Vapor Deposition for controllable growth of Nb2C MXenes.

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Chemical vapor deposition (CVD) is a promising alternative for wafer scale synthesis of transitional metal carbides or nitrides, i.e., MXenes. Unlike conventional top-down approaches, such as selective etching of MAX phases, CVD offers a bottom-up growth pathway that overcomes the use of hazardous etchants that typically results in unwanted surface functional groups and facilitates scalable, high yield and controllable MXene thickness.[1] Current CVD methods enables direct MXenes synthesis using two main approaches: i) traditional gas-solid precursor CVD and; ii) liquid metal CVD. In traditional CVD, gaseous precursors (e.g., $TiCl_4$ and CH_4) interacts with solid Ti substrate to yield Cl terminated MXenes. This has led to vertically aligned or three-dimensional flower-like morphologies of Ti_2CCl_2 and Ti_2NCl_2.[2] [3] This approach produces high quality and scalable MXenes, but it suffers from chlorinated surface terminations. In liquid metal CVD method, a catalyst metal (Cu) sits on a precursor transition metal substrate (e.g., Mo). When heated at high temperatures, the precursor diffuses into the liquid catalyst, reacting with carbon generated from the breakdown of hydrocarbon gases like CH_4 and facilitates regulated nucleation and lateral expansion of high quality 2D crystals.[4] This method can produce well-defined large area 2D termination free MXenes with controllable thickness by adjusting parameters such as catalyst thickness, CH_4 flow rate, growth temperature and growth time. However, further advancements of CVD methods for growing MXenes require overcoming alloy-related challenges and achieving better control over the diffusion process. In this work we present a novel surface-diffusion liquid metal CVD (SDLM-CVD) method for the direct synthesis of bare, few-layer Nb2C MXene. Nb2C is an emerging and promising MXene candidate for applications in energy storage, sensing, catalysis, and biomedicine. Unlike conventional CVD growth mediated by bulk diffusion in immiscible alloy systems, our approach employs a surface diffusion mechanism on liquid copper using a homemade showerhead CVD reactor. Our SDLM-CVD reactor ensured a uniform carbon concentration and Nb flux by adjusting the distance between the Nb source and substrate. Our results demonstrate the correlations between the growth parameters and crystal morphology, indicating that high-quality 2D Nb2C large-scale MXene films are achievable. We obtained ultra-thin, 2D layered and single crystalline Nb2C flakes with a trigonal structure. Moreover, triangular MXene flakes were found to self-assemble into large hexagonal islands that later merged into continuous films. Density functional theory calculations explained the mechanisms of the growt hand self-assembly behaviour. In summary, our SDLM-CVD system offers new opportunities to control and produce large-area and ultra-thin MXene flakes and films.

Keywords: MXenes, CVD, Lateral growth, 2D materials, Large Scale Synthesis

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X-Site Dependency of Optical and Electronic Properties in Ti3(C2-yNy)T*x* Carbonitride MXenes

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Abstract
While MXene properties are commonly tuned through M-site and surface termination engineering, systematic X-site substitution remains comparatively underexplored despite its unique potential to independently modulate bulk and surface electronic properties. Here, we demonstrate controlled carbon-to-nitrogen substitution in Ti3(C2-yNy)T*x* solid-solution MXenes, where a systematic X-site compositional change was achieved, including Ti3C2T*x*, Ti3C1.75N0.25T*x*, Ti3C1.5N0.5T*x,* Ti3C1.25N0.75T*x*, and Ti3CNT*x*, allowing for a direct correlation of X-site composition with their optical and electronic properties.
Systematic variation in X-site stoichiometry was found to influence multiple physicochemical properties simultaneously, often in nonintuitive and decoupled ways. Increasing nitrogen content led to a higher preference for halogen surface terminations, suggesting that nitrogen substitution renders the metal atoms more electropositive and stabilizes bonding to less directional halogen species relative to strong M=O bonds. The delaminated MXenes remained readily dispersible in water and exhibited a monotonic blue-shift in optical absorbance alongside enhanced light-matter interaction across the UV-vis-NIR range with increasing nitrogen content. Electrical conductivity decreased systematically (from 11,700 to 1,250 S cm-1) with increasing nitrogen substitution, consistent with decreased free-carrier concentration. Despite these pronounced optoelectronic variations, the work function remained nearly invariant (4.0 - 3.8 eV, in UHV and air) across all compositions, indicating that M-site and surface terminations are the primary determinants of the work function. Overall, X-site substitution is shown to strongly modulate bulk optical and electrical transport properties while leaving the surface-controlled work function largely unchanged. This reveals X-site engineering as a distinct and underutilized design lever in MXenes, enabling decoupled tuning of bulk and surface functionalities. Solid-solution carbonitrides therefore provide a promising pathway to tailor light-matter interactions and electronic behavior without substantially altering surface electronic energetics, opening new opportunities for rational MXene design in optoelectronic and energy-related applications.

Structural editing of layered transition metal carbides

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Key words: MAX phases; MXene; intercalation; delamination; Lewis acid molten salt;
Intercalated layered materials are usually produced by inserting guest species into the van der Waals (*vdW*) gaps of inherently layered materials such as graphite, hexagonal boron nitride (hBN), and transition metal dichalcogenides. The guest-host interaction alters the

electronic structure and enables property tailoring for energy storage, catalysis, electronic, optical, and magnetic properties. Intercalation in non-van der Waals (non-*vdW*) nanolaminated materials and their two-dimensional (2D) derivatives is, however, rare and lacks understanding of the chemistry and structural tunability involved. Here, we show a structural editing protocol for non-*vdW* layered ternary carbides and nitrides (known as MAX phases) and their *vdW* multilayer derivatives (MXenes). Gap-opening and species-intercalating stages are separately mediated by chemical scissors and guest intercalants, respectively. A large family of 3D MAX phases with unconventional components and structures as well as 2D MXenes with versatile termination species, is accomplished. Moreover, a reverse transformation from 2D MXenes to 3D MAX phases is realized through knockout of surface termination species by metal scissors and stitching of ceramic slabs by zero-valence metal atoms. This scissor-mediated structural editing would enable structural and chemical tailoring in a broad class of layered ceramics.

Bubble-assisted electrochemical synthesis of MXenes

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MXenes are fascinating materials that have gathered attention for diverse applications, from energy storage to biosensing. MXene are often produced with methods that require the use of hydrofluoric acid (HF). In the effort to decrease the use of toxic and hazardous substances, diverse synthesis routes have been explored. Electrochemical synthesis of MXene is a sustainable alternative, however, it often suffers from poor yield or control over the etching, resulting in large number of byproducts.

Recently, we have developed a novel electrochemical synthesis method which exploits the controlled formation of surface nanobubbles on the working electrode to deliver high quality electrochemical MXenes (EC-MXenes). [1,2]

The formation and eruption of SNs at the electrode interface restore the electrochemical activity, expanding the yield efficiency and improving the overall quality of the final product, which has been confirmed with extensive surface analytics (e.g., XPS, XRD, Raman). [1]

EC-MXene present the crystallographic (TEM), topographical (AFM), and nanomechanical (AFM) signatures of classic MXenes, however, their interface is populated with a low density of F- terminations, as appreciated with low energy ion scattering. [1]

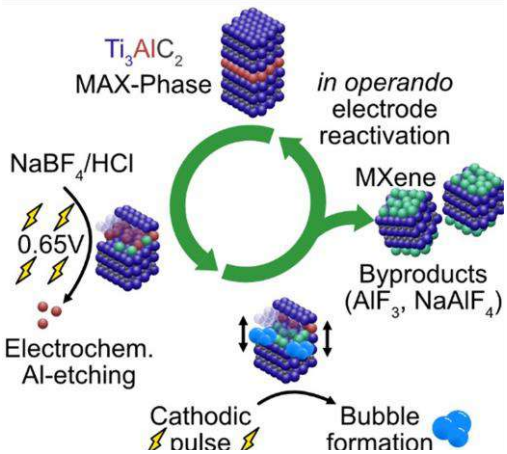

Figure 1 Bubble-assisted electrochemical synthesis of MXenes [1]

In addition, EC-MXene are able to function as solid lubricant, presenting a competitive coefficient of friction. [2] Surface analytics of the wear tracks and DFT calculation allowed us to propose a model to describe the mechanism drive the tribological performances. In a nutshell, it is critical to secure material transfer through adhesion on the counter surface to exploit the interlayer sliding of EC-MXene. [2]

In this talk I will present how interface science helped us achieving an important milestone in electrochemical synthesis of MXenes, showcase their tribological applications. Moreover, I will provide further information on our current research results in the direction to better

understand key questions such as how do SNs really interact at the MAX electrode during synthesis, or what are the nanomechanical properties of EC-MXene single flakes.

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MXenes: History, Science, Applications and Hype

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At this juncture there is no doubt that MXenes have captivated the world's interest and with good reason. The number of potential applications is quite numerous and diverse. The use, or addition, of MXenes can boost some properties sometimes to record levels; in other cases, it allows for herewith new applications for 2D materials. Their chemical diversity is also a huge attractor. In this talk I compare MXenes' stage of development with other high touted nanomaterials from bucky balls to graphene. I also differentiate between work done in the name of science that has little chance of applicability and other work that may lead to applications. As MXenes - like other new materials - get more popular, they are accompanied by hype. With hype comes responsibility. Hyping, or overpromising, is bad for the field in general and should be curtailed. The fundamental, and quite difficult problem to solve, with MXenes is that because we are dealing with essentially a few – 2, 3, 4 - of highly reactive transition metals layers interleaved with C or N, it will be quite difficult to render them oxidation resistant for extended times. It follows that applications where MXenes are placed in open, aqueous-based systems will be few and far between. Hyping such applications - while not simultaneously solving the stability conundrum for times commensurate with the time of use in said applications - is irresponsible since they fall under the purview of science. Another example of hype is work on MXene-based supercapacitors. To date, most of supercapacitor work on MXenes makes use of dilute aqueous-based electrolytes such as sulphuric acid. We have shown that in such electrolytes, the self-discharge rate is quite high which, in turn, would again greatly limit the scope of applicability of such devices. Other potential pitfalls will be discussed.

MXene Synthesis via Selective Gas-Phase Etching of MAX Phases

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The rise of two-dimensional (2D) transition-metal carbides and nitrides (MXenes) has allowed significant advancements in various fields such as energy storage, communication, electronics and healthcare. MXenes are traditionally synthesized using wet chemical selective etching of MAX phases that involves hydrofluoric acid (HF) or fluoride salts, which produce mixed O/OH/F surface-terminations. This work demonstrates a route for synthesis of various MXenes by gas-phase selective etching of MAX phases, allowing a safer and highly scalable approach that also reduces a water consumption. In-situ generated hydrogen chloride (HCl) vapor selectively removes the Al layer from the MAX phase. The synthesized Ti3C2Cl2 MXene was subsequently characterized using XRD, SEM, EDS, XPS, and Raman spectroscopy, confirming that the MXenes produced by this method have uniform halogen terminations, similar to those synthesized using the molten salt etching of MAX or chemical vapor deposition. Additionally, we demonstrated the successful etching of Ta4AlC3, Ti2AlC, Nb4AlC, Nb2AlC, and various carbonitride MAX phases, which are difficult to etch in acidic solutions. Furthermore, this technique can be used to produce multi-gram batches of MXenes, proving the scalability of the developed method. We anticipate that this novel gas-phase etching route will unlock the potential for unconventional MXene compositions to be produced from a variety of MAX phases.

Purpose-Driven Tailoring of MAX Phase and MXene Synthesis

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Since the discovery of MXenes in 2011, a variety of methods have been used to etch MXenes.
The most prominent among them are HF etching, in situ HF etching (usually using a mixture of hydrochloric acid and fluoride salts), and molten salt etching. Similarly, production of precursor MAX phase powders has been refined to produce high-quality powders with no competing phases, such as other MAX phases or binary carbide phases, and also to reduce MAX phase defects. An important development by Mathis et. al. in 2021 showed that adding a large excess of aluminum to Ti3AlC2 precursors led to a MAX phase that was highly pure and had reduced defects, thus providing a more stable MXene product. However, this method is not without its drawbacks. It requires extra aluminum, extra processing time to wash away the extra aluminum, and has proven harder to etch. Furthermore, while the MXene produced is very stable, it does not perform well for many post-processing functionalizations and other reactions. Here we have produced MAX phases with various amounts of extra aluminum to probe an optimal stoichiometry for stability, yield, and functionalizability. We have also expanded the stabilizing e□ects of extra aluminum to the carbonitride MXenes Ti2AlC0.5N0.5 and Ti3ALCN, showing that this is a good way to extend the stability of these notoriously more unstable phases.

Structural Engineering and High-Precision Inkjet Printing of Ti3C2Tx MXene Nanocomposites for Advanced RF Metadevices

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The integration of MXenes into next-generation radio-frequency (RF) systems requires both precise electronic modulation and scalable, high-fidelity manufacturing. In this work, we present a dual-pronged advancement: the development of structurally tunable MXene-biopolymer nanocomposites and high-stability organic inks for precision inkjet printing.
First, we demonstrate a highly tunable MXene-lignin architecture for RF metasurfaces. By tuning the sub-nanometer structure, we established a definitive negative correlation between the Hermans orientation factor (*f*) and the composite sheet resistance (*R*s). This structural control allows for the deterministic fine-tuning of electronic properties; while standard MXene composites typically exhibit broadband reflection, our *R*s-optimized layers facilitate a high-contrast narrow-band transparency at target RF frequencies. This selective transmission is highly promising for the development of frequency-selective surfaces and advanced RF modulators.
Complementing this structural tuning, we address the challenges of device integration through a novel additive-free organic solvent-based MXene ink designed for direct inkjet printing. This formulation offers superior colloidal stability and a significantly longer shelf life under ambient conditions compared to traditional aqueous or organic analogs. Utilizing the high-precision deposition capabilities of inkjet printing, we achieved high-resolution patterns on diverse substrates with excellent electrical continuity and uniformity. We demonstrate the versatility of this approach through the fabrication of various DC and RF components, ranging from transparent conductive coatings and thermal heaters to complex Fresnel lenses and Split-ring resonators. The combination of sub-nanometer structural engineering and high-precision additive manufacturing represents a solid step toward the practical deployment of stable, scalable functional MXene-based RF electronics.
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M- and X-Site Engineering of MXene Structure and Properties

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MXenes are defined by an unusually large compositional design space, yet much of the field has focused on a relatively small number of compositions. A central challenge is to understa nd how chemical complexity can be introduced deliberately, and how this complexity contro ls structure, surface chemistry, and functional properties. Mixed
metal MXenes provide one strategy for expanding this design space. By distributing multiple transition metals within the M layers, it is possible to modify bonding, lattice structure, elec tronic transport, optical response, and electrochemical behavior in ways that are not always predictable from the endmember compositions.
These materials also provide a chemical pathway to stabilize MXene structures that may be difficult or impossible to access using single-metal precursors alone.
A second, less explored strategy is X-
site engineering through carbonitride MXenes. Introducing nitrogen into the carbide sublatti ce changes the local metal-
X bonding environment and can influence surface termination chemistry, optical absorption, electronic conductivity, and surface electronic structure. Importantly, X-
site variation offers a design axis that is distinct from both metal-
site substitution and postsynthetic surface termination control.
Broad utilization of these approaches expands MXenes from compositionally tunable materi als into a broader platform for understanding how disorder, bonding, surface chemistry, and electronic structure interact.
The goal is to use chemical complexity not only to access new compositions, but also to dev elop clearer structure–property relationships that guide the rational design of MXenes for optoelectronic, electrochemical, and energy-related applications.

Hydrogen diffusion and hybrid orbital formation in Ti3C2 MXene

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Because of their outstanding physical properties, which originate from their two-dimensional structure, MXenes such as Ti3C2 are considered excellent candidates for sustainable energy applications. In fact, one aspect is the storage of energy by using hydrogen. To advance this field, a detailed understanding of hydrogen bonding and diffusion in MXenes is essential.
Commonly, chemical bonding of hydrogen is described by covalent, ionic, or multicenter bonds. However, the present study demonstrates that chemical bonding of hydrogen in Ti3C2 MXenes extends beyond this conventional framework. Using density functional theory (DFT), Ti3C2 MXene layers and surfaces were modeled in a slab geometry. Information on chemical bonding was obtained from the total and orbital projected density of states distributions. The calculations reveal that H atoms and molecules form multicenter bonds. At the surface these multicenter bonds are formed with adjacent Ti atoms. An example for H at the Ti3C2 surface is depicted in Fig. 1. However, at interstitial sites H and H2 form multicenter bonds with both titanium and carbon atoms. Notably, C–H bond formation involves s–p hybridization. The vibrational eigenmodes for all investigated hydrogen complexes were calculated using density functional perturbation theory yielding frequencies ranging from 890 to 1610 cm−1. These values indicating that the hydrogen multicenter bonds are stable.
For hydrogen-based energy storage applications, the transport mechanism for storing and releasing H and H2 is crucial. Therefore, hydrogen diffusion in Ti3C2 MXenes was examined using ab initio
calculations. To determine the temperature dependence of the diffusion coefficients for different migration mechanisms the migration barriers, hopping frequencies, vacancy formation enthalpies, and the vibrational entropy were calculated. As an example, Fig. 2 shows the change of the total energy as an H atom migrates along the surface of Ti3C2. The temperature dependence of the diffusion coefficients reveals that hydrogen diffusion is primarily governed by interstitial diffusion, while vacancy-mediated migration contributes negligibly.

