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POSTERS ABSTRACTS BOOK

#0

Enhancing Mechanical and Surface Properties of EP Copolymers with $Ti_3C_2T_x$ MXene Reinforcement

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Two-dimensional MXenes have emerged as highly promising nanomaterials due to their unique combination of high surface area, tunable surface chemistry, electrical conductivity, and mechanical reinforcement capability. Among them, $Ti_3C_2T_x$ has demonstrated remarkable potential as a multifunctional nanofiller in polymer-based nanocomposites [1–3]. This study investigates the fabrication of $Ti_3C_2T_x$ MXene/ethylene–propylene copolymer nanocomposite films via blade coating. $Ti_3C_2T_x$ was synthesized from the commercial MAX phase Ti_3AlC_2 using the MILD etching protocol and incorporated into the polymer matrix at loadings of 0.5, 1.0, 1.5, and 2.0 wt%. The coating parameters were optimized by controlling blade gap, coating speed, and substrate temperature.

Mechanical performance was strongly dependent on MXene content. For Vistamaxx 6102, hardness increased from 32.3 MPa (neat polymer) to 56.5 MPa at 2 wt% MXene, while for Vistamaxx 6202, hardness increased from 19.7 MPa to 51.6 MPa at 1.5 wt%, followed by a reduction at 2 wt% (29.3 MPa), indicating possible filler agglomeration at higher loadings. Elastic modulus exhibited distinct trends for each matrix. In Vistamaxx 6102, the modulus slightly increased from 0.214 GPa (neat) to 0.218 GPa at 1.5 wt%. In contrast, Vistamaxx 6202 showed an initial increase from 0.241 GPa to 0.270 GPa at 0.5 wt%, followed by a decrease at higher concentrations, suggesting concentration-dependent microstructural rearrangements. Nanotribological analysis revealed a significant reduction in the coefficient of friction (COF) with MXene incorporation. For Vistamaxx 6102, COF decreased from ~2.2 (neat) to ~0.7 at 0.5 wt%. Similarly, Vistamaxx 6202 exhibited a reduction from ~3 to ~1.3 at intermediate loadings. These results demonstrate that MXene incorporation enhances stiffness, hardness, and tribological performance, with optimal improvements depending on filler concentration, highlighting the importance of processing–composition interplay in blade-coated MXene/polyolefin films.

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#1

Label-Free Nb_4C_3, $Mo_2Ti_2C_3$, and Ta_4C_3 MXenes reprogram monocyte and macrophage activation toward an anti-inflammatory state

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Macrophages are central effectors of innate immunity whose phenotypic plasticity supports both inflammation and its resolution. However, dysregulated macrophage activation underlies a wide range of inflammatory, infectious, and degenerative diseases, making the identification of materials that can fine-tune macrophage responses of high therapeutic interest. Here, we show that three two-dimensional MXene nanomaterials, Nb_4C_3, $Mo_2Ti_2C_3$, and Ta_4C_3, are efficiently internalized by murine monocytes without compromising cell viability, while actively reprogramming their activation and differentiation toward an anti-inflammatory macrophage state .

Using an integrated approach that combines bulk RNA sequencing, flow cytometry, cytokine profiling, and single-cell mass cytometry (CyTOF), we demonstrate that these MXenes are not immunologically inert but instead induce a convergent immunomodulatory program. Transcriptomic profiling of MXene-treated monocytes reveals a shared signature characterized by downregulation of inflammatory and chemotactic genes, including *Cxcl9*, *Cxcl10*, *Ccl24*, *Il1b*, and *Il18*, together with reduced expression of the chemokine receptor *Ccr2*. In parallel, *Cd28* is consistently upregulated across all MXene treatments, suggesting engagement of regulatory pathways associated with restrained immune activation. Pathway enrichment analyses confirm broad suppression of cytokine production, interferon-related signaling networks, and macrophage activation programs.

At the protein level, secretion of CXCL10 and CCL24 is significantly reduced following MXene exposure, validating the transcriptional findings and indicating functional attenuation of pro-inflammatory and chemotactic outputs. In addition, transcripts linked to classical inflammatory polarization, including *Cd86*, *Stat1*, and *Nos2*, are decreased, while genes associated with regulatory or tissue-supportive programs show relative

enrichment. These coordinated changes indicate that MXenes do not simply redirect macrophages from one polarized state to another, but instead constrain excessive commitment to either inflammatory or alternatively activated phenotypes.

Functionally, early exposure of bone marrow precursors to MXenes increases the fraction of non-polarized (M0-like, $CD86^{-}/CD206^{-}$) macrophages after differentiation, while reducing both $CD86^{+}$ (M1-like) and $CD206^{+}$ (M2-like) subsets. Moreover, MXenes dampen basal macrophage activation and significantly attenuate LPS-induced CD69 upregulation, demonstrating the capacity to counteract strong pro-inflammatory stimuli without inducing cytotoxicity. Consistent with transcriptional downregulation of *Ccr2*, surface CCR2 expression is reduced, supporting a phenotype less prone to inflammatory recruitment.

A distinctive feature of Nb_4C_3, $Mo_2Ti_2C_3$, and Ta_4C_3 MXenes is their intrinsic detectability by CyTOF through natural metal isotopes, enabling simultaneous, label-free tracking of nanomaterial uptake and immune phenotype at single-cell resolution. Exploiting this property, we show that following intraperitoneal administration, peritoneal macrophages efficiently internalize MXenes while maintaining viability. In a thioglycollate-induced peritonitis model, MXene co-treatment partially attenuates the recruitment of monocyte-derived inflammatory macrophage subsets and stabilizes resident-like populations, in line with the observed suppression of chemokine production and CCR2-dependent trafficking pathways.

Collectively, these findings identify Nb_4C_3, $Mo_2Ti_2C_3$, and Ta_4C_3 as intrinsically immunoregulatory nanomaterials that promote a low-activation, low-recruitment macrophage state while remaining traceable without external labeling . By integrating immune modulation with high-dimensional single-cell tracking, these MXenes represent a versatile platform for the rational design of next-generation immunoengineered biomaterials aimed at controlling macrophage-driven inflammation in regenerative medicine and inflammatory disease settings.

Keywords: Macrophages, Monocytes, MXene, Biocompatibility, Nanomedicine.

#2

Aminosilane functionalised MXene enables a stable organic solvent based silk fibroin electrospinning formulation for nanofibrous bioelectronic scaffolds

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Abstract

MXenes are attractive for bioelectronic interfaces due to their high intrinsic electrical conductivity and surface chemistry, yet their integration with natural polymers remains challenging due to MXene nanosheets being prone to oxidation and aggregation during solution processing, which can compromise dispersion homogeneity and downstream electrical performance. Herein, we report an organic-solvent process route to fabricate electrospun silk fibroin (SF)/$Ti_3C_2T_x$ (MXene) fibrous scaffolds by first functionalising MXene with the aminosilane N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (AETMS) to grant a positive zeta potential and improve colloidal stability in an acidic organic solvent like hexafluoro-2-propanol (HFIP). Electrospinning formulations were prepared using 12% (w/v) SF while the AETMS-MXene content was varied from 3-10 wt% with respect to SF, yielding homogeneous spinning formulations and reproducible ECM-mimetic fibrous mats without visible agglomeration and bead formation. The resulting composite mats retain the characteristic nanofibrous morphology of electrospun SF and support robust handling. Specifically, the electrospun mats with higher MXene content exhibited increased tensile strength and ductility relative to those with lower MXene content. The electrical testing indicates signal transmission under a pulsed waveform (8 V, 100 Hz) indicating frequency-dependent electrical response (e.g., capacitive/AC charge transport), despite low DC conductivity (~10^{-10}-10^{-8} S/m) at the current formulation stage. In-vitro assays confirm cytocompatibility of the SF/MXene fibers with a mouse C3H10 fibroblast cell line, supporting their suitability as biocompatible scaffolds for future electrically active tissue engineering and biosensing applications. Collectively, this work establishes an aminosilane-enabled strategy to stabilise MXene in HFIP-based SF processing and provides a scalable platform for developing next-generation natural- polymer/MXene bioelectronic fibrous interfaces.