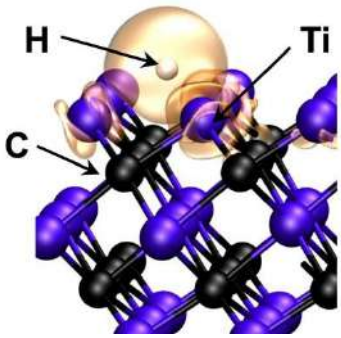

Fig. 1. Equilibrium position of atomic surface of unpassivated Ti3C2.

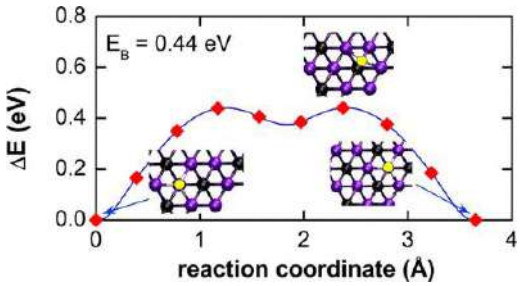

Fig. 2. Change of the total energy for H migration along the H on top of a Ti3C2 layer.

Direct CVD Synthesis of 2D Transition Metal Carbides via Sputtered Metal Precursors

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Keywords: MXenes, Transition metal carbides, CVD, Liquid metal CVD, sputtering, Large-scale Synthesis

Chemical vapor deposition (CVD) has emerged as a promising “bottom-up” approach for synthesizing 2D metal carbides and nitrides, referred as MXenes[1,2]. This method circumvents the limitations of conventional etching-delamination methods, such as small lateral flake size, structural defects, and uncontrollable surface terminations[3]. By enabling wafer-scale synthesis with high atomic economy, CVD represents a critical pathway toward the industrial-scale production of high-quality MXenes.
However, existing CVD methodologies face significant technical hurdles that limit their versatility. CVD growth of MXenes can be classified into two groups depending on the metal precursors adopted, named conventional CVD and liquid metal CVD (LM-CVD). Conventional gas-phase CVD often introduces chlorine terminations from metal halide precursors[2,4,5], which is detrimental for some applications. Another approach LM-CVD is restricted by precursor-substrate immiscibility and poor control over bulk diffusion[1,6]. These constraints have largely limited the success of liquid metal CVD approach to Mo-based systems and hindered the growth of other critical MXenes. To overcome this, our group has recently developed a novel surface diffusion liquid metal CVD (SDLM-CVD) approach in which the diffusion is better controlled when a thin metal wire was used as the metal precursor.
Here, we make further advancements of our SDLM-CVD by achieving successful growth of three distinct 2D carbide MXenes, Nb_2C, Mo_2C, and Ta_2C. By utilizing sputtered transition metal patterns on a copper surface, our method ensures a uniform distribution of source metal across the molten Cu catalyst surface. Comprehensive structural and chemical characterization, including XRD, XPS, AFM and SEM, confirms the formation of high-quality, large-scale 2D flakes and thin films. Furthermore, we elucidate the underlying growth mechanism through a combination of thermodynamic modeling and density functional theory (DFT) calculations. This SDLM-CVD technique overcomes the fundamental limitations of both chemical etching and previous CVD methods, providing a versatile platform for the large-scale synthesis of various MXenes compositions and accelerating their technological deployment.
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Carbene Terminations on 2D-Mo2C/Cu: A Method to Prepare MXene-Organic Interfaces?

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Ketones (R1R2C=O) react with bulk molybdenum carbide surfaces to form carbene (Mo=CR1R2)
terminations through carbonyl bond scission (deoxygenation). This chemistry is a result of the highly
oxophilic character of molybdenum-a property shared by the early transition metals found in Mxenes. The surface carbenes formed through deoxygenation of ketones or aldehydes display three important properties: extremely high thermal stability; excellent electrical contact via the double bond to the metal atom; additive chemistry in the sense that they serve as initiators for subsequent ring opening polymerization growth. As such, the deoxygenation approach offers unique opportunities to further enhance the properties of MXene materials by creating organic surface layers that grow out from the metal atoms. We will present studies of aldehyde deoxygenation modification of 2D-Mo2C/Cu-foil samples supplied by Prof. Wencai Ren (Shenyang National Laboratory for Materials Science).

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Solvothermal functionalisation of Ti3C2T*x* MXene for high capacity, ultralong-lifetime energy storage

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The tuneable surface chemistry of MXenes is one of their greatest assets, and tailoring the surface groups of MXenes for their intended application is critical to achieve their full potential. To this end, a fast, low-cost, and highly controllable microwave solvothermal treatment process was developed for Ti3C2T*x* MXene, using N,N-dimethylformamide and a controlled quantity of water. The resultant nitrogen-functionalised MXene is designated NMX. The solvothermal treatment causes pronounced morphological and chemical changes in the material, with TEM micrographs of NMX particles seen compared to pristine MXene (MX) in Figure 1a. The NMX forms microparticles with a nanoparticle decorated surface, which act as pillaring agents, giving NMX a 0.9 nm larger interlayer spacing than MX, as seen in Figure 1b. Mercury porosimetry and BET measurements also showed an internal volume 10 times larger for NMX compared to MX, with a peak pore diameter around 100 nm, corresponding roughly to the scale of the NMX particles and their interparticle space. Changes in surface chemistry were analysed using a combination of STEM-EDX as well as a range of synchrotron techniques, including XPS and NEXAFS. After optimising the treatment process for gravimetric capacitance, tuning both the water content and reaction time, there is a pronounced increase (over 30%) in capacitance in aqueous H2SO4, achieving over 500 F g-1 at 1 mV s-1, compared to MX's 380 F g-1. This is most likely due to the increased accessible surface area, as well as additional redox sites on the NMX surface. In addition to this significant increase in capacitance in aqueous acid, the NMX shows even greater performance in a Li ion system. Figure 1c shows the cycling performance of an NMX/CNT electrode in LP30 electrolyte at a high current density of 10 A g-1. Over 40000 cycles, the electrode increases in capacity by 148%, rising to 301 mAh g-1, while maintaining near-perfect coulombic efficiency. This increase is attributed to "opening" of the structure during repeated Li intercalation/deintercalation. In Figure 1d, the NMX's charge/discharge performance after 40000 cycles from 0.05 A g-1 to 100 A g-1 is shown. At low rates, the NMX reaches a maximum capacity of 682 mAh g-1, greatly exceeding typical values for MX (~300 mAh g-1), and higher than the theoretical capacity of graphite (372 mAh g-1), even up to 5 A g-1. At 10 A g-1, or 14.66C, NMX retains 321 mAh g-1, where graphite typically retains less than 300 mAh g-1 above 1C. Even at an extreme rate of 146.6C (100 A g-1), the NMX electrode retains 113 mAh g-1, showing supercapacitor-like speed with battery-like capacity. This exceptional performance, greatly exceeding typical anode materials in terms of capacity, longevity, and rate performance makes NMX an extremely promising candidate for

ultrafast, ultralong-life lithium-ion batteries, or as a replacement for graphite in lithium-ion capacitors, overcoming the significant rate and capacity limitations of that material.

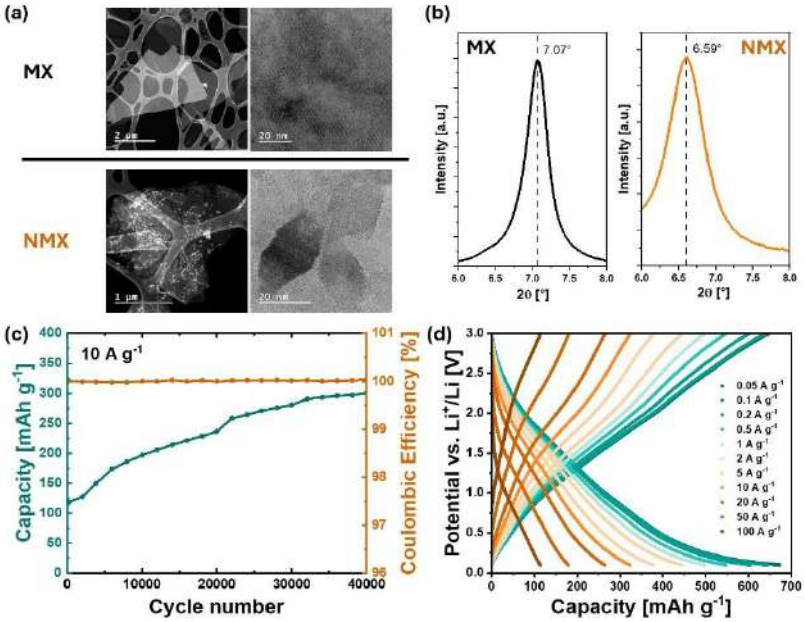

Figure 1: NMX. a: TEM micrographs of MX (top) and NMX (bottom) particles. b: XRD (002) reflections of MX and NMX. c: NMX cycling performance at 10 A g-1. d: Charge/discharge of NMX after 40000 cycles.

Development of Multifunctional MXene-Polymer Composites

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As new generations of technology continue to shrink in size and expand in scope, the need for lightweight materials that can provide multiple functionalities grows. Composites of polymers and nanomaterials offer a valuable solution, bridging the properties of both components to create multifunctional systems for a variety of applications. MXenes, a family of 2D transition metal carbides and nitrides, have attracted much attention in recent years in the field of nanocomposites. The unique electronic, mechanical, and optical properties, as well as the tunable surface chemistry of these nanomaterials, make them excellent candidates for multifunctional polymer composites. However, polymer selection for MXene composites is often limited by interfacial incompatibility with hydrophobic polymers. Typical methods for introducing MXenes into hydrophobic polymer matrices can involve excessive time and work, reduce the quality of MXene flakes, or utilize interfacial agents that alter the properties of the composite as a whole. The goal of this work is to explore alternative methods for developing MXene composites, using a functional polymer, hydrophobic polyvinylidene fluoride (PVDF) as a benchmark system. The relationships between processing, structure, and properties of composites will be thoroughly examined, as the variety of methods and materials used in the literature does not offer a clear story. By understanding the effects of MXene composition, surface chemistry, and composite processing on electronic, optical, and mechanical properties, guidelines will be established for fabricating systems tailored towards specific applications. Focusing on several distinct use cases, this work aims to provide a roadmap for developing multifunctional MXene-polymer composites, enabling future generations of high-performance materials.

Synthesizing MXene/conductive MOF heterostructure for sodium metal batteries

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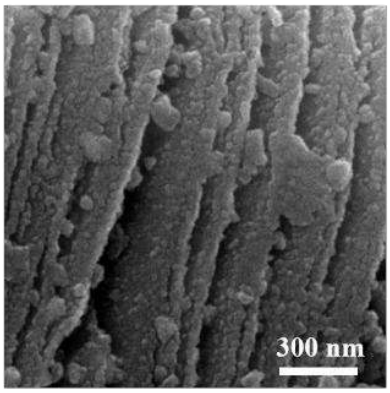
Assembling nanomaterials with different two-dimensional (2D) layered lattice structures can create heterostructure materials with unique properties that cannot be achieved by a singlecomponent material. Among these, the combination of inorganic and organic components offers new opportunities for constructing heterostructure materials with both excellent ionic and electronic conductivity. Herein, the controllable in-situ growth of conductive copper metalorganic framework (MOF) in the interlayer space of muti-layer iodine-terminated MXene is achieved. Multi-layer MXene exhibits host-like behavior, displaying a discrete yet regular structural configuration. The growth of the conductive copper MOF, as a guest with irregular size and shape, is guided and controlled by the physicochemical interactions of the terminating functional groups on the MXene layer surface. Due to in-situ MOF nucleation and generation, the MOF can effectively occupy and stabilize within the limited interlayer space of muti-layer MXene. The hydrophilic ends of MXene support the continuous growth of the copper-based MOF in the available 2D interlayer slits. The obtained 2D MXene/MOF heterostructure can accelerate the rapid transport of ions and electrons. Effective electronic interactions between MXene and the open surfaces of the nanoporous conductive copperbased MOF, including hydrogen bonding and coordination, enhance the electrochemical strength of the 2D MXene/MOF heterostructure, enabling the design of durable sodium metal anodes. The 2D MXene/MOF heterostructure-based sodium metal anode features controllable solid electrolyte interphase (SEI) composition and rapid ion and electron conduction, thus enabling the improved Na||Na symmetric batteries and Na||Na3V2(PO4)2F3 full batteries. The MXene-MOF heterostructure offers new insights for the development of high-performance sodium metal batteries.



SEM image of the obtained MXene/conductive MOF heterostructure

Morphology of MXene by topotactcic reactions

The metal fluxes can be effectively use for significantly increase the size of MAX and MAB crystallites from micron scale to millimeter by flux optimization. Beside the metal flux, the synthesis in transition metal sulfide can be used for synthesis of sulfur based MAX phases. Other approach to control the morphology of MAX phases is based on sue of suitable carbon precursors, which can produce MAX phase in ctorlled structures like tubes, which can be subsequently exfoliated to MXene tubular
structures [1]. The reaction of MAX phases and exfoliated MXene with various elements including halogen and chalcogen can be effective used for control of surface functionalization. The surface control is crucial for optimization of material performance for various electrocatalytic processes including HER and OER.

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Ultra-fast and selective silver (Ag^+) removal from complex water matrices using rationally designed MXene-$Mg(OH)_2$ nanocomposite

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The increasing discharge of silver ions (Ag^+) from industrial activities poses serious environmental and ecological risks, creating an urgent need for efficient removal strategies. In this study, magnesium hydroxide ($Mg(OH)_2$) and MXene-integrated $Mg(OH)_2$ composites (MgMX) were synthesized and evaluated for rapid and selective silver adsorption from aqueous systems. Among the prepared materials, MgMX-12.5% (MXene content of 12.5 wt.%) exhibited superior performance, achieving up to 97.5% Ag^+ removal with equilibrium attained within 3 minutes, outperforming pristine $Mg(OH)_2$. The enhanced performance is attributed to the synergistic interaction between $Ti_3C_2T_x$ MXene nanosheets and $Mg(OH)_2$ nanoflakes, resulting in increased surface area, improved dispersion, and abundant negatively charged functional groups. Adsorption kinetics followed the pseudo-second-order model, indicating chemisorption-dominated behavior. Temperature-dependent studies revealed an endothermic adsorption process for MgMX-12.5%, whereas pristine $Mg(OH)_2$ showed exothermic characteristics. Ionic strength and competitive ion experiments suggested an outer-sphere complexation mechanism. XRD analysis of the spent adsorbent confirmed in-situ reduction of Ag^+ to metallic Ag^0, demonstrating a combined electrostatic attraction and redox-driven removal pathway. The composite retained over 80% removal efficiency after six regeneration cycles using thiourea. Moreover, MgMX-12.5% demonstrated strong performance in real water matrices, including X-ray wastewater, jewellery effluents, greywater, and tap water. The silver-loaded adsorbent was further reutilized for iodine removal, highlighting its dual-functional and sustainable application. This work presents a robust MXene–hydroxide heterostructure for efficient silver removal and integrated wastewater remediation.

An MXene-Based Adhesive Tape for Multifunctional Electromagnetic Interference Shielding

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Flexible electromagnetic interference (EMI) shielding materials that can conformally adhere to diverse surfaces while maintaining electrical safety and mechanical compliance are highly desirable for next-generation wearable and skin-integrated electronics. In particular, EMI shielding materials in the form of adhesive tapes offer practical advantages for direct integration with devices, human skin, and irregular substrates, yet it remains challenging to simultaneously achieve strong adhesion, mechanical compliance, effective EMI shielding, and sufficiently high electrical resistance to avoid leakage currents or unintended electrical pathways. Here, we report a stretchable and self-adhesive EMI shielding tape in which MXene nanosheets serve as functional fillers within a soft polymer matrix. Unlike conventional highly conductive EMI shielding films, the material is engineered with a controlled microstructure that preserves high electrical resistance while enabling efficient electromagnetic attenuation. The resulting tape exhibits robust adhesion to diverse substrates, satisfactory EMI shielding performance, and a high electrical resistance that is maintained during repeated use. The combination of intrinsic adhesiveness, mechanical softness, and electromagnetic functionality allows the tape to be directly laminated onto diverse substrates without additional adhesives. Preliminary biocompatibility assessments further support its potential for long-term wearable use. Overall, this work presents a multifunctional MXene-based EMI shielding tape that integrates adhesion, electrical safety, flexibility, and shielding performance into a single material platform, offering a practical solution for wearable electronics, human-machine interfaces, and biomedical devices.

Towards scalable and sustainable methods for MXene synthesis – from theoretical and experimental perspectives

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About 15 years after the discovery of MXenes, research on their synthesis, characterization, and applications continues to expand. These two-dimensional (2D) transition-metal carbides and nitrides now form a rapidly growing materials family with diverse compositions, layer thicknesses, and surface chemistries. However, expanding the MXene chemical space beyond currently known structures requires new synthesis strategies that are both scalable and sustainable, supported by predictive theoretical frameworks. This talk presents recent advances that combine thermodynamic modeling with experimental synthesis to guide the discovery of new MXenes and related 2D materials derived from non–van der Waals solids. A vapor-based etching and transformation approach is introduced, in which layered MAX phases are selectively etched in reactive gas environments, enabling rapid, solvent-free synthesis of MXenes and related 2D carbides, nitrides, and carbonitrides while providing access to previously unexplored compositions. Together, these theoretical and experimental developments provide new routes for scalable MXene synthesis and broaden the design space for emerging applications in energy, catalysis, and electromagnetic technologies.

Rational design of high-performance double transition metal MXene catalysts for the hydrogen evolution reaction

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MXenes are a rapidly growing class of two-dimensional materials with the general formula Mn+1XnTx, where M is an early transition metal, X is carbon or nitrogen, and Tx represents surface termination groups. Owing to their compositional diversity, surface tunability, earth abundance, and high specific surface area, MXenes are highly attractive candidates for catalytic applications traditionally dominated by scarce and expensive noble metals such as Pt and Rh. Notably, Mo-based MXenes have demonstrated excellent catalytic performance for the hydrogen evolution reaction (HER), highlighting their potential as cost-effective alternatives in energy conversion technologies.
However, even Mo based MXenes have yet to reach the performance of Pt for the hydrogen evolution reaction (HER). Herein, using Density Functional Theory (DFT), we describe how double transition metal (DTM), M3C2 and M4C3 MXenes can be leveraged to close the gap between Pt and MXenes. We describe how the ordering of the two transition metals in the DTM MXenes can be used to tune the electronic structure and optimize the HER performance. We also describe how the DTM MXenes can be further tuned through surface functionalization to further optimize the HER performance. This work provides a roadmap for the design of high-performance MXene catalysts for energy conversion applications. Overall, this work establishes a rational design framework for high-performance DTM MXene catalysts and offers a pathway toward developing earth-abundant alternatives to noble-metal-based HER catalysts for next-generation energy conversion applications.

From Defect Mitigation to Defect Engineering in MXenes

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Our field of MXenes has evolved substantially over the past 15 years. Initially, we mainly aim ed to minimize defects as weak points or seal them to prevent degradation.
Now, as materials science advances toward harnessing defects for innovations in catalysis, e lectronics, and beyond, we have begunto better understand and control defects in MXenes. We now explore how defects can be leveragedto tune and enhance MXene properties for va rious applications.
In this talk, I will first discuss some of the current defect challenges we still face in MXenes a nd how we can address them.
Next, I will present how we can benefit from controlling defects to enhance MXene properti es. I will focus on controlling point defects, including vacanciesin the metal or nonmetal sites and substitutional defects. I will then discuss the formation of layered ceramic structures wi the oxygen bridging between MXene layers and how these modifications impact properties such as electrocatalysis and electrical conductivity. Finally, I will conclude with new evidence of defects beyond point defects in high-entropy MXenes.

Single-Atom MXenes: Versatile Platforms for Selective Cinnamaldehyde Reduction

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As an important organic intermediate, cinnamyl alcohol finds an extensive use across the perfumery and pharmaceutical industries. However, its conventional chemical synthesis suffers from significant drawbacks. While biosynthetic routes have been recomended as ecological and sustainable alternatives, the heterogeneous catalysts may offer a highly efficient pathway for the selective reduction of the carbonyl groups by H2 under mild and controlled conditions. In recent years, two-dimensional (2D) MXenes are being considered as versatile catalysts, particularly as versatile platforms for heterogeneous catalysis due to their peculiar and tailoring properties. Serving as supports for single-atom catalysts, MXenes allow for the uniform anchoring of isolated metal atoms. This architecture creates a new class of catalysts with tunable polarized active sites, significantly enhancing the catalytic activity. Based on this state of the art, this study reports the synthesis of MXene-supported single-atom catalysts, incorporating transition metals (e.g. Fe, Co) along with a less-explored element as Indium. The research systematically evaluates the catalytic performance of these materials in the chemoselective hydrogenation of cinnamaldehyde using molecular hydrogen.
Single-atom catalysts based on Ti3C2 Mxene were synthesized from a Ti3AlC2 MAX phase precursor. The process involved the selective etching of aluminum using Lewis acid metal halides (Fe, Co, In) within a molten NaCl/KCl salt medium. To ensure the atomic dispersion, the excess metal species was subsequently removed via washing with a concentrated aqueous acidic solution. The selective hydrogenation of cinnamaldehyde to cinnamyl alcohol was performed in a 16 mL stainless steel autoclave. In a typical run, 0.001 mol of cinnamaldehyde, 20 mg of catalyst, and 5 mL of isopropyl alcohol were charged into the reactor. The system was pressurized to 15 atm of H2 and maintained at 100 °C for a reaction duration of 5 hours under constant stirring. XRD analysis confirmed the successful formation of the Mxene phase, with characteristic harmonics dominating the patterns. Additionally, minor reflections attributed to the residual MAX phase could also be detected, indicating nearly complete conversion with only minor proportions of the precursor material remaining. No distinct phases corresponding to the modifiers (Fe, Co, In) were detected in the samples, suggesting that these metals are atomically dispersed and highly uniform across the Mxene surface, falling below the detection limit of XRD. In terms of stability, after the reaction, only a slight decrease in the intensity of the diffraction lines was observed, without any other structural change. The degree of structural disorder and surface defects evaluated with Raman spectroscopy was quantified using the ID/IG ratio. The values decreased in the following order: Fe(SA)- Ti3C2Clx (0.91) > Co(SA)-Ti3C2Clx (0.84) > In-Ti3C2Clx (0.69). Notably, the Fe(SA)-Ti3C2Clx catalyst exhibited the highest density of defects, which likely provides more active sites for catalysis. DRIFT spectroscopy of the spent single-atom Mxene catalysts reveals intense vibrational bands, confirming the strong chemisorption of reaction intermediates and products on the surface. The solid catalysts exhibited a bifunctional character, possessing both acid and base active sites on the surface. The capacity for hydrogen adsorption appears to be governed by a synergistic effect

between the electronegativity and atomic mass of the incorporated metal atoms: Co(SA)-Ti3C2Clx (1.31 mmoles·g−1) > Fe(SA)-Ti3C2Clx (1.17 mmoles·g−1) > In-Ti3C2Clx (0.19 mmoles·g−1). X-ray photoelectron spectroscopy confirmed that Fe, Co and In are present as atomically dispersed species on the Mxene surface. The observed binding energies indicate that these metals exist primarily in an oxidized state.

The TON revealed a striking disparity in catalytic efficiency among the modified Mxenes. The Co(SA)-Ti3C2Clx catalyst exhibited the highest activity with a TON of 807.71, vastly outperforming the Fe(SA)-Ti3C2Clx sample, which yielded a significantly lower value of 6.17. Meanwhile, the In-Ti3C2Clx catalyst showed intermediate performance with a TON of 391.63. The In-Ti3C2Clx catalyst achieved the highest selectivity toward cinnamyl alcohol, reaching 85.03%. The specific advantage of the single-atom dispersion was further underscored by a comparison with bulk In2O3, which exhibited a significantly lower selectivity of only 9.87% under the same conditions.

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Mo-Containing Ordered Double-Transition-Metal Carbide Mxenes: Composition and Substrate Effects Across OER, Pollutant Degradation, and CO2 Reduction

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Ordered Mo-containing double-transition-metal carbide MXenes provide a versatile platform for tuning catalytic behaviour through both intrinsic metal layering and extrinsic surface modification. In this work, we investigate Mo-Ti carbide MXenes together with the parent reference systems Ti3C2Tx and Mo2CTx, to understand how composition, secondary transition-metal modification, and electrode support jointly determine catalytic performance. Rather than treating these variables independently, we use them to build a unified picture of structure-activity relationships across three application spaces that are highly relevant to the MXene community: the oxygen evolution reaction (OER), pollutant degradation, and electrochemical CO2 reduction. Our study focuses on Mo-Ti ordered carbides, Mo2TiC2 and Mo2Ti2C3, and compares them directly with Ti3C2Tx and Mo2CTx. To tune the catalytic response, Mo2TiC2 and Mo2Ti2C3 were modified with Fe, Ni, NiFe, Cu, and NiCu. This compositional series allows us to probe how the electronic structure and interfacial chemistry of the Mo-Ti carbide scaffold are altered by mono- and bimetallic transition-metal modification, and how these changes affect performance relative to the undoped parent materials. In this way, the parent phases serve as important reference points for separating the influence of the ordered Mo-Ti framework from the contribution of the added catalytic components.
For OER, clear differences are observed across the modified and unmodified materials, confirming that the catalytic behaviour of Mo-based MXenes can be strongly tailored through transition-metal modification. However, one of the key outcomes of this work is that the activity trend is not fixed by composition alone. When the catalysts are evaluated on Ni foam, the ranking of the series differs from that obtained when the same materials are spray-coated onto carbon paper. This substrate-dependent reordering highlights the importance of electrode architecture in MXene electrocatalysis and shows that the support should be considered an active design parameter rather than a passive current collector. The different trends likely arise from changes in catalyst-support electronic coupling, film morphology, wetting, ion and gas transport, and the possible electrochemical participation of the Ni foam under anodic conditions. The practical consequence is significant: catalyst screening performed on one support cannot be assumed to translate directly to another, even when the nominal catalyst composition is identical.
The same family of transition-metal-modified materials was also explored for pollutant degradation, where composition-dependent differences were again observed. These results demonstrate that the catalytic utility of Mo-based MXenes is not limited to water oxidation but extends to environmental remediation processes in which surface redox chemistry and efficient interfacial charge transfer are equally important. The ability of the same Mo-Ti carbide platform to operate in both OER and pollutant degradation suggests a broader multifunctionality that is especially attractive for integrated energy and environmental

applications. It also indicates that transition-metal modification can be used as a general strategy for adapting MXene surfaces to distinct oxidative reaction environments.
In parallel, we evaluated the parent carbides, the Mo-Ti series, and their Cu-containing composites for electrochemical CO_2 reduction. This part of the study expands the role of these materials from anodic oxidation chemistry to cathodic carbon conversion and provides a second, complementary test of how composition engineering changes surface reactivity. Comparison with $Ti_3C_2T_x$ and Mo_2CT_x helps isolate the specific contribution of the ordered Mo-Ti architecture, while the inclusion of Cu-containing composites introduces an additional handle for promoting CO_2 activation and tuning reduction pathways. Taken together, these results show that the catalytic behaviour of Mo-based MXenes can be redirected across fundamentally different electrochemical reactions by changing both the metal composition and the interfacial environment.
Overall, this work identifies three tightly connected design variables for Mo-based MXene catalysts: the parent carbide chemistry, the choice of transition-metal modification, and the substrate used for electrode assembly. By systematically comparing $Ti_3C_2T_x$, Mo_2CT_x, Mo-Ti ordered carbides, and Fe-, Ni-, NiFe-, Cu-, and NiCu-modified derivatives across OER, pollutant degradation, and CO_2 reduction, we show that catalytic trends emerge from the interaction of composition and device configuration rather than from composition alone. These findings provide a practical framework for the rational design of multifunctional MXene-based catalysts and support the development of Mo-containing ordered carbides as adaptable materials for both energy-conversion and environmental-remediation technologies.

MXenes as versatile 2D materials for next-generation catalysis

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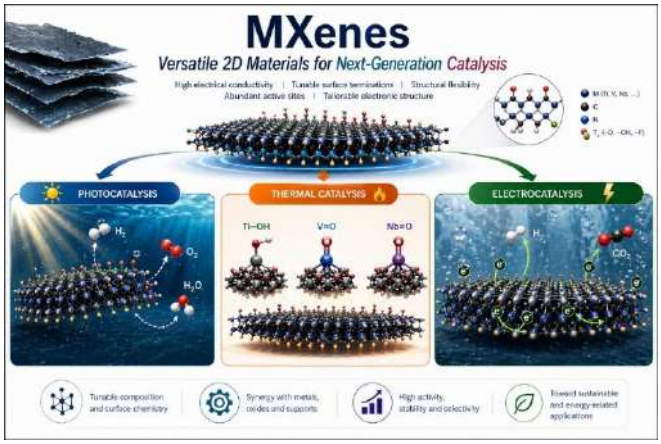
MXenes, a rapidly expanding family of two-dimensional transition metal carbides and nitrides, have recently emerged as versatile platforms for catalytic applications due to their unique
combination of metallic conductivity, tunable surface chemistry, and structural adaptability. In this contribution, we present a comprehensive study of MXene-based materials across three key catalytic domains: photocatalysis, thermal catalysis, and electrocatalysis.
In photocatalysis[1][2][3][4], we demonstrate that controlling the size and surface terminations of MXenes enables the transition from metallic to semiconducting behavior, allowing their use either as standalone photocatalysts or as cocatalysts in heterojunction systems. Density functional theory (DFT) calculations reveal that both quantum confinement and surface functionalization critically influence the band gap, which can be tailored to match specific redox reactions.



For thermal catalysis[5][6][7], we exploit the intrinsic similarities between MXene surface terminations (–O, –OH, –F) and classical metal oxide active sites (e.g., Ti–OH, Nb=O), while introducing a distinct electronic environment arising from the underlying C/N framework. This duality enables the design of catalytic systems with modified adsorption and activation properties, which we probe through benchmark reactions.
In electrocatalysis[8][9], MXenes exhibit outstanding performance due to their high electrical conductivity, hydrophilic surfaces, and ability to form hybrid structures with metals and porous materials. We highlight the role of MXene-based heterostructures in enhancing charge transfer and catalytic efficiency in reactions such as hydrogen evolution and CO_2 reduction.
Overall, this work establishes MXenes as a unifying platform bridging classical catalysis and emerging nanomaterials, where electronic structure and surface chemistry can be precisely engineered to drive catalytic performance.

Surface-engineered Ti3C2Tx MXene/Cu2O Photocathodes for Highly Selective Photo-electrocatalytic CO2 Reduction to Ethanol

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Carbon dioxide reutilisation has gained significant relevance in the last decade due to the increase of the greenhouse effect and the necessity of finding alternatives to fossil fuels. Cu2O is inexpensive p-type semiconductor that can promote photo-electrocatalytic CO2 reduction reaction (PEC CO2RR). But while its low bandgap (2.2 eV) enables photoexcitation by visible light, the long-term stability remains limited due to its quick charge recombination and photocorrosion.
Here, we developed strategies for promoting charge separation and extraction by combining Cu2O with surface-engineered MXenes. We prepared a series of electrodes combining Cu2O with 10-50 wt% of Ti3C2Tx-MXene. To engineer the MXene surface, we varied the atmosphere and temperature of ml-Ti3C2Tx thermal annealing. Under an oxidizing atmosphere, TiO2 particles formed on the MXene surface, thus promoting a p-n heterojunction with Cu2O. In inert and reducing atmosphere, TiO2 was not formed, however, the annealing caused decrease of -F terminal groups.

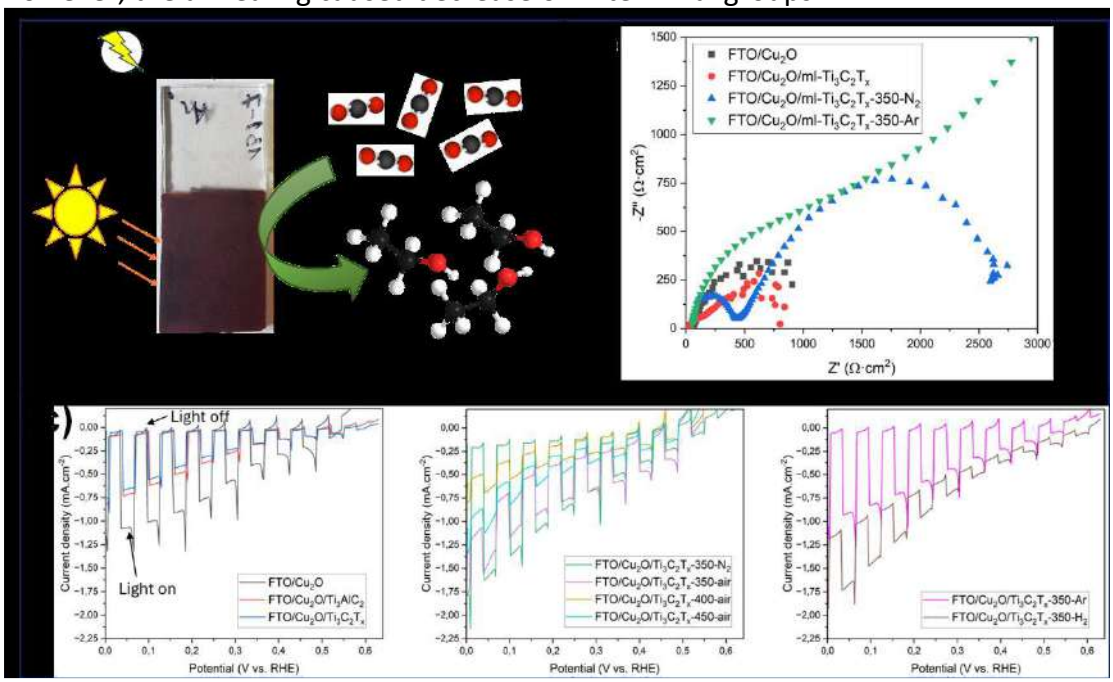

Figure 1: (a) Scheme of photo-electrocatalytic CO2RR over FTO/Cu2O/MXene photocathodes; (b) Nyquist plots from electrochemical impedance spectroscopy (EIS) reveal markedly lower charge-transfer resistance and improved carrier transport in Cu2O/MXene-350-N2 composites compared to pristine Cu2O; (c) Linear sweep voltammetry (LSV) curves of bare Cu_2O, Cu2O/Ti3AlC2, and Cu2O/MXene electrodes under CO2-saturated conditions and chopped illumination, showing reduced charge recombination and enhanced photocurrent density upon MXene addition.
In PEC CO2RR, the photo-cathode containing 10 wt% of MXene with a balanced amount of TiO2 on the multilayered Ti3C2Tx surface outperformed the best Cu2O/Cu-based materials reported thus far, reaching a

rate of 25.56 mM.g-1.h-1, corresponding to 0.096 mM.cm-2.h-1. Moreover, the improved MXene coverage of Cu2O (50 wt% MXene) further increased the highly selective ethanol production rate up to 0.112 mM.cm-2.h-1 after 2 hours. Importantly, it significantly stabilized the photocathode, maintaining 76% of this production rate even after 6 hours. Therefore, surface-engineered MXenes with interfacial modifications unlock the full potential of Cu2O for selective photoelectrocatalytic CO2 reduction.