Acknowledgements

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#3

Operando XAS investigation of CuCo hybrid catalysts on V_2CT_x and $V_4C_3T_x$ MXenes: Structure-Activity Relationships in Oxygen Evolution Reaction

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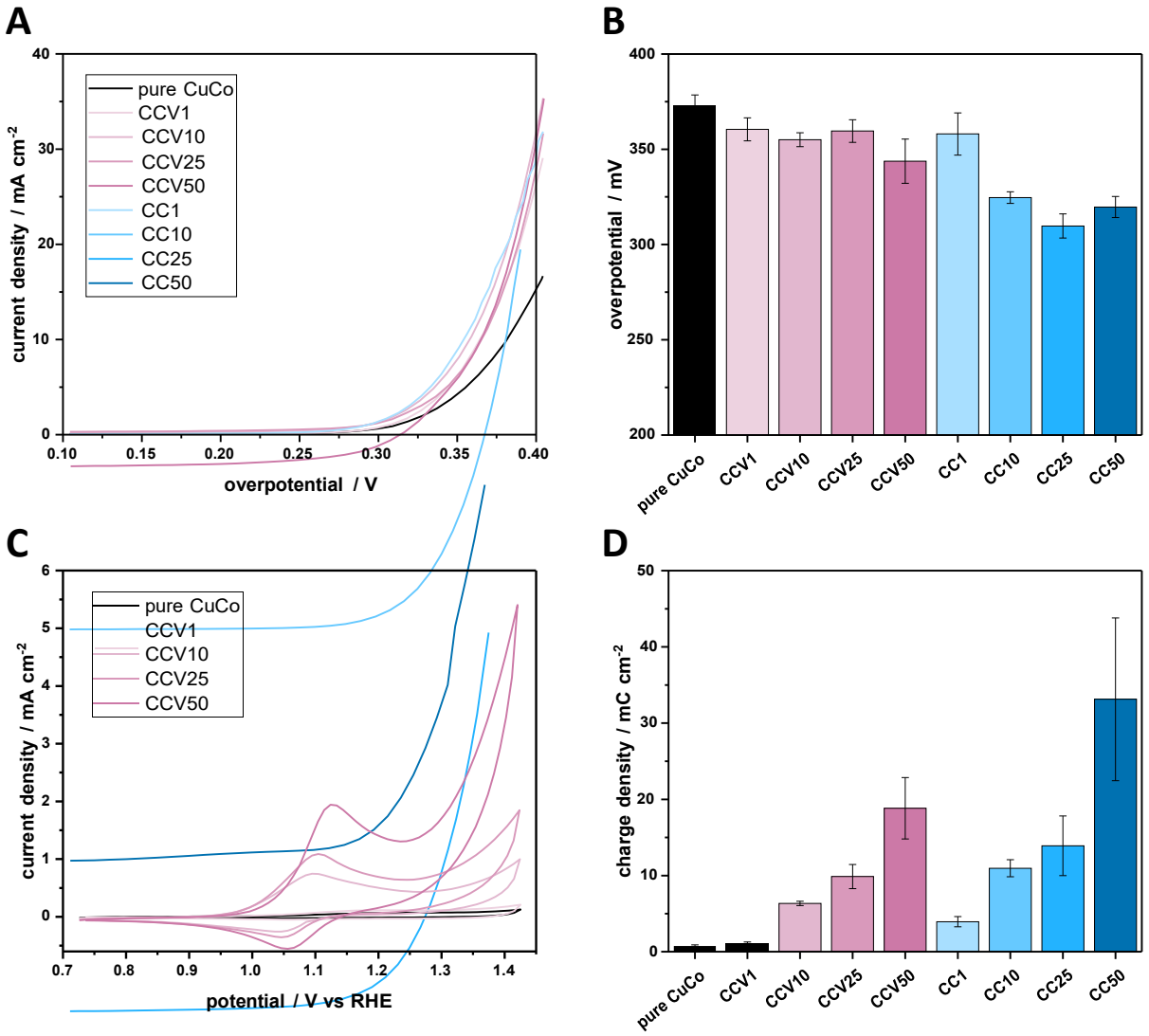
Keywords: V_2CT_x, $V_4C_3T_x$, MXene, oxygen evolution reaction, operando XAS, transition metal hydroxide

Abstract

Vanadium-based MXenes offer promising alternatives to Ti3C2Tx as conductive supports for oxygen evolution reaction (OER) electrocatalysts.[1,] While V2CTx-supported CuCo hydroxides have shown excellent performance, the influence of MXene layer thickness and composition remains largely unexplored. Here, we systematically compare V2CTx and V4C3Tx as supports for identical CuCo hydroxide catalysts, combining electrochemical characterization with operando X-ray absorption spectroscopy to probe electronic structure evolution during OER.

CuCo@V4C3Tx composites (1, 10, 25, 50 wt% MXene) were synthesized using identical methods to our CuCo@V2CTx materials, enabling direct comparison. Structural characterization confirms Kolwezite-type copper-cobalt carbonate hydroxides with MXene incorporation and progressive $Cu^{2+} \rightarrow Cu^{+}$ reduction (0-22%) increasing with loading. Electrochemical evaluation reveals that V2CTx-supported catalysts consistently outperform V4C3Tx counterparts by 30-
50 mV at 10 mA cm^{-2}, Figure 1. The optimal V2CTx composition (CC25: 310 mV overpotential)
achieves significantly better performance than the best V4C3Tx sample (CCV50: 344 mV). Both
MXene types produce similar cyclic voltammetry signatures: comparable Co(II)→Co(III) oxidation potentials and Tafel slopes, yet V2CTx composites generate 1.4-1.8× higher charge densities. This paradox suggests electronic differences emerge at higher potentials relevant to active OER catalysis.



OER catalysts. A. Linear sweep voltammograms of CC and CCV series in 1.0 M NaOH at 1 mV s^{-1}, 1600 rpm. **B.** Overpotential at 10 mA cm^{-2} showing V_2CT_x supported catalysts outperform $V_4C_3T_x$ counterparts by 34-51 mV. **C.** Cyclic voltammograms of CC and CCV series at 40 mV s^{-1}. **D.** Integrated anodic charge density demonstrating 1.4-1.8× higher charge density for V_2CT_x composites compared to $V_4C_3T_x$ at equivalent loadings.