Photothermal nitrogen reduction to ammonia over multi-layered Ti3N2 MXene catalysts

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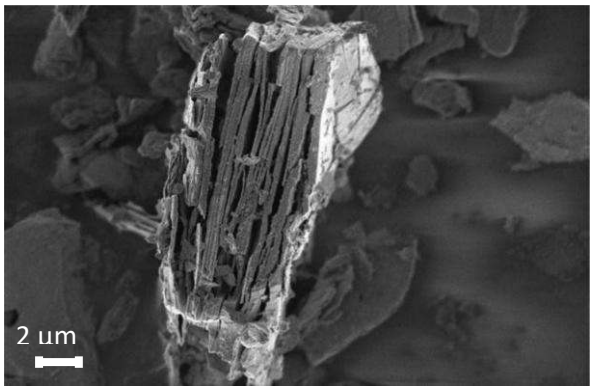
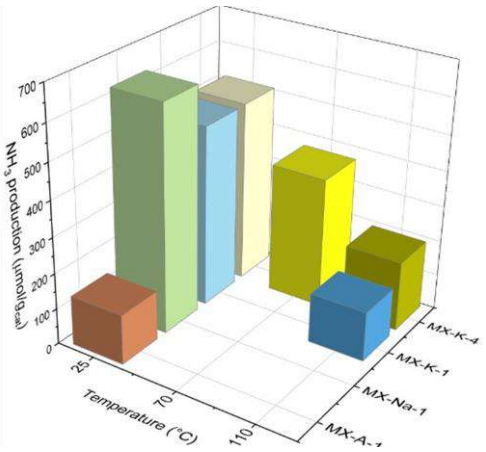
Transition metal MXenes have emerged as a versatile class of two-dimensional materials for energy conversion and heterogeneous catalysis since their first report in 2011. MXenes features combine metallic conductivity, high surface area, and chemically tunable terminations within a layered architecture.
While early studies focused mainly on carbide MXenes, nitride counterparts have recently attracted increasing interest due to their distinct electronic structure and adsorption energies, plus stronger metal-nitrogen bonding, and enhanced structural stability, making nitride MXenes particularly promising for nitrogen reduction reactions (NRR).[1] Nevertheless, their development has been limited by synthetic challenges and instability under conventional etching conditions, resulting in only a few experimentally reported multilayered nitride phases. Recently, computational investigations on M2N systems (M = Mo, Ta, Ti) indicate favorable surface energetics for N2 adsorption and activation, highlighting the largely untapped potential of nitride MXenes in ammonia synthesis under mild pressure conditions.[2]
This work arises in part from the European DAM4CO2 Project's interest in the management and valorisation of combustion gas by-products, such as CO2 and N2. To this end, the present study focuses on the synthesis and application of multi-layered Ti3N2 Mxenes for the photothermal nitrogen fixation reaction to form ammonia.
Pure and partially oxidized TiNα crystalline structures were obtained from the fluorine-free etching of Ti3AlN MAX phase,[3] coupled with a tailored purification protocol to control surface chemistry and structural integrity (Figure 1a). The role of the oxidizing agent was systematically evaluated by comparing different persulfate salts (NH4+, K+ and Na+), varying their concentration, and modulating the purification temperature to establish clear structure–property–activity correlations. Extensive physical and chemical characterization of the materials was performed to get a comprehensive structural and electronic properties of each Ti3N2 Mxene. Nitrogen reduction was evaluated in batch and continuous-flow reactors under light and dark conditions to distinguish between photothermal and thermal effects, while the catalyst stability was verified under reaction conditions. 15N2 isotope-labelling experiments, combined with in situ illumination XPS analysis, confirmed the catalytic origin of ammonia and provided evidence for a surface-mediated hydrogenation pathway.
Notably, the best photocatalyst achieved a high ammonia yield of 633.6 µmol/gcat, after 20 h of reaction under solar-simulated light irradiation (Figure 1b).





a) *b)*

Figure 1. a) HRSEM of a purified Ti3N2 MXene and b) photocatalytic NH3 production at 20h of reaction over multi-layered Ti3N2 MXenes.

Catalytic Performance of V2Oy/Ti3C2Ox MXene in Formaldehyde Production

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Active and selective materials are essential for the low-temperature oxidative activation of methane into value-added products. In this context, two-dimensional metal carbides known as MXenes have attracted increasing attention due to their promising catalytic properties [1,2]. These materials exhibit a unique combination of characteristics, including high electronic conductivity, hydrophilicity, and resistance to chemical attack and high-temperature oxidation. Such properties are closely related to their rich surface chemistry, which originates from the wet-etching synthesis process and results in surface terminations such as –O and –OH groups.
In this study, we report the selective formation of formaldehyde from direct selective oxidation of methane using Ti3C2Ox-MXene as support for V2Oy species and molecular oxygen at low temperatures and ambient pressure. The compositional and structural features of the catalytic system were comprehensively investigated by XRD, Raman spectroscopy, SEM, TEM, transient operando Xray photoelectron spectroscopy, and diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS).
The unique synergy between the carbide framework and the dispersed oxide components, together with the intrinsic two-dimensional architecture of Ti_3C_2Ox MXene, enables a remarkable formaldehyde selectivity of 70% at 250 °C under ambient pressure. This enhanced performance can be attributed to the strong interfacial interactions between the Ti_3C_2Ox MXene support and the V2Oy species, which promote efficient activation of methane while suppressing total oxidation pathways. The conductive carbide layers facilitate charge transfer processes, whereas the surface terminations (–O, – OH, and other functional groups) contribute to the stabilization and modulation of active sites. The 2D morphology further ensures high surface accessibility and short diffusion paths, both of which are crucial for selective oxidation reactions.
Despite these promising results, the dynamic surface and structural transformations occurring under reaction conditions remain insufficiently understood. In particular, the evolution of surface terminations, oxidation states, and subsurface rearrangements during methane activation is likely to play a decisive role in determining catalytic efficiency and selectivity. To address this knowledge gap, we recently conducted an in-depth investigation using operando and in situ techniques.
We monitored the surface and subsurface dynamics of $Ti_3C_2O_x$ MXene under steady-state O_2 and/or CH_4 atmospheres over a temperature range from room temperature to 250 °C. The results reveal that controlled surface modifications of $Ti_3C_2O_x$ occurring during both catalyst synthesis and catalytic operation lead to the formation of highly active interfacial sites.

These dynamic rearrangements appear to optimize the balance between methane activation and selective oxidation, thereby favoring formaldehyde formation over deep oxidation products.
Overall, the findings highlight the crucial role of structural flexibility and surface adaptability of MXene-based systems in governing their catalytic function.

Adapting MXene Models for Catalysis and Sensing: Lessons from Theory and Experiment

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Since their discovery in 2011, MXenes have inspired both theoretical and experimental investigations, progressing in tandem. This talk will explore how computational models of MXenes have developed over the past decade and a half, with particular emphasis on catalytic and sensing applications.
The evolution of these models has been guided by three intertwined forces. Curiosity drives researchers to explore beyond what is experimentally accessible, predicting hundreds of potentially stable MXenes while only a few tens have been synthesized.[1] Necessity arises when simplified virtual models fail to capture experimental behaviour, prompting adjustments such as incorporating mixed surface terminations to reconcile theory with observations.[2] Finally, experimental reality induces model refinement. For instance, newly discovered MXene structures, such as oxycarbides, immediately inspire theoretical investigations to include novel atomic configurations and probe their properties.[3] Through examples such as these, this talk highlights the dynamic interplay between theory and experiment in advancing MXene research and shaping models that guide future applications in catalysis and sensing.

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Electrochemically Formed Single-Atom Centers of MXenes as a New Class of Electrocatalysts for Energy Conversion and Storage

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Single atom catalysts (SACs) have emerged as a new class for the development of active and selective catalysts.

These materials are commonly based on anchoring a noble transition metal to some kind of carrier. It has been shown that MXenes—two-dimensional materials with application in energy storage and conversion— spontaneously form SAC-like sites under anodic polarization conditions, using the applied electrode potential as a probe to transform the MXene basal plane into a SAC-type structure [1]. Combining ab initio molecular dynamics simulations and electronic structure calculations in the density functional theory framework, we demonstrate that the SAC sites rather than the basal planes of MXenes are highly active and selective for the oxygen or chlorine evolution reactions, respectively [1,2]. Our findings may simplify synthetic routes toward the formation of active and selective SAC-like sites and could pave the way for the development of smart materials by incorporating fundamental principles from nature into materials discovery: while the pristine form
of the material is inactive, the application of an electrode potential activates the material by the formation of active and selective single-atom sites.

The MXene-SAC motif enables the selective transformation of several electrocatalytic processes relevant for sustainable energy under anodic polarization [3]—including oxygen evolution [4], hydrazine oxidation [5], and ammonia oxidation [6]—or electrochemical nitrogen reduction by pulsing the electrochemical potential [7]. This talk provides an overview of the application of in situ formed SAC-like sites on the MXene basal planes and gives an outlook on future work.

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Rapid electrothermal heating and molten salt etching to produce Ti3C2 MXenes

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Rapid, out-of-oven techniques for MXene synthesis are of great interest and would allow for easier production of this exciting class of 2D materials. MXenes are typically synthesized by etching MAX phases with strong acids for long times, sometimes exceeding 40 hours. Electrothermal synthesis techniques can reduce heating time of materials; here we utilize Joule heating with molten salt etching precursors to etch MAX phase into multilayered (ML) Ti3C2Tx MXenes. An inert environment was used to etch the MAX phase in 30 minutes at 750-800 °C. SEM/EDS and XRD confirmed etching of the material. XPS, FTIR, and Raman were compared to conventional LiF-HCl ML- Ti3C2Tx, showing similar spectra to Joule heated ML-Ti3C2Tx material. Most importantly, this new out-of-oven Ti3C2Tx synthesis decreased etching time by 98% from molten salt etching and reduced energy usage from 1.56 x 107 J/g to 1.01 x 106 J/g per batch, paving the way for commercialization of MXene etching.

MXenes: from the passive nanomaterials to targeted bullet

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Since their discovery in 2011, MXenes (2D transition-metal carbides/nitrides) have emerged as a versatile nanomaterial platform for biomedical applications, spanning photothermal and photodynamic therapy (PTT/PDT), antimicrobial interventions, biosensing/bioimaging, targeted drug delivery, and electrically conductive scaffolds for tissue regeneration. A major driver of this interest is their strong absorption in the near-infrared (NIR) region and efficient conversion of optical energy into heat, enabling rapid, localized hyperthermia. Across multiple in vitro and in vivo studies, MXenes have demonstrated potent anticancer and antibacterial activity under NIR irradiation, often outperforming conventional nano-photosensitizers due to higher optical absorption and photothermal conversion efficiency. These attributes position MXenes among the most promising PTT agents for effective tumor ablation or bacteria removal.
However, the clinical translation of MXene-mediated PTT remains constrained by non-specific biodistribution, limited accumulation at the tumor site, and the potential for off-target toxicity, particularly under intensive or repeated irradiation regimens. To address these barriers, we and
others have focused on engineering actively targeted MXene systems to improve selectivity and therapeutic index. Active targeting leverages ligand–receptor interactions (e.g., receptor overexpression on malignant cells or bacteria) to promote preferential uptake and retention at the disease site, moving beyond passive accumulation mechanisms such as the enhanced permeability and retention effect and offering a more controlled route toward specificity and safety.
Here we summarize a “passive-to-bullet” concept in which MXenes are converted from broadly distributing nanoheaters into disease-anchored, on-demand effectors by adding (i) a biocompatible interface layer that stabilizes the flakes in biofluids and provides robust bioconjugation handles,
and (ii) a targeting ligand that pre-defines where heat will be released. In our melanoma model, Ti3C2Tx sheets were coated with polydopamine (PDA) and conjugated with anti-CEACAM1 antibodies to recognize CEACAM1-overexpressing malignant cells. This design preserved baseline biocompatibility while enabling antigen-dependent binding and selective photothermal killing of CEACAM1-positive melanoma cells, with minimal effect on CEACAM1-negative counterparts under identical irradiation.
In vivo, antibody functionalization shifted biodistribution toward the target tumor, increasing tumor titanium content and tumor-to-normal tissue ratios, while reducing non-specific uptake in clearance organs (liver, lung, spleen) compared with pristine MXene after systemic delivery.

Intratumoral administration further confined the material to the tumor and led to negligible accumulation in major organs, supporting a safety-by-design route for local or image-guided PTT.

A parallel challenge exists in antimicrobial MXene research, and we demonstrate that externally triggered MXene-assisted PTT provides rapid bacterial eradication, including complete killing in vitro and improved healing in an infected wound model. Critically, antibody-functionalized MXenes enabled targeted ablation of E. coli in mixed bacterial environments, sparing non-target bacteria and thereby reducing the risk of dysbiosis – an analogue of “off-target” complications in oncology.

Mechanistically, the bactericidal effect is dominated by localized heating at the bound pathogen surface (often exceeding ~50 °C), with minimal reliance on ROS chemistry, which may also help limit collateral host damage.

Looking forward, translating MXene “targeted bullets” will require converging materials engineering and clinical constraints: (1) standardized synthesis and purification to control oxidation state and eliminate etching residues that confound bioactivity; (2) colloidal stabilization and corona-aware targeting to maintain ligand accessibility in vivo; (3) rational selection of NIR-I vs NIR-II windows and laser dosimetry tailored to tissue depth and heat diffusion; and (4) integration with multimodal imaging, immunotherapy, or drug delivery to leverage MXenes as theranostic hubs.

Collectively, these advances position actively targeted MXene platforms as a broadly extensible strategy for precision photothermal oncology and pathogen-specific disinfection with a widened therapeutic window and reduced off-target burden.

Non-irritant profile, single-cell detection, and anti-inflammatory potential of Nb_4C_3 MXene for skin applications

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MXenes have gained significant attention for their potential in skin-contact applications. Their exceptional electrical conductivity, flexibility, hydrophilicity, and surface tunability make them promising materials for wearable electronics, biosensors, antimicrobial coatings, wound dressings, and smart dermal interfaces. In particular, niobium-based Nb_4C_3 MXene has attracted increasing interest due to its chemical stability and reported redox-modulating properties; however, its impact on skin cells and tissues has not been systematically investigated.

Here, we comprehensively evaluated the biocompatibility, cellular interactions, and irritation potential of Nb_4C_3 MXene through an integrated multiscale approach combining physicochemical characterization with in vitro, reconstructed human epidermis, and in vivo models. High-quality delaminated Nb_4C_3 nanosheets (~250 nm lateral size) were synthesized and validated prior to biological testing. Human dermal fibroblasts, immortalized keratinocytes (HaCaT), and primary normal human epidermal keratinocytes (NHEK) were used to assess cytotoxicity, oxidative stress, cytokine production, and wound-healing dynamics. Nb_4C_3 exposure did not affect cell viability across all models, confirming its low cytotoxicity. Notably, Nb_4C_3 reduced intracellular reactive oxygen species and modulated IL-6 and IL-8 secretion in a predominantly anti-inflammatory direction, without eliciting a broad pro-inflammatory response. While higher concentrations transiently delayed keratinocyte migration under low-serum conditions, proliferative capacity and overall wound closure were preserved, indicating concentration-dependent but non-detrimental modulation of re-epithelialization processes.

An innovative aspect of this study was the application of mass cytometry (CyTOF) to detect Nb_4C_3 uptake in skin-derived cells at single-cell resolution by exploiting its intrinsic ^{93}Nb isotopic signature. This label-free, high-sensitivity approach enabled simultaneous quantification of nanomaterial internalization and cell viability. We

quantified the MXene associated with cells after 24 h exposure, observing higher uptake in HaCaT compared to primary keratinocytes.

In reconstructed human epidermis (EpiDerm™, OECD TG 439), Nb_4C_3 did not induce irritation or compromise tissue viability, preserved normal epidermal architecture, and reduced pro-inflammatory cytokine release. Complementary in vivo intradermal administration in rats confirmed excellent local tolerance, with no persistent inflammation or structural damage up to 7 days post-exposure.

Collectively, these findings identify Nb_4C_3 MXene as a biocompatible, non-irritant, and redox-modulating nanomaterial. Beyond establishing its dermatological safety, this work introduces a robust single-cell analytical framework for tracking metal-based 2D materials in cutaneous systems, supporting the rational development of Nb_4C_3 for wound healing, anti-inflammatory therapies, and next-generation skin-interfaced biomedical technologies.

Single molecule biosensing with MXene energy transfer

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Single-molecule detection offers exceptional sensitivity in bioanalysis by resolving the behavior and interactions of individual molecules. Among available approaches, fluorescence-based energy transfer methods are particularly suited for probing nanometer-scale distances, which are central to structural biology and membrane biophysics. Conventional Förster Resonance Energy Transfer (FRET) employs paired donor and acceptor fluorophores and operates most effectively over distances of ~3-10 nm, yet accurate distance quantification remains challenging.

Graphene-based energy transfer (GET), where graphene serves as a broadband energy acceptor, extends the measurable range to approximately 10-40 nm and enables quantitative single-molecule analysis [1]. However, graphene's hydrophobic surface chemistry and fluorescence lifetime variations arising from multilayer structures limit its reproducibility and compatibility with biological systems.

To address these limitations, we investigate titanium carbide ($Ti_3C_2T_x$) MXenes as alternative two-dimensional quenchers and as substrates for biomolecular systems. Our work began by examining MXene-DNA interactions through fluorescence spectroscopy combined with molecular dynamics simulations [2]. Two key findings emerged. First, DNA adsorption onto MXene is primarily mediated by hydrated salt bridges, in contrast to the combined hydrophobic and hydrogen-bonding interactions typical for graphene. This type of interaction suggests reduced perturbation of biological structures and improved biocompatibility. Second, real-time surface hybridization experiments revealed a measurable fluorescence increase during conversion of single-stranded to double-stranded DNA. Simulations indicated that this transition altered the fluorophore-surface separation by less than 0.3 nm, demonstrating that MXenes can resolve sub-nanometer positional changes.

We next employed single-molecule fluorescence microscopy in combination with DNA nanotechnology to position fluorophores at precisely defined distances from MXene-coated glass substrates [3]. Within a 1-8 nm window, MXenes exhibited strong distance-dependent quenching, with fluorescence almost fully restored at ~8 nm. The energy transfer efficiency followed a cubic distance dependence, consistent with Förster-type mechanisms, and was largely independent of MXene film thickness. These observations confirm that MXene-based energy transfer enables quantitative distance sensing with sub-nanometer sensitivity in the biologically relevant 1-10 nm regime.

Finally, we applied this approach to supported lipid bilayers (~5 nm thick), widely used as minimal models of cellular membranes. MXene substrates enabled leaflet-resolved fluorescence readout at the single-molecule level, a long-standing challenge in membrane biophysics. This capability demonstrates the suitability of MXenes for interrogating nanoscale organization and asymmetry in biomembranes.

In summary, MXenes combine the short-range sensitivity characteristic of FRET with the quantitative advantages of graphene-based platforms, while offering superior direct biocompatibility and robustness. These properties establish MXenes as promising quenching platforms for advanced fluorescence microscopy, particularly in membrane biophysics and nanoscale biointerface research.

Acknowledgements

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ELECTROACTIVE BIOMIMETIC 3D-PRINTED MXENE SCAFFOLDS FOR CENTRAL NERVOUS SYSTEM REPAIR

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INTRODUCTION

Neurotrauma leads to the disruption of neuronal connections, inflammation and repair-inhibitive scarring and no effective treatment currently exists. The multifaceted therapeutic benefits of electrical stimulation of neural tissues present opportunities to develop multifunctional electroactive tissue engineering scaffolds for neurotrauma repair. The hypothesis of my work is that the architecture of electroconductive scaffolds can be designed to enhance delivery of electroactive signalling to drive neural repair.

Specifically, the aim of this work is to 3D-print tunable conductive microstructures capable of enhanced delivery of electrical stimulation, by functionalizing melt-electrowritten polycaprolactone (PCL) microfibre structures with highly conductive Ti3C2TX MXene nanosheets. These electroconductive microstructures were then incorporated into a previously developed macroporous scaffold consisting of hyaluronic acid (HA) functionalized with neurotrophic proteins. The capacity of these novel composite scaffolds to enhance the delivery of electrical stimulation to neurons is now being examined.

MATERIALS AND METHODS

Multilayer Ti3C2TX MXenes were etched from Al-rich Ti3AlC2 MAX phase and dispersed into delaminated sheets and centrifuged to form a concentrated MXene ink. To 3D-print conductive microstructures, a microfibrous PCL mesh was melt-electrowritten (MEW) with a rectilinear pattern containing fibre spacings of 500, 750 and 1000 µm (corresponding to High, Medium and Low fibre densities, respectively) and then functionalized with the MXene ink to form a conductive composite MXene/PCL structure. These 3D-printed microstructures of varying fibre density were then embedded within the neurotrophic HA-based matrix (ECM), containing collagen type-IV and fibronectin, to produce soft, biomimetic (0.6 - 3.25 kPA) composite MXene-ECM scaffolds [1]. The MXene-ECM scaffolds were then seeded with human neuronal cells or murine stem cell-derived neurospheres and electrically stimulated in for up to 7 days.

RESULTS

The electroconductive properties of the MEW MXene/PCL microstructures were highly tunable through changing fiber density and MXene content (0.081±0.053 - 18.87±2.94 S/m) and exhibited electrochemical properties equivalent to metallic electrodes. Neurons exhibited significantly increased neurite length (a 1.47 ± 0.14-fold increase) following

electrical stimulation (200 mV/mm) within the MXene-ECM scaffolds. Stem cell-derived neurospheres, electrically stimulated on MXene-ECM composite scaffolds with higher microfibre densities, exhibited a >2-fold ($p<0.05$) increase in maximum axonal length compared to lower density scaffolds and increased expression of βIII-tubulin, a marker of neuronal differentiation.

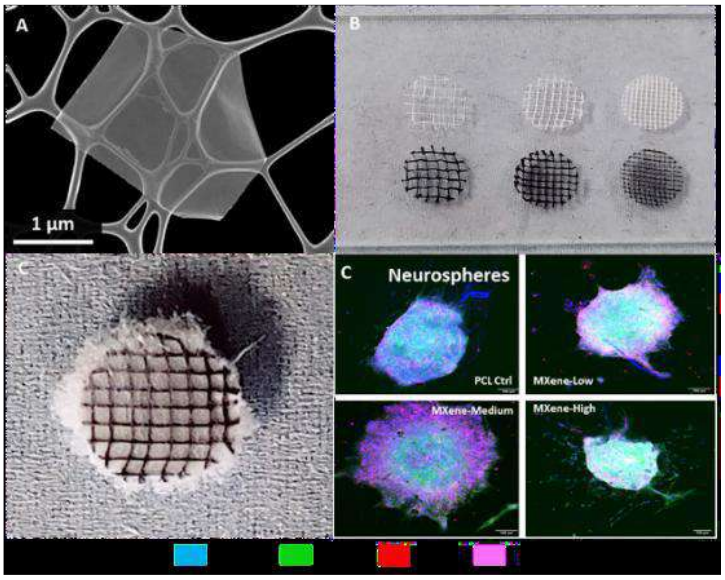

Figure 1 MXene-HA Composite Scaffolds. (A) 2D MXene nanosheets. (B) PCL & MXene/PCL MEW microstructures (C) MXene-HA Scaffold. (D) Neurospheres stimulated on MXene-HA scaffolds.

DISCUSSION

This study describes the incorporation of a highly conductive nanocomposite microstructure within a neurotrophic and immunomodulatory biomimetic scaffold, producing a novel multifunctional tissue engineering implant capable of driving key repair-relevant behaviours in neurons and neuronal stem cells by enhancing the therapeutic characteristics of exogenous electrical stimulation [2]. The biocompatibility of a MXene interface with several neural cell types is established and a tunable, electroconductive, 3D printable scaffold material for tissue engineering applications was developed. Furthermore, these findings indicate that the spatial organization of conductive materials plays an essential role in regulating repair-critical cellular responses to electrical stimulation and demonstrates the broad therapeutic potential of 3D-printable electroconductive scaffolds. This 3D-printed scaffold platform forms a key tool for the further exploration of the mechanisms that underly the pro-reparative potential of electrical stimulation which may provide novel biomaterial solutions to CNS repair.

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Selective Antibacterial Photothermal Ablation via MXene-Antibody Nanocomplexes

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The rapid emergence of antibiotic-resistant microorganisms necessitates the development of alternative antibacterial strategies that do not rely on conventional antibiotics. Photothermal therapy (PTT) has emerged as a promising non-antibiotic approach capable of inducing localized microbial destruction through light-to-heat conversion1. Among advanced photothermal nanomaterials, Ti_3C_2Tx MXene demonstrates high photothermal conversion efficiency, strong near-infrared absorption, and good biocompatibility2. To enhance selectivity and reduce off-target damage, we developed an antigen-targeted MXene-based system for precise bacterial ablation.

In this study, Ti_3C_2Tx was functionalized with polydopamine (PDA) to create a versatile surface for biomolecule immobilization3. The resulting Ti_3C_2Tx-PDA nanocomplexes were conjugated with anti-Escherichia coli (E. coli) polyclonal antibodies (ABIN3027591), generating a targeted Ti_3C_2Tx-PDA-Ab platform. The antibody was selected for its specificity toward E. coli surface antigens, enabling selective recognition of the target microorganism. Staphylococcus aureus (S. aureus) was used as a control species, as it lacks the corresponding antigen and therefore does not bind the antibody-functionalized complex. Mature biofilms of E. coli and S. aureus were established following 24-hour incubation. After removal of non-adherent bacteria, biofilms were incubated with the Ti_3C_2Tx-PDA-Ab complexes to allow selective binding. Unbound nanomaterials were washed away prior to irradiation to ensure that photothermal effects resulted exclusively from targeted attachment. Samples were then exposed to near-infrared laser irradiation at 4 W and 50 Hz for 10 minutes to induce localized heating and bacterial destruction.

The results demonstrated complete eradication of antibody-positive E. coli following targeted PTT. No bacterial growth was detected in the treated E. coli group by either resazurin assay or agar plating. Fluorescence microscopy confirmed extensive membrane disruption consistent with irreversible bacterial death. In contrast, S. aureus biofilms remained viable after identical treatment conditions, demonstrating preserved metabolic activity and colony formation. This confirms that the observed antibacterial effect was antigen-specific and not due to nonspecific photothermal damage.

These findings highlight the advantages of combining the strong photothermal properties of Ti_3C_2Tx MXene with antibody-mediated targeting. The incorporation of antibody specificity enables localized heat generation exclusively at antigen-positive bacterial sites, significantly improving therapeutic precision and reducing collateral damage. These results support the

translational promise of antibody-functionalized MXene nanoplatforms for the treatment of localized infections and biofilm-associated diseases, particularly in the context of increasing antibiotic resistance.

Keywords: MXene, antibacterial, photothermal therapy, targeted delivery

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Effect of fiber orientation and MXene integration in 3D scaffold for cardiac tissue regeneration

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Keywords: MXene, aligned, randomly, electrospun membrane, electrical conductivity, iPSC

Considering the rise in heart failure incidence and the persistently high mortality attributable to cardiovascular disease, the limited regenerative capacity of adult myocardium, heart transplantation remains the only established definitive therapy. However, broad clinical implementation is constrained due to legal, financial, and medical constraints, and tissue engineering has emerged as a promising approach for developing effective regenerative therapies [1].

In cardiac tissue engineering, the scaffold plays a key role by providing a porous three-dimensional environment for cell delivery, adhesion, and organization, as well as mechanical support and integration with host tissues to restore the mechanical and electrical function of the myocardium. Since native myocardium has a pronounced anisotropic microarchitecture with directional orientation of cardiomyocytes and collagen fibers, reproducing this structural organization in engineered scaffolds is critical for achieving functional tissue regeneration [2].

Taking into account current understanding of scaffold anisotropy and electrically conductive modifications, we investigated how fiber orientation and MXene incorporation modulate the physicochemical and biofunctional properties of electrospun polycaprolactone (PCL) scaffolds. Predominantly aligned and randomly oriented nanofiber scaffolds were fabricated with and without MXene and systematically compared the contributions of architectural cues and electroactive modification to cardiomyocyte viability, cytoskeletal organization, and functional maturation. This two-factor study evaluates two key design parameters for next-generation cardiac patches: fiber alignment and electroactivity within a single experimental framework, providing insight into their individual and combined contributions to scaffold performance.

Our results show that the electrospun membrane with randomly oriented fibers (PCL-R) exhibited significantly higher porosity (23.6 ± 0.9%) compared to aligned membrane (PCL-A) (17.6 ± 2.1%). Following MXene (MX) deposition, the porosity decreased to 6.2 ± 1.7% in PCL-A-MX and to 9.2 ± 1.5% in PCL-R-MX, corresponding to deeper infiltration of MXenes into interconnected pores. Notably, MXene integration increased the conductivity of the PCL-R scaffold (from an insulating state to ~1 S/m-1) and rendered the PCL fibers superhydrophilic. The aligned MXene-PCL fiber scaffolds induced elongated, parallel alignment of cultured cardiomyocytes, closely mimicking the architecture of natural heart muscle. In contrast, scaffolds with randomly oriented fibers provided a more isotropic structure, which, although it promoted cell growth and proliferation.

Overall, the randomly oriented, MXene-enriched scaffold exhibited the strongest combined effect by integrating anisotropic topographical guidance with a conductive and bioactive surface. This dual functionalization enhanced cardiomyocyte proliferation, alignment, and structural maturation, while eliciting a balanced immune response characterized by controlled immunostimulatory activation accompanied by compensatory regulatory feedback. Collectively, these findings support the development of advanced electroconductive, immunomodulatory scaffolds for functional myocardial regeneration. This research was funded by Horizon Europe MSCA-2021-SE-01 project ESCULAPE (#101131147) and the "Latvian Post-doctoral" research project (No 1.1.1.9/LZP/1/24/142). The Ministry of Education and Science of Ukraine provided financial support research grants No 0126U000875.

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Tailoring MXene Flake Morphology via Aerosol Jet Printing for Biological and Strain Sensor Applications

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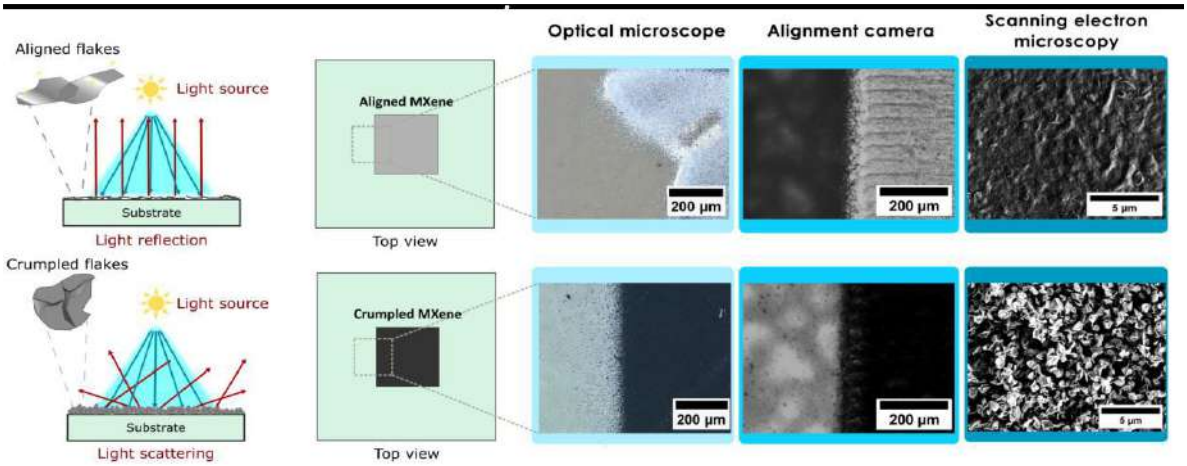
MXenes are commonly known for their 2D dimensions and single flake high-surface area, however, typical fabrication techniques can promote the restacking of flakes, limiting the available surface area and real-world applications. Due to their large aspect ratio, MXene flakes may also favour the formation of 3D structures in certain conditions, turning into crumpled particles with yet underexplored properties. This study leverages high-resolution Aerosol Jet printing (AJP) technology to precisely control MXene ($Ti_3C_2T_x$) flake morphology, and introduces a novel method for rapid in situ monitoring of the deposition of aligned and crumpled flakes. By repurposing the in-built alignment camera, we could rapidly evaluate the flake morphology based on the printed appearance: aligned flake networks exhibited a metallic lustre, whereas crumpled networks appeared darker and duller. Systematic analysis of the printing parameters revealed the critical role of the mass flow, nozzle size and ink concentration to obtain either flake type. Furthermore, the applicability of the developed method was tested with other 2D materials, including liquid phase and electrochemically exfoliated graphene and also molybdenum disulfide, demonstrating the versatility of this approach. The properties of both morphologies were also evaluated. Aligned MXene flakes obtained conductivities of up to 2672 ±125 (S/cm), while crumpled MXene films displayed enhanced hydrophilic properties and roughness. Both morphologies demonstrated potential for the development of neural interfaces, exhibiting excellent biocompatibility in several cell types, including human induced pluripotent (iPSC) derived-cells, while showing enhanced antimicrobial activity against Staphylococcus aureus when crumpled MXenes were used. Furthermore, evaluation of strain sensors based on the crumpled morphology also yielded enhanced gauge factors in the low strain regime when compared to aligned and hybrid architectures.
Overall, these results demonstrate that precise control of 2D material morphology during 3D printing is key to engineering functional properties required for manufacturing of multifunctional biomedical devices. Importantly, this low-cost strategy can be seamlessly integrated into existing AJP platforms, paving the way for scalable, high-resolution manufacturing of morphology-controlled 2D materials.