Operando X-ray absorption spectroscopy at the Cu and V K-edges reveals distinct behaviors between the two MXene supports during potential cycling through the OER region. Cu K-edge analysis shows that both MXenes systematically modify copper electronic structure compared to pure CuCo, but with different dynamics. V_2CT_x composites exhibit relatively consistent copper edge positions throughout potential cycling with high structural reversibility based on EXAFS analysis. $V_4C_3T_x$ composites, particularly at high loading, show more pronounced potential-dependent edge evolution, suggesting greater copper redox participation during OER operation.

However, this dynamic behavior correlates with reduced structural reversibility compared to V_2CT_x systems.

V K-edge measurements provide complementary insights into support stability. V_2CT_x at intermediate and high loadings demonstrates minimal spectral changes throughout the OER potential window, with near-complete reversibility after cycling. EXAFS indicates preservation of structural features characteristic of layered MXene coordination. In contrast, $V_4C_3T_x$ shows progressive spectral evolution toward higher vanadium oxidation states during potential increases, with more limited reversibility. EXAFS reveals greater structural transformation compared to V_2CT_x, suggesting more extensive oxidation of the MXene framework. While $V_4C_3T_x$ oxidation improves interfacial charge-transfer resistance, it does not translate to optimal OER overpotentials.

These operando measurements, which will be complemented by Co K-edge analysis, suggest that optimal MXene-catalyst performance may correlate with maintaining electronic and structural stability during OER operation. V_2CT_x appears to provide more stable electronic environments for both copper sites and the support framework itself, whereas $V_4C_3T_x$ enables more dynamic but less reversible transformations. The relationship between electronic stability, structural reversibility, and catalytic performance suggests important considerations for rational MXene-catalyst design, where support oxidative behavior and electronic coupling must be carefully balanced. This systematic operando XAS comparison of vanadium carbide MXenes provides insights into how they influence not only conductivity but also the dynamic electronic structure of supported electrocatalysts during operation.

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#4

Heat transport of two-dimensional $Ti_3C_2T_x$ MXene flakes

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Keywords: MXene, heat transport, 2D materials, $Ti_3C_2T_x$

The fundamental understanding of heat transport across MXenes is a key determinant of device performance in applications such as electronics, thermoelectric energy harvesting, and thermal insulation[1–3]. A deeper understanding of the thermal conductivity in the out-of-plane direction is crucial in these applications, as heat dissipation and temperature gradients are governed by interlayer pathways and interfaces.

The state-of-the-art related to thermal analysis of MXenes focuses primarily on thin films made of a stack of flakes[4]. These show wide variability in the reported thermal conductivities, which could be due to misaligned flakes that make it difficult to decouple in- and out-of-plane contributions and to disentangle the influence of different interfaces. In addition, the variability could be due to the use of different synthesis strategies. Therefore, there are key research questions that remain unanswered about the mechanisms that govern heat transport in MXenes flakes[5,6]. These relate to the heat carriers that dominate out-of-plane heat transport – phonons vs electrons – and the dependence of the thermal conductivity on flake thickness and temperature, which in turn depend on the underlying microscopic phonon scattering mechanisms.

To address these questions, we present a systematic study of the out-of-plane transport in single $Ti_3C_2T_x$ flakes using frequency domain thermoreflectance (FDTR). Our results[7] show a thermal

conductivity of 0.18 ± 0.02 W m^{-1} K^{-1} at room temperature, which is thickness independent in the range of 15 nm to 75 nm. When varying temperature from 150 K to 450 K, the thermal conductivity displays a non-monotonic trend, increasing up to 375 K before decreasing at higher temperatures with an approximate T^{-1} dependence. These results evidence a diffusive scattering and confirm phonon-dominated heat transport instead of electrons. Additionally, the in-plane thermal conductivity of these flakes was also studied[8], showing a value of 13.5± 0.6 W m^{-1} K and confirming also a phononic behavior within this heat transport direction. Overall, these findings provide fundamental insights of the thermal properties of 2D - $Ti_3C_2T_x$ flakes, helping us to define future MXenes based thermal management strategies.

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#5

In situ (S)TEM study of thermally induced phase transitions in Titanium-based MXene

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MXenes are a class of two-dimensional transition metal carbide and nitride compounds with a chemical formula of $M_{n+1}X_nT_x$ (n = 1-4) where M, X, and T_x denote the transition metal, carbon and/or nitrogen, and surface termination, respectively[1][2]. They were first synthesised in 2011 and displayed a variety of electronic, optical, chemical, and mechanical properties[3][4].With their unique and tuneable 2D transition metal carbide (or nitride) structures, MXenes have emerged as promising anode materials for Li-ion batteries[5]. The wid e interlayer spacing (~1 nm) of MXenes could potentially enable rapid Li^+ intercalation with minimal lattice distortion, enhancing the rate performance and cycling stability of Li- ion batteries. Besides, MXenes possess excellent mechanical properties (e.g. the effective Young's modulus of monolayer $Ti_3C_2T_x$ MXene was 0.33 ± 0.03 TPa)[3][6], which make MXene one of the most promising reinforcing 2D nanomaterials for ultra-high temperature ceramics (UHTCs)[7] . However, the thermal degradation behaviour of MXenes at high temperatures remains poorly understood, which is crucial for expanding their high- temperature applications in UHTCs.

Early investigations into the thermal degradation of MXenes have employed a combination of techniques such as X-ray diffraction (XRD), thermogravimetric analysis (TGA), and X- ray photoelectron spectroscopy (XPS) to elucidate the structural and chemical evolution of MXene upon heating. Although these methods have provided valuable insights into the phase transformation behaviour of $Ti_3C_2T_x$ MXene, atomic-scale, real-space information on the transformation process remains lacking, which is crucial for elucidating the phase transformation mechanisms of MXenes.

Therefore, this study employs in situ scanning transmission electron microscopy (STEM) method to investigate the thermal degradation behaviour of $Ti_3C_2T_x$ MXene over a

temperature range of 25 °C to 1200 °C. The results offer high temporal and spatial resolution insights into the dynamic structural disruption and degradation of MXene's 2D morphology at elevated temperatures, while also revealing the phase transformation mechanism of $Ti_3C_2T_x$ into TiC.

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#6

Ultrafast electron cooling in $Ti_3C_2T_x$ MXene revealed by time-resolved photoemission spectroscopy

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Abstract

MXenes are emerging two-dimensional materials whose transport metrics have advanced rapidly, yet direct investigation of ultrafast electron dynamics remains scarce. In our experiment, we have used time-resolved photoemission spectroscopy (tr-PES) to directly track the nonequilibrium occupied electronic distribution in a $Ti_3C_2T_x$ thin film and to quantify ultrafast electron cooling via the time-dependent electronic temperature.

To this end, delaminated $Ti_3C_2T_x$ flakes were prepared by selective etching of a Ti_3AlC_2 MAX precursor followed by washing, delamination and centrifugation to isolate single and few-layer flakes. Thin films were spray coated from a methanol-based dispersion onto Si substrates capped with 230 nm SiO_2, yielding a thickness of about 20 nm. Ultrafast electron dynamics were then measured at room temperature under ultrahigh vacuum using a pump-probe scheme with 800 nm near-infrared excitation and an extreme- ultraviolet probe generated by high-harmonic generation at 26.5 eV. The overall temporal resolution was 110 fs and the pump fluence was 250 μJ/cm^2.