Rapid imaging of Aerosol Jet printed crumpled and aligned MXene films (Ti3C2Tx). Left: Light scatters on AJP-printed crumpled flakes (dark patterns) and gets reflected on aligned MXene printed films (glossy patterns). Right: Images captured by optical microscopy, the repurposed alignment camera, and scanning electron microscopy (SEM) on AJP-printed aligned (top) and crumpled MXene films (bottom).

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Quantitative Defect–Property Correlations in Ti3C2Tx MXenes via Precursor-Controlled Defect-Engineering

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Defect engineering offers significant potential for tailoring the multifunctional properties of MXenes. However, quantitative correlations between defect structures and material performance remain largely unexplored due to the lack of reliable strategies for precisely controlling defect densities. Here, we demonstrate that the defect density of Ti3C2Tx MXenes—including titanium vacancies, carbon vacancies, substitutional oxygen defects, and associated lattice strain—can be systematically controlled through precursor engineering. Specifically, defect densities are tuned by adjusting the carbon stoichiometry during TiC precursor synthesis and the aluminum content during Ti3AlC2 MAX phase formation. These defects propagate from the precursor phases to the resulting MXenes, enabling the fabrication of a series of Ti3C2Tx MXenes with systematically controlled defect densities. This approach enables, for the first time, a quantitative correlation between defect density and multifunctional properties, including electrical and thermal conductivity, infrared emissivity, electromagnetic interference shielding effectiveness, Joule heating performance, and oxidation stability. The defect-minimized Ti3C2Tx MXene exhibits record-high performance, including an electrical conductivity of 26,000 S cm^{-1}, thermal conductivity of 57 W m^{-1} K^{-1}, electromagnetic shielding effectiveness of 90.5 dB, Joule heating up to 263 °C at 1.5 V, ultralow infrared emissivity of 0.05, and superior oxidation resistance with an activation energy of 72 kJ mol^{-1}. Furthermore, this work establishes a comprehensive quantitative framework linking defect structures to multifunctional properties and environmental stability in MXenes.

FIB-SEM sample preparation and subsequent atomic-scale chemical and structural analysis of MAX/MXene systems by correlated STEM imaging and spectroscopy

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MXenes present complex structural and chemical heterogeneity, driven by selective etching, surface terminations, and residual precursor phases. Resolving these features requires simultaneous sensitivity to both heavy and light elements at atomic resolution. Additionally, MXenes are notoriously sensitive to air which is one of the main challenges limiting their long-term stability and applications. When MXenes are exposed to air, they oxidize, lose conductivity, and eventually structurally degrade and decompose. In this work, we present high-resolution characterization of representative MAX-derived and MXene specimens, including V-based MAX-derived structures (V–Ga–Al system) and $Ti_3C_2Cl_x$ MXene lamellae, prepared with a focused ion beam (FIB-SEM).

A low-damage FIB-SEM workflow was applied for the preparation of TEM specimens using a 16 kV stepwise thinning strategy. A key guiding principle in this approach is that, for MXene and other beam-sensitive materials, exposure to 30 kV milling should be minimized, with a transition to low-kV conditions implemented as early as possible to reduce ion beam–induced damage. The process begins with coarse milling to ~150 nm at 16 kV, followed by intermediate thinning to ~100 nm at 8 kV. Final thinning is performed at 5 kV, which constitutes the most critical stage for minimizing surface damage. A second key factor in this workflow is the use of a gas injection system (GIS) W-deposited cap layer, which provides enhanced protection against ion beam damage and enables extended low-kV milling at 5 kV without compromising specimen integrity.

This approach effectively preserves the MXene chemical composition. Additionally, keeping the transfer time of the lamellae between FIB-SEM preparation and TEM imaging to an absolute minimum was key in preventing specimen degradation and contamination.

Atomic resolution STEM imaging at 200 kV, combining HAADF, ABF, and iDPC, enables direct visualization of both heavy-element sublattices and light-element distributions within the same field of view. In particular, ABF and iDPC imaging reveal the presence or absence of light elements within atomic columns that are not accessible via Z-contrast HAADF imaging alone.

Simultaneous EDS and EELS acquisition provides complementary chemical sensitivity, enabling column-by-column compositional analysis. In the V-based MAX system, correlated spectroscopy reveals spatial variations in Ga, Al, and V occupancy, while confirming negligible In incorporation, despite its presence during synthesis. These results highlight the ability to resolve subtle substitutional chemistry across individual atomic columns. For $Ti_3C_2Cl_x$ MXene, combined STEM-EDS/EELS mapping identifies the

spatial localization of Cl terminations, with its signals confined to specific regions which correlate with contrast variations in HAADF imaging.

Overall, this work demonstrates that low damage FIB-SEM sample preparation and subsequently correlative high-resolution STEM imaging and spectroscopic mapping enables robust characterization of both atomic structure and chemistry in MXenes and their parent MAX phases. These approaches provide direct insight into termination chemistry, elemental substitution, and structural variability, which are central to understanding and tailoring MXene functional properties.

TEM sample preparation was carried out on a Helios 5 UC DualBeam, and the STEM work was carried out with an Iliad 300 STEM with Iliad EELS Energy Filter and Ultra-X EDS at the Thermo Fisher Scientific Eindhoven site in collaboration with the Nicolosi group at Trinity College Dublin.

Atomic SIMS Where It Should Not Work: MXene Aerogels

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Atomic-scale depth resolution in SIMS is considered feasible only for layered materials with crystallographic planes aligned parallel to the sample surface [1,2]. Under such geometry, the sputtering front intersects atomically flat planes, enabling layer-by-layer profiling with atomic precision. For two-dimensional materials processed as dense films or restacked flakes, this requirement is typically fulfilled. However, for three-dimensional architectures such as MXene aerogels, the assumption of preferential alignment clearly breaks down. Random orientation of flakes should, in principle, destroy the conditions required for atomic-scale depth resolution.

Yet this conclusion may be too categorical.Even in a randomly organized aerogel, individual flakes or local stacks can be oriented nearly parallel to the macroscopic surface. The challenge is therefore not the absence of suitable domains, but their identification within a large heterogeneous volume. In this work,we demonstratethat atomic-scale SIMS analysis can be extended to MXene aerogels by combining large volume three-dimensional acquisition with post-acquisition structural selection.

We acquire 3D SIMS datasets over areas of 500 x 500 µm2and approximately 1 µm in depth. The reconstructed volume is then segmented to identify local domains in which the sputtering front intersects MXene layers under near parallel geometry. By restricting depth profile analysis to these regions of interest, the effective depth resolution approaches that of conventionally aligned layered systems. This strategy converts a geometrical limitation into a statistical search problem and enables atomic-scale profiling within an otherwise randomly oriented 3D material.

This approach was applied to Ti3C2T*x*-based MXene aerogels in three configurations relevant to hydrogen storage: pristine aerogels,aerogel with Mg incorporation,and aerogel with Ni incorporation.The atom resolved depth profiles reveal three distinct hydrogen storage behaviors.

In the pristine aerogel, hydrogen is detected predominantly within the intralayer region corresponding to the M–X framework. Guided by atomistic simulations, we attribute this to hydrogen trapping in Ti vacancies stabilized by oxygen. In this scenario,hydrogen binds to oxygen located in Ti vacancy sites inside the structural layer, rather than to terminal surface groups. While SIMS cannot directly resolve the exact atomic configuration, the depth distribution is consistent with intralayer defect-mediated trapping rather than simple surface adsorption.

In the Mg-containing aerogel, SIMS indicates thatthe dominant storage mechanism appears to involve either classical hydride formation within Mg domains embedded in the MXene scaffold or enhanced physisorption and polarization of hydrogen at magnesium sites. The MXene network acts primarily as a high surface area support, while hydrogen is localized atmagnesium-rich sites.

In contrast, the Ni-modified aerogel exhibits a different behavior. The depth profiles and chemical signatures are consistent with catalytic dissociation of H2on Ni followed by hydrogen spillover onto MXene. A substantial fraction of hydrogen is associated with oxygen-terminated sites, suggesting conversion of O terminations into OH groups. This indicates a surface redox-mediated storage mechanism, distinct from both defect trapping in the pristine system and hydride formation/physisorptionin the Mg case.
Taken together, these results suggest that hydrogen storage in MXene aerogels is not governed bya single universal mechanism but depends strongly on the incorporated metal species and local defect chemistry. The combination of large volume 3D SIMS acquisition with domain selective reconstruction provides a powerful route to probe such mechanisms at atomic depth resolution,even in geometrically disordered 3D architectures.
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Self-Assembled Moiré Superlattices in Ti3C2Tx MXene: Atomic-Scale Insights for Twistronic Applications

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Nanoscale periodic moiré superlattices in two-dimensional heterostructures provide a powerful platform to engineer emergent electronic and quantum phenomena absent in their single-layer or bulk counterparts. However, an atomic-scale understanding of moiré superlattices remains largely unexplored in MXenes, one of the fastest-growing families of 2D materials. Such insight is essential for controlling their electronic functionality and enabling MXene-based quantum technologies. Here, we systematically investigate self-assembled moiré superlattices in the prototypical MXene Ti3C2Tx by combining high-resolution scanning tunnelling microscopy and spectroscopy with density functional theory calculations. Three distinct moiré patterns with periodicities of 2.52 nm, 2.39 nm, and 1.25 nm are identified. Both experiments and theory reveal that the 1.25 nm moiré superlattice exhibits pronounced spatial modulation of the density of states in the conduction band arising from electronic interlayer coupling. These results provide the first atomic-scale insight into MXene moiré superlattices and establish a foundation for twistronics based on MXenes (MXetronics), opening new opportunities for quantum device applications.

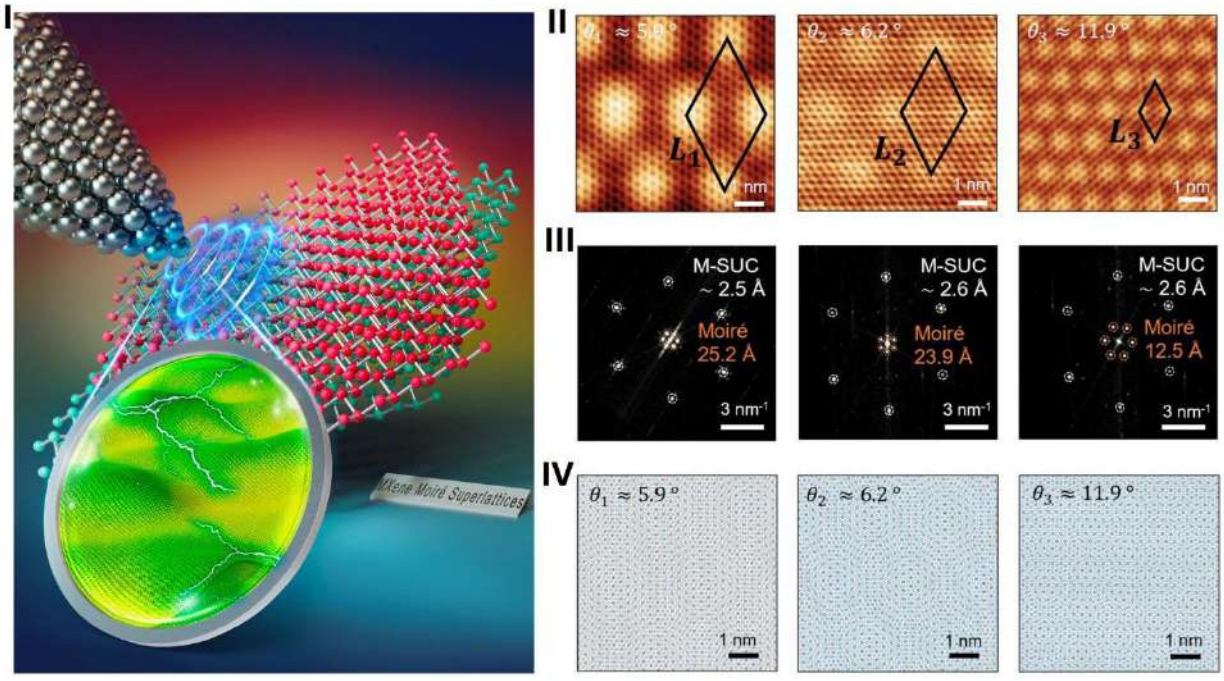

Fig 1. (I) Artistic illustration of the STM tip and twisted MXene layers. (II) STM topographic images showing Moiré patterns in MXenes at different angles (ϑ1 = 5.9°, ϑ2 = 6.2°, and ϑ3 = 11.9°, from left to right), with black rhombuses indicating the supercell. (III) Fast Fourier transform of the STM topographic images in II, where M-SUC corresponds to the MXene single unit cell. (IV) Model of simulated Moiré patterns (7 × 7 nm) of the STM topographic images in (II).

Atomic and Nanoscale Engineering of MXenes and Related 2D Materials for Energy Applications

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MXenes constitute a large family (>90 phases) of two-dimensional (2D) transition metal carbides and
nitrides with the general formula $M_{n+1}X_nT_x$, where M is an early transition metal, X is carbon and/or nitrogen, n = 1–4, and Tx represents surface terminations. Owing to their exceptional electrical conductivity, tunable surface chemistry, redox activity, and ion-hosting capabilities, MXenes have emerged as highly promising materials for electrochemical energy storage and conversion. Moreover, their layered structure and chemically active surfaces provide a versatile platform for atomic- and nanoscale engineering tailored toward targeted applications. In this presentation, we highlight how pre- intercalation strategies can profoundly alter the electrochemical behavior of MXenes by tuning interlayer spacing, ion transport, and charge-storage mechanisms, while also enabling nanoconfined synthesis. We also discuss additional atomic-level engineering approaches that enhance MXene performance in energy storage systems and electrocatalytic hydrogen evolution reactions (HER). Finally, we introduce 2D Transition Metal Carbo-Chalcogenides (TMCCs), that can be considered as MXenes but with chalcogen termination. Unlike conventional MXenes, TMCCs can be synthesized through a simple acid-free solid-state route that enables scalable production without hazardous etching chemistries. This safer and more scalable synthesis strategy opens new opportunities for expanding the landscape of 2D materials beyond traditional MXenes.

X-ray chemical imaging of electrochemical reactions on single MXene flakes

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Two-dimensional transition metal carbides, called MXenes, are an ideal platform to explore fundamental electrochemical processes under 2D confinement due to their tunable interlayer spacing and hydrophilic surface. Especially, MXenes exhibit a pseudocapacitive behavior upon cycling in aqueous electrolyte, which origin remains under discussion. Investigating MXene electrodes composed of assembly of individual MXene micro-sized flakes limits the understanding of intrinsic MXene properties that may be screened by extrinsic properties from the thick MXene film.
In this talk, I will present the nanoscale chemical imaging of individual Ti3C2Tx MXene flakes during (electro)chemical reactions. To this aim, synchrotron-based in situ scanning X-ray microscopy (SXM) will be introduced, enabling X-ray absorption spectroscopy characterization with sub-50 nm spatial resolution.1 The intercalated species can be imaged at the single MXene flake level using an in situ holder enabling imaging in liquid.2 In situ X-ray imaging during an electrochemical reaction is also possible to monitor faradaic reactions at the MXene surface.3 We will compare spontaneous and electrochemical intercalation of protons and Li+ ions in MXene flakes and discuss related chemical changes of the Ti chemical bonding. Chemical imaging of few-layered Ti3C2Tx MXene flakes will be compared to monolayered MXene flakes to discuss the effect of confinement. Finally, electrochemical reaction occurring at the sub-flake level will be imaged using SXM.

Acknowledgment
This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 947852).
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Smart Molecular Bridges for 2D MXenes

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MXenes, a family of 2D transition metal compounds, have emerged as promising materials due to their tunable surface chemistry and exceptional electrical properties, making them ideal candidates for flexible electronics and sensor applications. In this work, we present a versatile strategy to adjust interlayer spacing and interfacial interactions within Ti3C2Tx - MXenes through molecular cross-linking, achieved by sequential ligand exchange with homologous diamines. Initially, oleylamine ligands were employed to exfoliate and stabilize MXene flakes in organic solvent, facilitating their uniform dispersion. The delaminated flakes were then reassembled into thin films through controlled cross-linking using diamines with varied aliphatic chain lengths, enabling precise modulation of interlayer spacing. Grazing incidence X-ray scattering (GIXRD/GIWAXS) revealed a systematic increase of interlayer distance with increasing chain length, while density functional theory (DFT) calculations corroborated these results, indicating precise tunability based on a molecular length scale. We performed charge transport measurements of the resulting films, demonstrating a strong correlation: as the interlayer spacing increases, the electrical conductivity shows a distinct trend. Notably, longer ligands led to more separated layers, which introduced broader tunneling barriers, while shorter linkers improved inter-flake coupling, increasing conductivity.1 Beyond conductivity, the cross-linked MXene films exhibited promising chemiresistive sensing behavior.
When exposed to volatile organic compounds and water vapor, they responded with significant resistance changes. A pronounced selectivity towards H2O was observed. This selectivity is attributed to the modified interfaces of MXenes, where molecular cross-linkers act as both spacers and functional moieties, facilitating the adsorption of polar analytes and enabling rapid, reversible chemiresistive responses. By strategically tuning interlayer spacing, interface structure, and surface chemistry through molecular cross-linkers, this work demonstrates how molecular design directly influences both electronic transport and chemiresistive sensing properties in MXene systems.1

Keywords: MXene, Charge transport, Density Functional Theory (DFT), Hybrid nanomaterials, Molecular Cross-linking, Vapor sensing
Reference:
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A Cost-Effective Route to High-Purity Ti3AlC2 for High-Performance Ti3C2Tx MXene and MXene/NiO Supercapacitors

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MXenes are emerging two-dimensional materials with versatile physicochemical properties and strong potential for supercapacitor applications. However, their transition from laboratory-scale synthesis to commercial viability remains challenging due to high production cost, limited material lifespan, and severe self-stacking behavior. Previous efforts to reduce synthesis cost by using TiO2 as a precursor often led to the formation of impurity phases such as TiC, TiAl, and Ti2AlC, thereby hindering the formation of high-purity Ti3AlC2 and offering limited advantage over conventional, expensive Ti/TiC precursors. Herein, we present a cost-effective synthesis strategy for producing ultra-high-purity Ti3AlC2 MAX phase through optimization of the TiO2:Al:C molar ratio, controlled calcination conditions, and post-synthesis HCl washing. The synthesized MAX phase was subsequently converted into high-purity Ti3C2Tx MXene using a mild etching process, which contributes to improved structural stability and extended lifespan. To further overcome MXene restacking and enhance electrochemical performance, an MXene/NiO composite was fabricated via a simple bath-sonication method. Electrochemical measurements show that pristine Ti3C2Tx MXene delivers a specific capacitance of 358.5 F g-1, while the MX/NiO composite achieves a significantly higher capacitance of 892 F g-1 at a current density of 1 A g-1 within a potential window of −0.6 to 0.4 V in a 2 M H2SO4 electrolyte. Density functional theory (DFT)-based theoretical capacitance analysis of the MAX phase, MXene, and MX/NiO composite supports the experimental electrochemical results. By addressing the critical challenges of cost, purity, stability, and restacking, this approach provides a viable pathway for bridging laboratory-scale research and large-scale commercial production of MXenes, thereby unlocking their full potential for high-performance supercapacitor applications [1].

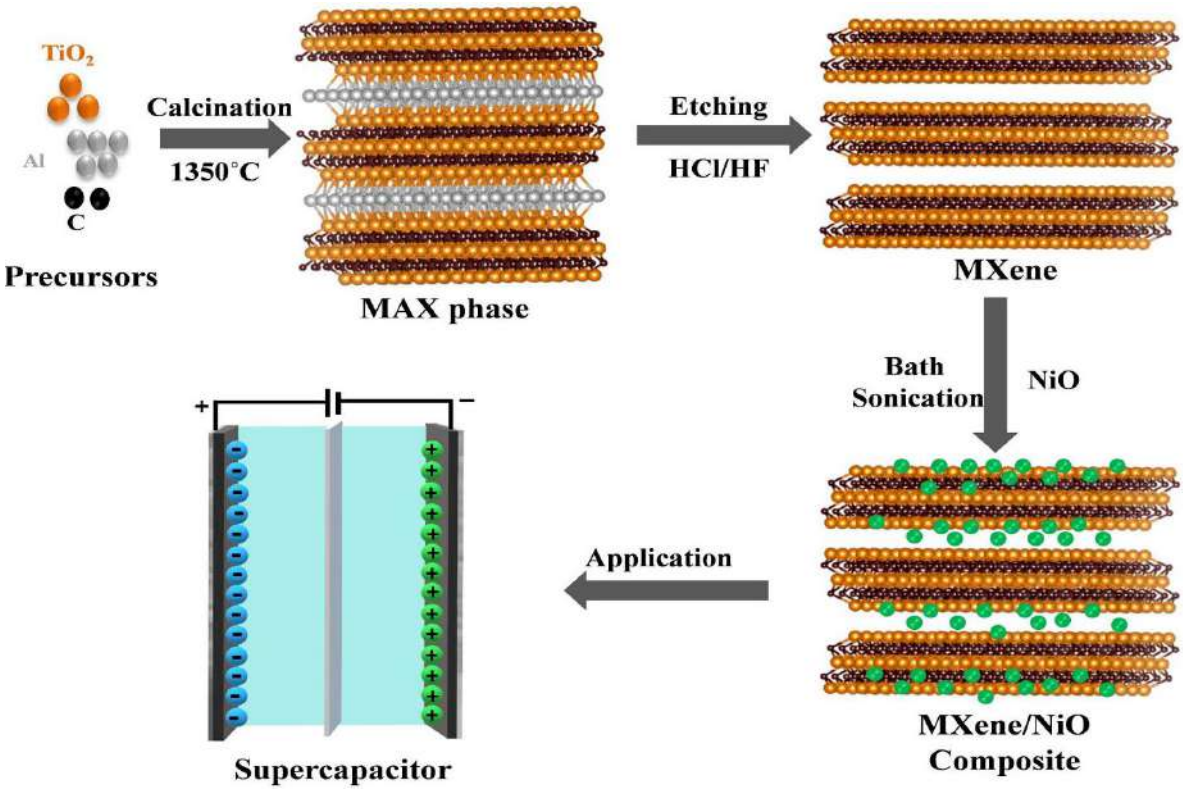

Fig.1 Schematic representation of the synthesis and electrochemical performance

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Tuneable electroconductive biomaterials for bioelectronic interfacing with human iPSC-cardiomyocyte contractility and structural organisation

Bioelectricity pervades through all biological systems from the micro cell scale to large scale tissues. Appreciating and incorporating this into biomaterial design was an underappreciated but now widely applied approach. Conductive hydrogels can replicate key bioelectrical cues of the myocardium and, when formulated as bioinks, can be shaped into microarchitectures that mimic the structural complexity of the heart. Here, we developed a tuneable electroconductive matrices and bioinks in which pH-based gelation is harnessed to regulate electrostatic interactions during mixing, so that the formulation remains printable while forming a stable hydrogel after extrusion. These biomaterials combine the electrical conductivity of conductive fillers (such as MXene and PEDOT:PSS) with the biocompatibility, biodegradability, and mechanical strength of naturally derived biomaterials (collagen type I and silk fibroin, while supporting bioprinting, matrix support and non-invasive electrical stimulation (ES) of human iPSC-derived cardiomyocytes (iCMs).

Silk fibroin (SF) gelation was strongly pH-dependent. Mixing SF with acidic PEDOT caused rapid, inhomogeneous gelation with phase separation and poor extrudability. In contrast, pH neutralisation induced a uniform composite and extended the printing window to ~10-15 minutes, with improved flow behaviour (viscosity ~100 Pa.s). The optimised formulation maintained structural integrity after extrusion and achieved high print fidelity, as shown by filament-collapse testing and printability metrics (Pr ~0.9-1.1). Separately the combination of MXene and collagen type I required pre-treatment of MXene flakes with naturally derived gelatin.

MXene/collagen type I biohybrid films enhanced iPSC-derived cardiomyocyte maturation, adhesion and inhibited microbial activity. They also exhibited mechanical, electrical, degradation and swelling properties that were directly correlated with MXene content %. Printed SF/PEDOT:PSS constructs were porous and swelled under physiological conditions, which softened the gels from ~200 kPa to ~120 kPa (functionally relevant for iCMs). iCMs showed improved contractility and sarcomere organisation on softer, more conductive SF/PEDOT hydrogels with higher PEDOT content (0.26%) compared with stiffer formulations with 0.12% PEDOT, with no major change in spontaneous beat rate.

We further applied non-invasive capacitive-coupling ES using a 10 kHz biphasic square-wave carrier (18 V) delivered in 5 ms bursts at 2 Hz (generated as an arbitrary waveform in MATLAB). While stimulation did not pace beating to the input frequency, the stimulated groups showed an increase in beating rate compared with non-stimulated controls. Qualitative observations also indicated improved structural organisation in stimulated groups, with no clear differences between bioink formulations spanning conductivity and stiffness. Overall, the SF/PEDOT bioink platforms were found to be compatible with non-invasive ES and supported preliminary bioprinting with hiPSC-derived cardiac fibroblasts showing good post-print viability, highlighting its potential for bioprinted cardiac bioelectronic interfaces.

Acknowledgements
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Deeper understanding of Zn electrodeposition mechanisms on Ti3C2Tx MXene

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The development of electrochemical energy storage systems based on chemistries beyond lithium-ion technology is attracting increasing interest. In this framework, zinc-ion batteries (ZIBs) and hybrid zinc-ion supercapacitors (ZISCs) stand out as promising alternatives due to the favorable characteristics of zinc chemistry, such as high energy density, rapid charge–discharge capability and improved safety compared to lithium-based systems [1]. Nevertheless, during the charging process, the electrochemical reduction of Zn^{2+} ions to metallic zinc often results in inhomogeneous nucleation on the anode surface, triggering dendritic growth and leading to premature cell failure. Surface modification strategies that enhance the zincophilic nature of the electrode have been proposed as an effective approach to mitigate these issues and regulate zinc deposition behavior [2].
MXenes, and in particular $Ti_3C_2T_x$, have recently emerged as attractive interfacial materials capable of promoting uniform and highly reversible Zn plating/stripping processes [3]. Although lattice matching between hexagonal Zn and $Ti_3C_2T_x$ has been suggested as a key factor driving smooth and preferentially oriented Zn growth, the interfacial electrochemistry of Zn^{2+} at MXene surfaces remains only partially understood. In this work, we have investigated the electrochemical response of inkjet-printed $Ti_3C_2T_x$ MXene thin films in $ZnSO_4$ electrolyte, with a specific focus on zinc storage mechanisms in both the underpotential deposition (UPD) and overpotential deposition (OPD) regimes. Electrochemical analyses combined with morphological and microstructural characterization indicate that Zn deposition in the UPD region is governed by a combination of surface-controlled and solution-controlled processes. In particular, in situ Raman spectroscopy and electrochemical atomic force microscopy (EC-AFM), together with X-ray photoelectron spectroscopy (XPS), provide evidence for metallic Zn underpotential deposition occurring within a narrow potential window preceding bulk Zn plating. In addition, the effect of MXene flake size on Zn crystal growth is examined, revealing that smaller flakes can negatively influence the development of well-defined hexagonal Zn crystals [4]. We, in fact, demonstrated that the lateral size of $Ti_3C_2T_x$ MXene flakes plays a decisive role in regulating Zn nucleation and growth: electrodes composed of larger flakes form interconnected conductive networks with fewer defects and more homogeneous charge distribution, which favors epitaxial-like Zn deposition along the stable (002) plane. As a result, these electrodes enable long-term, dendrite-free cycling for more than 600 hours with stable Coulombic efficiency.

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Chlorine Terminated MXenes Based Separators for Advanced Li-S Batteries

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Lithium–sulfur (Li–S) batteries have emerged as one of the most promising next-generation energy storage systems due to their exceptionally high theoretical energy density (~2600 Wh kg^{-1}), natural abundance of sulfur, and low material cost compared to conventional lithium-ion batteries based on transition-metal oxides.1 Sulfur offers a high theoretical specific capacity of 1675 mAh g^{-1} through the multielectron conversion reaction between sulfur and lithium. These advantages make Li–S batteries highly attractive for applications ranging from electric vehicles to grid-scale energy storage. However, despite their theoretical potential, practical implementation remains hindered by several critical challenges. The most significant among these is the "polysulfide shuttle effect," where intermediate lithium polysulfides (Li_2S_x, $4 \leq x \leq 8$) dissolve in the electrolyte and migrate between the cathode and anode. This results in active material loss, low Coulombic efficiency, rapid capacity fading, and poor cycling stability.2

In this context, two-dimensional (2D) materials known as MXenes have gained considerable attention. MXenes are a family of transition metal carbides, nitrides, or carbonitrides derived from MAX phases, where "M" represents an early transition metal, "A" is a group 13 or 14 element, and "X" is carbon and/or nitrogen. Since the first successful synthesis of Ti3C2Tx from Ti3AlC2 in 2011, MXenes have demonstrated exceptional properties, including metallic conductivity, hydrophilic surfaces, high mechanical strength, tunable surface chemistry, and large specific surface area. 3

Our work demonstrates the modification of pristine polypropylene separator with Ti2CCl2-based MXenes. The high electronic conductivity and large surface area of Ti2CCl2, along with chlorine surface terminations "T_x," provide abundant active sites, accelerating the transformation between soluble polysulfides and insoluble Li_2S/Li_2S_2 species. Second, the polar surface functional groups on MXenes provide strong chemisorption toward lithium polysulfides, effectively immobilising them and mitigating their diffusion to the lithium anode. This chemical confinement significantly suppresses the shuttle effect and enhances Coulombic efficiency. Moreover, it is noteworthy that within the operational voltage range of Li-S batteries (1.7- 2.8 V), the Ti_2CCl_2 catalyst does not undergo lithium self-deintercalation, remaining electrochemically inactive in Li–S battery reactions while exhibiting excellent structural stability. Moreover, the layered 2D structure of MXenes forms a dense yet ion-permeable network when coated onto conventional polypropylene separators. This architecture creates a physical barrier that prolongs polysulfide diffusion pathways while still allowing efficient lithium-ion transport. The interlayer spacing of MXenes can also be tuned to optimise ionic conductivity and electrolyte wettability. Moreover a facile spray coating strategy is used to coat the MXenes flakes on top of the separator. This technique enables the formation of uniform and ultrathin coatings, ensuring homogeneous coverage of active materials along with tunable thickness. Figure 1 presents the galvanostatic charge/discharge curves of Li-S batteries containing Ti2CCl2 coated

separator. A very high initial capacity of 1285 mAh/g was achieved at 400mA/g of current density, after 135 continuous charge/discharge cycles, 1030 mAh/g of capacity was achieved, with 80.1% of capacity retention and a low decay rate of 0.15%/ cycle.

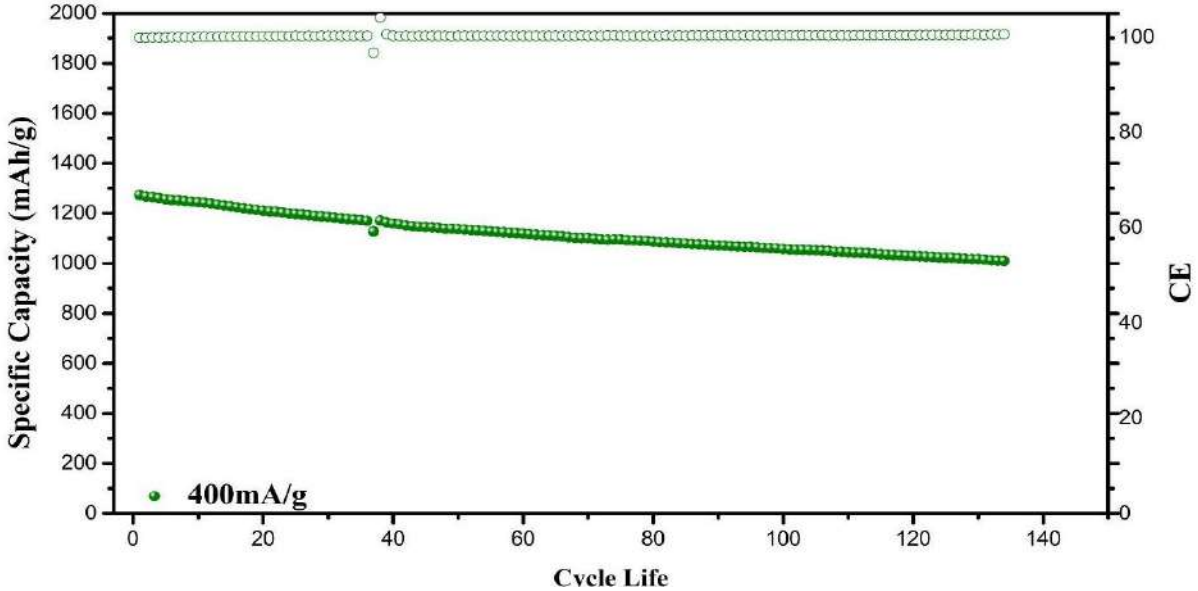

Fig. 1 Galvanostatic charge/discharge curves of Ti2CCl2 MXene-based separator for Li-S battery.

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Plasma Surface Engineering of 2D Metallic Carbides for Advanced Supercapacitors

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The Supercapacitor (SC), an advanced energy storage device, is essential for modern power applications; however, its energy performance still requires significant improvement for widespread commercialization.
Considering the key role of advanced electrode materials in enhancing energy storage properties, 2D
MXenes are emerging as frontrunners. Even though 2D MXenes, derived from their MAX precursors, exhibit ultra-high intrinsic conductivity, a unique stacked structure, and excellent electrochemical properties, non-essential surface terminations and the tendency to restack are bottlenecks to using MXene as a stand-alone material for SCs. Besides, the presence of undesirable fluorine terminations on MXenes resulting from conventional synthesis routes, typically involving hydrofluoric acid etching of MAX phases, can hinder ion diffusion, compromise structural stability, and reduce the number of electrochemically active sites, thereby limiting electrochemical capacitance. Engineering the interlayer spacing within the stacked structure of MXenes or selectively switching the surface terminations are promising approaches to addressing these challenges, thereby improving both charge storage performance and cycling life of the material. This is commonly achieved by modifying the termination groups on the MXene surface. In this work, we propose controlled surface engineering of MXenes using a plasma-assisted soft-chemistry approach, enabling the incorporation of heteroatoms and switching of functional groups without compromising MXene structural integrity. Plasma-surface modification has demonstrated high potential for altering the surface chemistry of 2D materials [1,2], including MXenes, by enabling stoichiometric control of
their elemental composition, thereby allowing the functionalization of MXene with desired surface terminations. Herein, the rapid plasma dry process using a sulfur-containing environment enables the incorporation of sulfur into the MXene surface and is completed in just 5 minutes, offering significant advantages, including a short reaction time, high energy efficiency, and reduced hazardous byproducts.
Furthermore, electrochemical energy storage analysis demonstrates a significant ten-fold increase in specific capacitance (733 F g-1 vs 62 F g-1 for sulfur-treated Ti2C vs Ti2C) and superior rate capability due to these controlled changes in surface terminations and interlayers. Additionally, the fabricated asymmetric device demonstrated good energy storage capabilities with energy-power densities, highlighting the advantages of plasma surface engineering. These findings reveal that a fast, facile, and cost-effective plasma surface-engineering process establishes a promising pathway for scalable surface modification of MXene-based electrodes, enabling their practical application in high-performance supercapacitors.