Upon excitation, a prompt redistribution of spectral weight appears around Fermi level (E_F). Energy distribution curves near E_F were fitted at each pump-probe delay using a Fermi-Dirac distribution convoluted with a Gaussian to account for the experimental energy resolution (118 meV FWHM). Figure 1a compares representative spectra before and after excitation together with the corresponding fits. This yields the time-dependent electronic temperature $T_e(t)$ and its pump-induced change $\Delta T_e(t)$ relative to the pre-pump baseline, as shown in Figure 1b. The electronic response rises rapidly and reaches a maximum within about 200 fs from onset to peak, followed by a fast decay. Modelling $\Delta T_e(t)$ with an instantaneous rise and an exponential decay convolved with the instrument

response gives a characteristic energy relaxation time of 138 fs and the peak electronic temperature increase of about 220 K.

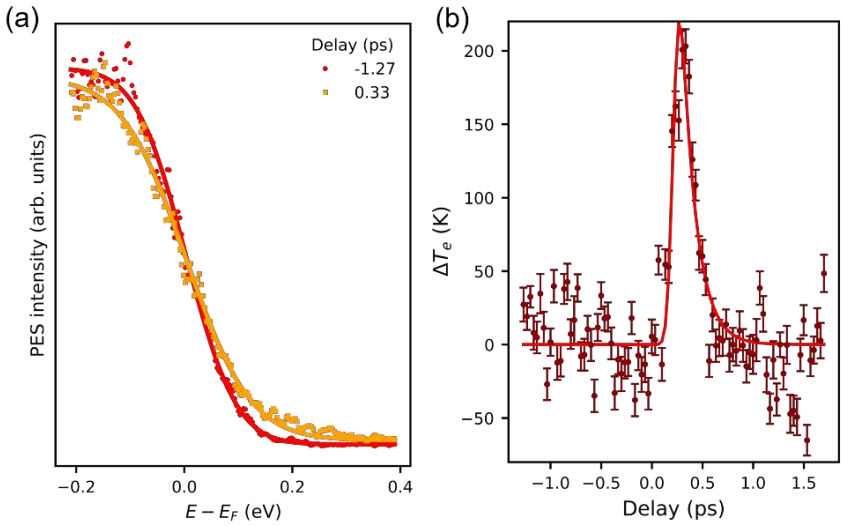

Figure 1. (a) Photoemission spectra (shown as points) around the Fermi level taken at different temporal intervals of the pump-probe delay and fitted with a Fermi-Dirac distribution convoluted with a Gaussian function, shown as solid line. (b) The extracted electron temperature change (ΔT_e) as a function of pump-probe delays.

The extracted relaxation time places $Ti_3C_2T_x$ among materials with exceptionally efficient electron-to-lattice energy transfer. The rapid rise is consistent with electron-electron scattering that establishes a quasi-thermal Fermi-Dirac distribution, while the subsequent decay reflects electron-phonon cooling. We connect the measured timescale to longitudinal optical (LO) phonon channels using Raman spectroscopy, which shows prominent modes near 708 cm^{-1} and 191 cm^{-1} assigned to LO vibrations, corresponding to phonon energies of about 87 meV and 23.6 meV. At room temperature, Bose occupation factors strongly favour emission over absorption for the 708 cm^{-1} mode, making it an efficient cooling pathway, while the lower-energy mode remains more thermally populated. The measured relaxation time is consistent with electron-phonon coupling strengths inferred from other ultrafast optical studies. This further supports a picture in which LO phonon emission dominates the early-time energy loss.

By providing a tr-PES view of nonequilibrium electron cooling in $Ti_3C_2T_x$ thin films, this work establishes a quantitative benchmark for modelling ultrafast energy flow in MXenes. The sub-150 fs hot-electron lifetime implies that device responses beyond this timescale will be governed by near-thermal carriers and heat transport. This favours photothermal and bolometric concepts and sets constraints on approaches that require long-lived hot carriers for energy harvesting or hot-carrier injection, guiding the design of MXene-based optoelectronic and electronic platforms.

#7

$Ti_3C_2T_x$ MXene-Induced Performance Enhancement of MoS_2 Cathode in Aqueous Zinc-Ion Batteries

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Abstract: Developing cathode materials with fast charge transport and structural robustness remains a key challenge for high-performance zinc-ion batteries [1]. Although layered MoS2 possesses a favourable two-dimensional structure for ion intercalation, its poor electrical conductivity and limited electrolyte affinity severely constrain its electrochemical efficiency and cycling durability [2]. In this study, a MoS2/Ti3C2T*x* MXene composite is prepared via a one-step hydrothermal synthesis, enabling the vertical growth of ultrathin MoS2 nanosheets on conductive Ti3C2T*x* layers. The resulting architecture forms a continuous electron transport network while exposing abundant active sites for Zn^{2+} storage. The hydrophilic and highly conductive Ti3C2T*x* framework enhances electrolyte penetration, accelerates charge-transfer kinetics, and alleviates the structural stress of MoS2 during repeated Zn^{2+} insertion/extraction. Owing to this synergistic integration, the composite achieves a high specific discharge capacity of 186.55 mAh g-1 at 0.1 C, significantly surpassing that of pristine MoS2 (129.02 mAh g-1), along with excellent cycling stability. These findings demonstrate that constructing MXene-based heterostructures is an effective strategy for improving the capacity, rate capability, and durability of cathode materials in zinc-ion batteries.

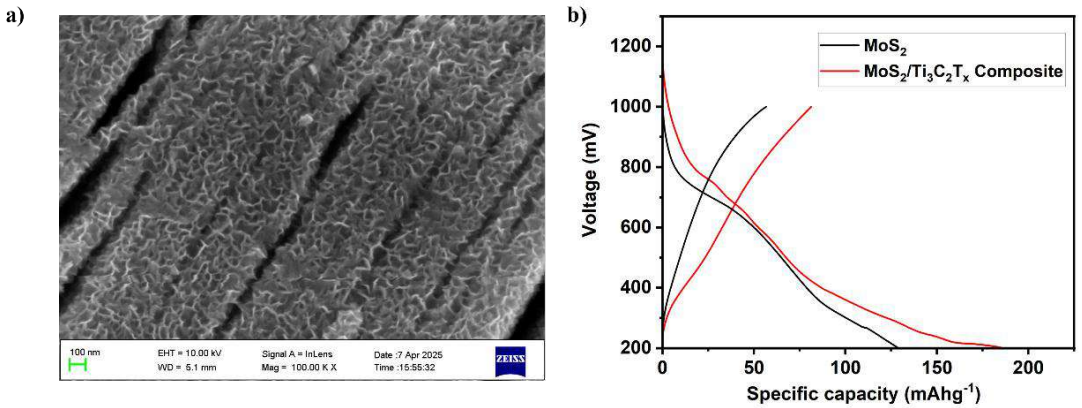

Figure 1. FESEM image of $MoS_2/Ti_3C_2T_x$ MXene composite b) Comparison of galvanotactic charge/discharge curves of MoS_2 and $MoS_2/Ti_3C_2T_x$ MXene composite

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#8

In Situ Decoration of 0D-Nickel Boride on Stacked 2D-Vanadium MXene Composites: An Advanced Electrode Material for High-Energy-Density Supercapacitors