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$Mo_2V_2C_3T_x$ Free-Standing Films as Nucleation Layers for Zero-Excess Sodium Metal Batteries

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Sodium metal batteries (SMBs) offer a exciting pathway toward low-cost, high-energy electrochemical storage due to the natural abundance of sodium, low redox potential (–2.71 V vs. SHE), and high theoretical specific capacity of Na metal (1166 mAh g^{-1}). In particular, anode-free sodium metal batteries, where Na is plated in situ onto a bare current collector, present a transformative opportunity to maximise gravimetric and volumetric energy density by eliminating excess metallic sodium from the cell architecture. However, the practical implementation of both Na metal and anode-free configurations remains severely constrained by unstable Na nucleation, high interfacial resistance, dendritic growth, and rapid depletion of active sodium during cycling. These issues are strongly influenced by the chemical and electronic properties of the substrate onto which Na is plated. Conventional metallic or carbon-coated current collectors provide limited control over Na nucleation kinetics and interfacial energy, often resulting in heterogeneous deposition, localised current hotspots, and morphological instability, particularly under high current densities and high areal capacities. MXenes offer a promising materials platform for interface engineering in sodium metal systems. Their high intrinsic electronic conductivity, tunable surface terminations and layered morphology make them attractive candidates for regulating alkali metal nucleation. Importantly, bimetallic MXenes introduce additional compositional degrees of freedom, enabling modulation of electronic structure and surface adsorption energetics beyond what is achievable with single-metal systems. This compositional tunability provides a rational pathway to optimise Na nucleation behaviour and suppress dendritic growth under demanding electrochemical conditions.
Here, we report the synthesis of $Mo_2V_2C_3T_x$ MXene via HF etching and its fabrication into free-standing ultrathin films using vacuum-assisted filtration. When evaluated as sodium metal hosts, $Mo_2V_2C_3T_x$ films demonstrate a substantially reduced Na nucleation overpotential (14.32 mV) compared to identically prepared $Ti_3C_2T_x$ films (25.73 mV), indicating enhanced sodiophilicity and improved Na–substrate interaction. Under high-rate conditions (5 mA cm^{-2}, 5 mAh cm^{-2}), the bimetallic films exhibit excellent cycling stability and reversible Na plating/stripping behaviour. Post-mortem analysis reveals homogeneous Na deposition and effective dendrite suppression, confirming improved interfacial regulation relative to monometallic counterparts. These findings highlight the potential of bimetallic MXenes as high-rate sodium metal hosts and establish a materials design strategy for controlled Na nucleation. Ongoing work focuses on integrating these architectures into anode-free Na||Prussian blue analogue full cells, advancing toward practical zero-excess sodium metal battery configurations.

Mapping delocalized faradaic processes at isolated MXene flakes using correlative single-entity electrochemistry

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Due to their unique properties, MXenes are promising building blocks for the fabrication of high-performing electrodes in energy conversion/storage devices. MXene electrodes typically consist of 3D networks, often displaying porosity, which presents significant challenges when attempting to investigate and correctly interpret chemical motifs or factors that give rise to optimal performance. Correlative methods that enable characterization of single entities by electrochemistry and microscopy/spectroscopy are therefore increasingly needed to elucidate structure-function relationships of MXenes and other 2D nanomaterials with applications in electrochemical systems.1-3
In this presentation we discuss a novel methodology for probing the electrochemical response of individual $Ti_3C_2T_x$ MXene flakes and correlating it to thickness and chemical changes. First, carbon thin films with homogeneous surface chemistry are introduced as high-performing conductive substrates that provide outstanding topographic and electrochemical contrast for the characterization of isolated 2D nanomaterials.3 Initial validation of the capabilities of these sample architectures via studies of the capacitive response of individual flakes using scanning electrochemical cell microscopy (SECCM) was recently reported.2 Building on this, we demonstrate that this sample architecture also enables correlative characterization via Scanning X-ray Microscopy (SXM) and SECCM. SXM in transmission and total yield modes at the Ti- and O-edges can be used to map changes in chemical composition resulting from electrochemical probing with exquisite spatial resolution (<50 nm). We demonstrate SXM-SECCM mapping of the reaction fronts arising from localized (<1 μm2) electrochemical stimuli that trigger long-range (>10 μm2) proton-coupled faradaic reactions across the surface of individual $Ti_3C_2T_x$ monolayers. We hypothesize that fast surface proton diffusion is at the origin of delocalization and discuss how SXM-SECCM can be used to probe the role of interfacial water as well as possible implications for the design of MXene 3D networks.

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Understanding the Role of MXenes in Beyond Conventional Catalysts for the Oxygen Evolution Reaction

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In the Electrocatalysis Synthesis to Devices Group at Helmholtz-Zentrum Berlin, our research is focused on combining MXenes, Figure 1, and water splitting active materials to create the next generation Oxygen Evolution Reaction (OER) catalysts. Metal oxides, e.g. Ni oxides, are known to be the most active materials for the OER in alkaline media but lack high conductivity and exhibit only average OER overpotentials. On the other hand, MXenes are highly conductive but oxidise readily under several conditions due to its termination sites and don't contain OER active sites.1, 2 To overcome these issues, we employ several strategies in our group to combine these two materials to make one material which is OER active and highly conductive. Furthermore, by blocking the MXene termination sites with metal-based materials, this may lead to less oxidation of the MXenes structure.
This presentation will focus on the development of hybrid MXene materials for the OER through various fabrication methods to produce Green H2.3-6 In this talk, the research conducted in this area from our group will be shown and vital information on optimizing MXenes for the OER will be discussed.

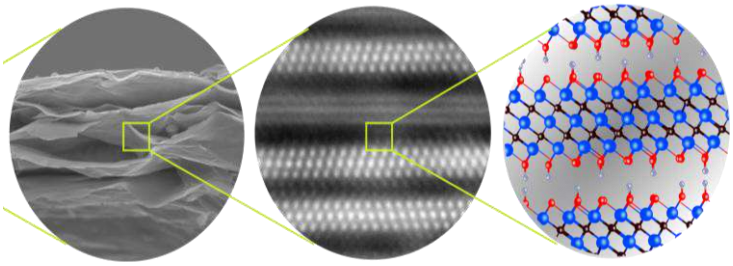

Figure 1. Ti3C2Tx MXene

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(2) Current Opinion in Electrochemistry, 34, 101021 (2022)
(3) Electrochimica Acta, 490, 144269 (2024)
(4) ChemElectroChem, e202400656 (2025)
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(6) Advanced Functional Materials, 2503842 (2025)

In-operando probing of MXene interfacial reactivity using machine-learning simulations with first-principles accuracy

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The surface functional groups of Mxenes are of particular interest, as they result from the interaction between the material and its environment and are therefore strongly influenced by the operating conditions. This is especially important, as during electrochemical screening. the functional groups undergo protonation and deprotonation processes, contributing to the exceptionally high pseudo capacitance of Mxenes.
Density functional theory (DFT) calculations are a powerful tool for gaining atomic-scale insight into
MXene behavior and are essential for rationalizing experimental observations obtained from techniques such as cyclic voltammetry, X-ray photoelectron spectroscopy (XPS), and X-ray absorptions pectroscopy (XAS). However, to date, the applicability of these simulations to realistic experimental conditions has been limited. Largely due to computational cost, most studies have been restricted to vacuum calculations, poorly controlled electrode potentials, and simplified or unrealistic surface compositions.
Building on previous studies that have elucidated the complex interplay between pH, electrode potential,and surface group composition in $Ti_3C_2T_x$ [1,2], we propose to develop a machine-learning (ML) interatomic potential based on the MACE architecture and fine-tuned using DFT. This potential will be used to construct a model of $Ti_3C_2T_x$ with a realistic -O/-OH functional-group coverage (Fig. 1.a), in contact will an aqueous electrolyte subjected to a well-defined potential and pH.
Using this model, we will be able to perform long Molecular Dynamics (MD) simulations, in the
nanosecond range, usually unachievable for ab initio MD, while supporting DFT calculations will allow us to track the electrode potential during the simulations (Fig. 1.b). In particular, we will investigate processes such as the charging and discharging behavior of $Ti_3C_2T_x$ and the interaction between ions and surface functional groups, thereby providing deeper insight into the underlying mechanisms at play.

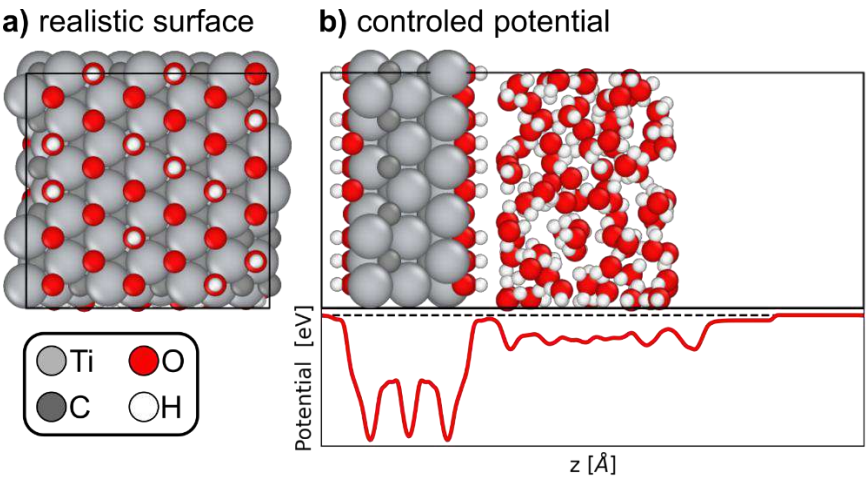

Figure 1: atomistic model, in a) the realistic functional group covering of $Ti_3C_2T_x$, and in b) a description of the Mxene/electrolyte model, the DFT calculations provide a method for obtaining the electrode potential.

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Porous MXenes for Gas Applications

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Porous MXenes are interesting prospective materials that are yet to be properly explored for adsorptive applications. They have a range of characteristics that makes them quite distinctive from other porous materials – they have high electrical and thermal conductivities, high mechanical strength, chemical stability and hydrophilicity, which are derived from their unusual combination of ceramic and metallic features. Porosity is key for many applications and making more of the MXene surface available increases performance in many applications, including catalysis, energy storage or gas applications. MXenes also offer a wide range of compositional varieties, since they can be made many different elements. To date, more than 30 MXenes have been synthesised but many more are predicted to exist theoretically.
We have successfully adapted strategies from heterogeneous catalysis to create porous MXenes. These techniques involve the use of pillaring agents between MXene layers, which increase the surface area of the materials and their interlayer spacings, achieving BET surface areas as high as 235 m2 g-1 and interlayer spacings up to 3.2 nm. In the past, we have shown how CTAB and DDA-TEOS can be intercalated in MXene materials and have tested these materials as hybrid capacitors for Zn-, Na- and Li-ion [1,2,3], where they showed better capacities and stability compared with non-modified MXenes. There are many advantages in exploring porous MXenes for adsorption applications, as MXenes can display properties that are unique in comparison with the porous materials that are typically used. Adsorption is key for applications related to gas storage and separations, and materials' enhancements are critical to enable new technologies coming to the fore, such as hydrogen storage or carbon capture. Both these applications represent two of the main challenges currently facing the research community and are critical to address problems related to clean energies.
In this talk, we will show different techniques for creating porosity in MXenes. These include the use of different intercalants such as ammonium precursors (butyl ammonium, octyl ammonium, dodecyl ammonium), amines and silica, coupled with thermal treatments, which increase porosity and interlayer distances. We also explore other techniques such as organic templating to obtain MXenes with increased surface areas. The resulting materials are characterised with techniques that include powder X-ray diffraction, Raman spectroscopy, SEM, elemental analysis and nitrogen adsorption. We show how different synthetic strategies lead to different interlayer spacings (which can be controlled depending on the intercalant), different BET surface areas and different pore size distributions. Some of the materials show high increases in BET surface areas, going from essentially a non-porous material to a material that has a BET surface area in excess of 200 m2 g-1.
MXenes have been proposed as prospective hydrogen storage materials, as the interlayer spacings can be tuned to maximise interactions with molecular hydrogen [4]. We show results for hydrogen adsorption in porous MXenes under a wide range of temperatures and up to 200 bar, and their surface properties, including porosity and chemical composition, are correlated with their hydrogen uptake.

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Aerosol Jet Printed MXene Microsupercapacitors for Flexible and Washable Textile Energy Storage

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The increasing demand for miniaturized and flexible wearable electronics is driving the rapid growth of research into materials for electronic textiles (e-textiles). In this context, microsupercapacitors (MSCs) are becoming essential as energy storage solutions, offering high-power density and extended lifespans. Herein, a novel approach is introduced using aerosol-jet printing (AJP) to fabricate e-textiles with additive-free, pseudocapacitive Ti3C2Tx MXene ink. AJP offers superior resolution and cost-effectiveness for rapid prototyping, while Ti3C2Tx exhibits excellent electrical conductivity, solution-processability, electrochemical activity, and mechanical flexibility. Our printed flexible MXene@Fabric electrodes achieve high areal capacitance of up to 4.4 F cm-2, high rate capability, excellent cyclability, and good washability. The fabricated current collector-free symmetrical MSCs on cotton deliver an areal capacitance of 381 mF cm-2 (at 2 mV s-1) in poly(vinyl alcohol)/sulfuric acid gel electrolyte, outperforming current printed MXene/textile-based MSCs. These findings demonstrate the transformative potential of integrating MSCs via AJP, paving the way for enhanced energy storage in a wide variety of flexible, breathable, and washable textile-based devices, thereby catalyzing a paradigm shift in wearable electronics.

Reassessment Hypotheses of Physicochemical and Electrochemical Aging Mechanisms in $Nb_4C_3T_x$ MXene for Energy Storage Applications

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During the sintering process of the MXene precursor, the formation of vacancies within the carbon sublattice may occur. The degradation rate of delaminated MXenes in aqueous colloidal suspensions can qualitatively reflect the defect concentration present in the corresponding MAX phases.1 Furthermore, the long-term performance stability of niobium-based MXenes remains a critical barrier to their practical implementation in electrochemical energy storage technologies. While previous research has focused on strategies to mitigate performance loss 2,3, such as electrolyte engineering, the fundamental physicochemical aging processes remain poorly understood. In this work, we undertake a systematic analysis of previously acquired experimental data to unravel the probable aging mechanisms of Nb2CTx and Nb4C3Tx MXene and their impact on electrochemical behavior. EDS spectra and EDWS images reveal the presence of oxygen in freshly prepared MAX phase samples that were previously exposed to ambient conditions prior to analysis. Oxidation processes could be started at the precursor stage and progressively intensified throughout the post-etching washing and delamination steps, persisting during storage. This possibility can intensively affect the galvanostatic cycling operation. Other degradation possible processes are interlayer collapse, delamination, and relevant associated impedance growth in at least one magnitude degree. To synthesize MAX phases used in this work, Nb, C, and Al were used as raw materials, in approximately stoichiometric proportions, in powder form. This powder mixture is compressed and synthesized in an oven at temperatures between 1550 and 1700 °C, depending on the planned MAX phase (Nb2AlC in the lower range or Nb4AlC3 in the upper range). MILD method was used to obtain Nb2CTx and Nb4C3Tx MXene: MAX phase, LiF, and HCl were stirred at 50 ºC for 96 h. After the reaction, the material was washed with DI water until pH ~ 6, and was added to TMAOH, stirred for 12 h at room temperature, and was washed with DI water again to reach a pH ~ 6. Finally, MXene was dispersed in deionized water and deposited onto glassy carbon via drop-casting. Furthermore, freshly synthesized and aged Nb4C3Tx samples were prepared and characterized by a suite of complementary analytical techniques, including scanning electron microscopy (SEM), electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and galvanostatic charge–discharge (GCD) analysis. In this focus, it was possible to isolate and examine specific signatures of degradation that arise over time, independently of electrolyte additives. EIS analysis indicates a notable increase in charge-transfer resistance and changes in solution resistance metrics as aging progresses, if compared with the previous work of this research group4. Galvanostatic charge and discharge measurements further indicated the possibility that structural and interfacial

changes correlate with diminished ionic accessibility and reduced pseudocapacitive performance. It is an exception when using water-in-salt electrolyte. Comparing EIS data from that previous work4 and this, it is important to notice that the real and imaginary components of electrochemical impedance increased around 10 times (including before and after GCD cycling). Both of them showed external and lamellar double-layer sequenced behaviour. However, the aged material showed one more component effect: pore presence influenced more in this one. Furthermore, these data can suggest possible targets for future investigation about stabilizing strategies of MXenes in energy storage contexts.

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