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Vanadium carbide-MXene (V_2CT_x) is considered a rising star among 2D materials and is an ideal electrode material for energy storage due to its unique features. However, oxidation and layer restacking can impair specific capacity (Cs) and cycling performance. Considering this challenge, we have developed a composite material consisting of amorphous nickel boride (Ni_xB NPs) and V_2CT_x. To prevent oxidation and restacking of the layers and to improve the performance of the supercapacitor, Ni_xB was decorated between the gaps and the surface. The V_2CT_x and its composites were prepared by simple etching and direct liquid-phase methods. Under the optimized conditions, the Ni_xB/V_2CT_x-75 modified nickel foam exhibited an improved Cs value of 705.9 C g^{-1} and a rate capability of 53.8 % at a current density of 10 A g^{-1}; the excellent cycling stability was 120.5% after 10,000 cycles at 10 A g^{-1} in 3 M KOH. The improved Cs values shortened ion diffusion paths, swift electron transfer, and excellent cycling stability of the composites are due to the V_2CT_x layers surface entrapped/gaps filled by the Ni_xB NPs. Form practical application, an asymmetric device with Ni_xB/V_2CT_x-75 and reduced graphene oxide (rGO) as positive and negative electrodes was fabricated. The Ni_xB/ V_2CT_x-75//rGO device achieved a maximum energy density of 50.22 Wh kg^{-1} at 800 W kg^{-1} and 26 Wh kg^{-1} at 16000 W kg^{-1}. the capacity retention was 89.98 % and the Coulombic efficiency was 99.9% after 20,000 continuous cycles at 8 A g^{-1}. These results emphasized that the developed 0D/2D Ni_xB/V_2CT_x electrode materials with novel composite architecture are suitable for advanced energy storage applications.

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#9

"Facile Room-Temperature Synthesis of $Ti_3C_2T_x$ MXene-S/Se Cathodes for High-Performance Li-S Batteries"

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Abstract: The high theoretical energy density and material abundance make Li-S batteries the next generation of high-density energy storage devices. However, the electrical insulation behavior, dissolution of intermediate polysulfides and polyselenides, and significant volumetric expansion during cycling poise a great challenge for the practical applicability of Li-S battery. This study provides a facile synthesis of cathode materials by anchoring sulfur and selenium nanoparticles onto the 2D-MXene nanosheets (Ti3C2Tx) under room temperature conditions. This synthesis provides a greener approach for preparing high S/Se-loading cathode materials without requiring extreme heat treatment. The synthetic approach ensures uniform distribution and strong adherence of nanoparticles onto the surface of MXene.[1] The electronic conductivity of MXene sheets ensure the entrapment of intermediate polysulfide and polyselenides, enhancing the cycling stability of battery by suppressing the shuttle effect.[2] The S/Se nanoparticles also improve the active material utilization and accommodate the volume expansion. The prepared cathode material demonstrates high initial capacity and a sustained cycling stability of over 400 cycles, while exhibiting robust performance under faster charge-discharge conditions. The room temperature synthesis along with high energy density and long-term cycling stability of the prepared MXene-S/Se hybrid cathodes offers a platform for the scalability and practical applicability in advanced Li-S batteries.

Keywords:

$Ti_3C_2T_x$ MXene, Li-S Battery, Room-Temperature Synthesis, Nanoparticles, S/Se alloy

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#10

Single-element and multiple-elements MXenes for supercapacitor application

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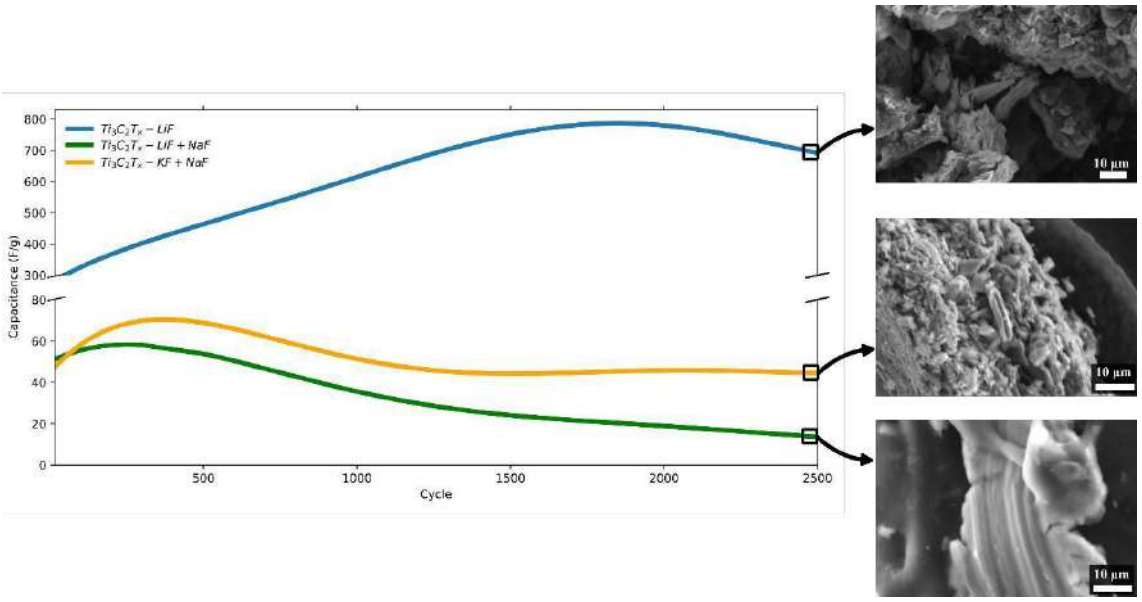
Since the early investigations on MXenes, these bidimensional nanomaterials standed-out for applications in energy conversion and storage. High surface area, high capacitance and high electrical conductivity of MXenes make them suitable for supercapacitor application. In the present investigation, $Ti_3C_2T_x$ MXene was synthesized by modified MILD (minimally intensive layer delamination) route into which different fluoride salts (LiF, LiF + NaF, and LiF + KF) were investigated aiming to improve the delamination and the electrode performances. More effective delamination was obtained when the NaF + LiF was used, followed by LIF and LiF + KF. Conversely, the highest capacitance was obtained for LiF which yielded 380 F/g at the first charge / discharge cycle, reaching around 800 F/g after 1800 cycles, due to further delamination. In

another approach, a novel composition of MXene $(TiVNbZrTa)_2CT_x$ was synthesized aiming to enhance the electrochemical performance due to a variety of different surface redox sites. In this MXene, the measured capacitance was 320 F/. The interplay between the electrode performances, microstructures and surface chemistry of the MXenes produced was discussed.



Capacitance over charge / discharge cycles at 0.3 A/g and the SEM image of the electrode materials after 2500 cycles.

Keywords: MXenes; supercapacitors; synthesis.

#11

Mixed-Metal Carbonitride MXenes: A New Design Lever for Stabilizing Previously Inaccessible Chemistries

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MXenes continue to expand as a versatile family of two-dimensional carbides, nitrides, and carbonitrides with tunable electronic and optical properties. However, the accessible compositional space of carbonitride MXenes is constrained by thermodynamic stability limits associated with conventional MAX-phase chemistry. Many mixed carbonitride compositions are considered unstable or inaccessible according to equilibrium phase diagrams, restricting the development of new MXene chemistries. Here, we demonstrate that mixed-metal carbonitride MXenes can exceed the thermodynamic stability limits of conventional MAX phase systems, resulting in emergent functional behavior. By leveraging mixed metal incorporation, we access previously inaccessible carbonitride compositions that would not be expected to form under conventional thermodynamic assumptions.

Beyond simple compositional expansion, mixed-metal chemistry fundamentally alters the stability window and functional response of the resulting MXenes. They exhibit composition-dependent optical absorption and electrical conductivity, alongside unexpectedly enhanced resistance to ambient degradation relative to conventional MXene analogues. The observed stability and property evolution cannot be fully rationalized by simple rule-of-mixtures behavior, suggesting emergent effects arising from solid-solution metal mixing and configurational complexity. Overall, this work reframes thermodynamic limits as tunable boundaries, demonstrating that compositional complexity can be intentionally leveraged to stabilize new, previously inaccessible, two-dimensional materials with tailored properties.

#12

The Emerging Landscape of MXene Life Cycle Assessments: Hotspots and Knowledge Gaps

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This review consolidates current knowledge on MXene environmental sustainability as determined through life cycle assessment and reveals recurring methodological patterns and limitations within the field. The primary outcome of the scrutiny is that the application of LCA to MXenes remains highly underdeveloped, with only six dedicated studies available and a disproportionate focus on $Ti_3C_2T_x$, even as the broader MXene family continues to expand rapidly.

Across studies, environmental hotspots consistently emerge from high electricity demand—especially during MAX phase synthesis—and from the use of hazardous etchants such as HF. Upstream processes, notably titanium production via the Kroll route, can account for more than 70 % of chemical-related impacts, further amplifying resource depletion burdens.

A central insight of this review is the presence of performance–impact trade-offs. Comparative analyses mapping environmental single-scores against bulk electrical conductivity reveal a "high-desirability" region where favourable conductivity aligns with lower environmental burdens. While some synthesis routes fall within this optimal domain, others deliver superior electrical performance only at the expense of substantially higher impacts. Paradoxically, the widely perceived "safer" LiF–HCl etching route may exhibit impacts up to 3.7 times higher than traditional HF etching due to longer reaction times.

Persistent methodological gaps include an over-emphasis on climate change indicators, inconsistent yield reporting, and the absence of characterisation factors for MXenes. Moreover, existing assessments primarily focus on cradle-to-gate boundaries and rely on laboratory-scale inventories that omit use-phase behaviour, regeneration, and end-of-life management.

To advance the field, future LCA efforts must adopt prospective approaches incorporating scale-up modelling, toxicity metrics, and realistic end-of-life scenarios. Expanding environmental assessment beyond Ti-based systems to non-Ti MXenes and nitride MXenes (TMNs) is essential, particularly given the higher formation energies associated with M–N bonding. Standardised procedures for recovery, regeneration, and safe disposal will be indispensable to mitigate long-term risks associated with MXene degradation.

#13

Er^{3+} ion doped V_2CT_x MXene quantum dots as a multifunctional sensing platform of 4-aminohippuric acid through a fluorescence turn-on response, and cobalt ions via both colorimetric and fluorescence turn-off mechanisms

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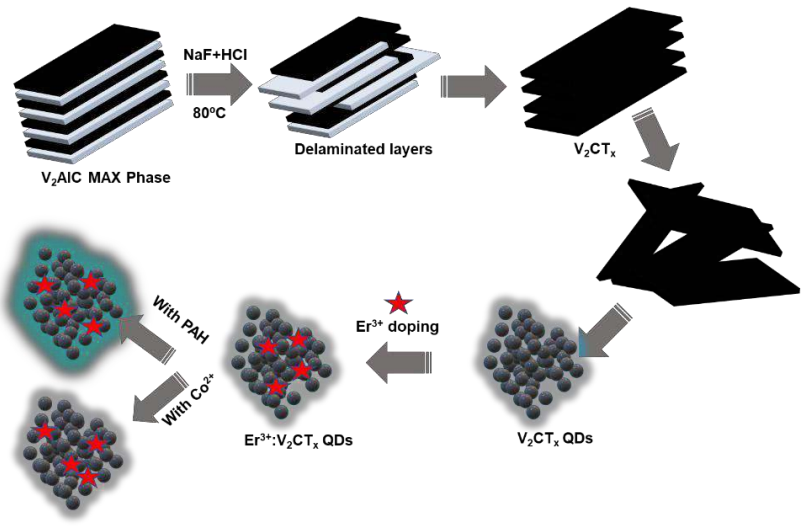
Abstract:
Strategic engineering of MXene-based materials enables synergistic advantages, including enhanced catalytic performance, heterojunction formation, and improved charge-carrier transport, while also offering protective and molecular-sieving enrichment layers. In this work, erbium ion doped vanadium carbide MXene quantum dots (Er^{3+}:V2CTx MXene QDs) were synthesized for the detection of *ρ* -amino hippuric acid (PAH) in biological samples and Co^{2+} ions in pharmaceutical formulations. The synthesized Er^{3+}:V2CTx MXene QDs exhibited bluish-green fluorescence under 365 nm UV illumination offering λEx/Em : 390/468 nm. The average particle size was determined to be 5.22 ± 1.99 nm. Notably, the fluorescence intensity of the Er^{3+}:V2CTx MXene QDs increased significantly with increasing PAH concentration in the range of 0.05–2.5 μM, achieving a low limit of detection of 45.70 nM. The proposed probe was successfully applied to the determination of PAH in human biofluids, demonstrating excellent accuracy and reliability. Furthermore, the developed system functions as a dual-mode sensor for Co^{2+} detection via both fluorescence and colorimetric pathways. The presence of Co^{2+} induced pronounced fluorescence quenching along with a distinct bathochromic shift toward the green region in the UV– visible absorption spectrum, mediated by a complex-assisted sensing mechanism. The method exhibited linear responses over the concentration ranges of 0.5–10 μM and 5–100 μM, with detection limits of 11.31 nM and 38.26 nM from fluorescence and colorimetric measurements, respectively. Overall, Er^{3+}:V2CTx MXene QDs emerge as a promising dual-functional sensing platform for the sensitive and precise quantification of PAH in biological fluids and cobalt ions in pharmaceutical tablets.

Keywords: Vanadium carbide, Erbium, MXene QDs, *ρ*-amino hippuric acid, fluorescence.



Scheme 1. Schematic representation for the synthesis of Er^{3+}:V_2CT_x MXene QDs and its sensing application against PAH and Co^{2+} ion

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#14

Controlled MXene Synthesis via Lewis Acid Molten Salt and Dry Selective Etching: Mechanistic Insights for Energy Storage

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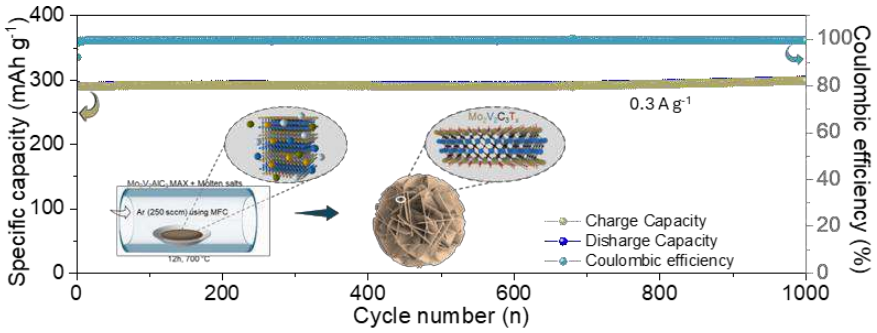
ABSTRACT

The synthesis of MXenes has undergone significant evolution from conventional wet chemical etching toward more controlled, sustainable, and selective strategies. Traditional hydrofluoric acid–based routes, while effective, suffer from limitations including hazardous processing conditions, uncontrolled surface terminations, and environmental concerns . Recent advancements such as Lewis's acid molten salt (LAMS) etching, have introduced fluorine-free pathways that enable tunable surface chemistries and improved structural integrity, although challenges in delamination and scalability remain. Concurrently, the emergence of dry selective etching techniques—including gas-phase and vapor-assisted extraction—offers a transformative route for MXene production by enabling solvent-free processing, precise control over termination groups, and enhanced compositional selectivity. Meanwhile, the development of high-performance and environmentally benign anode materials is essential for advancing lithium-ion battery technologies. In this work, we present a unified perspective on the evolution of MXene synthesis, integrating our previously reported LAMS-based methodology with a newly developed dry selective etching approach. The proposed strategy bridges the gap between molten salt chemistry and vapor-phase extraction, enabling controlled removal of A-layer elements from MAX phases while preserving crystallinity and tailoring surface functionalities. This hybrid framework facilitates improved yield, reduced defect density, and customizable interlayer chemistry, which are critical for next-generation energy storage applications. The resulting MXenes exhibit enhanced electrochemical performance, driven by optimized surface terminations, increased conductivity, and improved ion transport kinetics. This study not only highlights the transition from wet to dry etching paradigms but also establishes a viable route toward a safe, scalable, and environmentally benign pathway for synthesizing high-quality MXenes. The insights provided herein offer a foundation for the rational design of MXene synthesis routes, aiming to advance their applications in batteries, supercapacitors, and beyond.

Keywords: Sustainable synthesis, Dry selective etching, Molten salt etching, synergistic effect, 3D MXene; Li-ion batteries.

Graphical Abstract



Link to publication

1. Monodispersed flower-like Mo2V2C3Tx MXenes synthesized via Lewis acid molten salt ching with exceptional capacity retention for lithium-ion batteries - ScienceDirect

#15

A comparative exfoliation study of $(V_{1-y}Nb_y)_2AlC$ (y = 0.0, 0.5 & 1.0) MAX phases using different etching routes

Vaibhav Joshi and Christina S. Birkel*

MXenes which are commonly derived from MAX phases, offer expanded compositional diversity resulting in a unique combination of high electrical conductivity, tunable surface chemistry, mechanical flexibility, and excellent electrochemical performance, making them promising candidates for energy storage, sensing, and electromagnetic applications. However, their physicochemical properties are strongly dependent on the choice of etching chemistry, which translates directly into their functional properties and potential applications. In this work, we systematically investigate and compare the reaction of $(V_{1-y}Nb_y)_2AlC$ MAX phases (y = 0.0, 0.5 & 1.0) with three different etchants: concentrated aqueous hydrofluoric (HF) acid, *in-situ* HF (using LiF-HCl) under hydrothermal conditions, and molten-salts based on $CuCl_2$ as the Lewis acid (Figure 1). We compare the etching behavior of the three different MAX phases with varying *M*-element based on X-ray diffraction and electron microscopy coupled with elemental analysis. All successfully synthesized multi-layered MXenes are subsequently delaminated into few- and single-layer sheets. Their properties are compared by spectroscopy techniques to probe the influence of the etchants on their behavior. The results not only shed light on the influence of the *M*-element on their properties but also provide significant insights into the chemistry of each etching method.

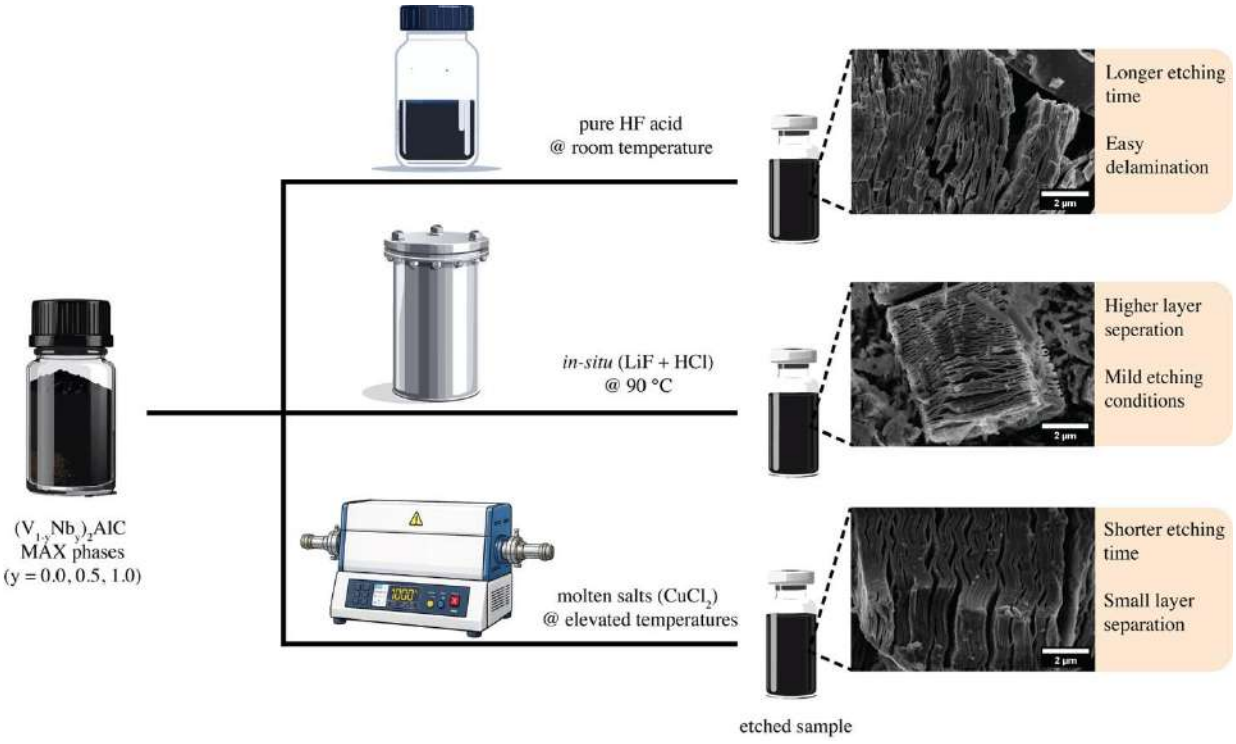


Figure 1: Systematic study of MAX phase exfoliation using: pure HF etching, *in-situ* hydrothermal etching and molten salts etching.

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#16

Size- and Surface-Dependent Electronic and Optical Tunability in MXene Quantum Dots

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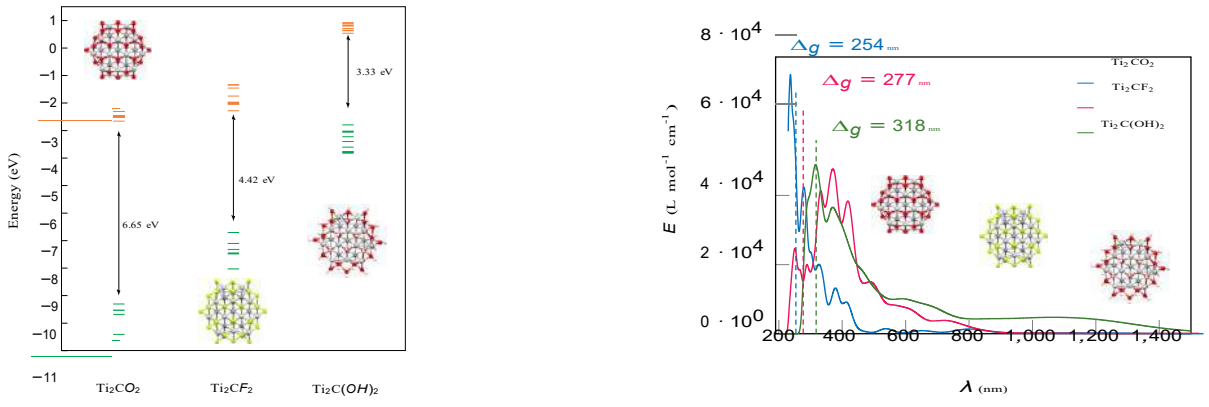
The quantum confinement effect in quantum dots (QDs) leads to significant modifications of their physical properties compared to bulk and two-dimensional (2D) materials. Reduced dimensionality alters charge distribution and electronic structure, resulting in pronounced size-dependent electronic and magnetic behavior. These characteristics make low-dimensional systems highly attractive for both fundamental research and advanced technological applications. [1]

In this work, we investigate the electronic structure of selected MXene-based quantum dots with different metal compositions and surface terminations. We show that the energy gap decreases systematically with increasing quantum dot size, reflecting the weakening of quantum confinement. Changes in metal composition and surface functionalization represent an additional means of modifying the electronic properties of the system. We further analyze their magnetic and optical behavior. Spin polarization is primarily observed in smaller quantum dots, indicating that strong quantum confinement stabilizes magnetic ground states, whereas larger dots exhibit weaker magnetic response. [2] The optical properties are studied using time-dependent density functional theory, where we observe a pronounced red shift in the absorption spectra induced by surface functionalization. In contrast, decreasing the size of the quantum dots leads to a significant blue shift, associated with enhanced quantum confinement. [3]

These results demonstrate how quantum dot size and chemical composition jointly govern the electronic, magnetic, and optical properties of MXene-based quantum dots, highlighting their potential for nanoelectronic, spintronic, and optoelectronic applications.



(a) (b)

Figure 1: Energy level diagrams and corresponding band gaps (a) together with calculated absorption spectra (b) of Ti_2C-based quantum dots with different surface functionalizations.

Acknowledgements: This contribution has been produced with the financial support of the European Union under the LERCO project (number CZ.10.03.01/00/22_003/0000003) via the Operational Programme Just Transition.

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#17

How Surface Oxygen Controls Catalysis: From Passivation to Activation of Mo_2C

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MXenes are highly promising catalysts whose reactivity is critically determined by surface terminations. Pristine Mo_2C binds reaction intermediates too strongly, resulting in excessive reactivity, whereas full oxygen coverage passivates the surface, suppressing adsorption and catalytic activity. Optimal catalysis therefore requires a delicate balance in oxygen coverage, with computational studies playing a key role in interpreting and predicting the properties of these versatile materials [1].

Density functional theory combined with reaction energy profiling and transition-state calculations was used to investigate the forward and reverse water–gas shift (WGS) reactions on Mo_2C MXenes with varying surface terminations. Fully O-terminated Mo_2CO_2 is largely inactive as the oxygen overlayer blocks surface Mo sites, weakens adsorbate interactions, and imposes prohibitively high dissociation barriers. Reducing oxygen coverage, either through mixed O/F terminations or termination vacancies [2,3], restores catalytic activity by partially exposing Mo sites. Partial oxygen termination enables moderate adsorption energies, lowers bond dissociation barriers, and reshapes reaction energetics toward the Sabatier optimum.

This mechanistic understanding explains why experimentally relevant Mo_2CT_x catalysts, which naturally feature mixed terminations or vacancies, exhibit significant forward or reverse WGS activity [4], despite predictions of inactivity for fully terminated surfaces. More broadly, surface oxygen coverage emerges as a decisive factor for tuning Mo_2C MXene reactivity, providing practical guidance for the rational design of high-performance catalysts.

Acknowledgements:

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#18

Nb_2C MXene as a Peculiar Catalyst for the One Pot Oxidation/Hydrogenation Reaction

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Since their discovery in 2011,[1] the two-dimensional 2D MXenes have attracted interest in a wide range of applications in electrocatalysis, optoelectronics, renewable energy storage, or biomedicine, leveraging their diverse chemical compositions and tunable characteristics. It has been shown that MXenes are also a promising platform for thermal catalysis. However, to identify the existing research gaps in the MXene-based heterogeneous catalysis more investigations are still necessary.

In this study we have investigated the catalytic performance of Nb-based MXenes, specifically focusing the selective aniline oxidation to azoxybenzene and hydrogenation of azoxybenzene to azo compounds. Nb_2C MXene was synthesized through the hydrothermal Al etching using a commercial Nb_2AlC precursor.[2] This process followed an *in situ* HF treatment, generated by the reaction between $NaBF_4$ and HCl. Delamination of Nb_2C MXene occurred via intercalation of DMSO during 24 h, followed by an ultrasonic treatment. After drying the solid at RT, the solid was exposed to a subsequently thermal activation at 350 °C, under a nitrogen flow for 1 hour leaving to an increased surface functional groups.

The produced MXene exhibited a surface area, ranging from 2.5 to 2.7 m^2/g with absence of microporosity. A noticeable difference was detected between the chemisorbed and physisorped H_2. XPS analysis identified the presence of structural defects, while the low density of the weak-to-moderate acid-base sites (*ca*. tens of $\mu mol \cdot g_{catalyst}^{-1}$) was confirmed by NH_3 and CO_2-TPD profiles. Also, the XPS survey spectra of the Nb_2C samples indicated the presence of Nb and C framework, along with F, O, and S atoms likely originating from the surface terminations and residual etchant species. According to ICP-OES chemical analysis, the residual Al content decreased significantly from 17.96% in the Nb_2AlC precursor to just 1.41% in the Nb_2C MXene, with an Nb loading increasing from 39.95% to 52.11% in the produced Nb_2C MXene, reflecting the selective Al removal. Upon Al etching, the diffraction lines characteristic of the Nb_2AlC MAX phase diminished significantly, confirming its successful transformation into Nb_2C MXene, with a new broadened *002* reflection at $2\theta=6°$ confirming the expansion of the interlayer spacing. Upon the excitation with a 413 nm laser, the Raman spectra of the Nb_2C MXene exhibited prominent peaks at 235 and 664 cm^{-1}, alongside a characteristic shoulder at 957 cm^{-1} attributed to the Nb(III) vibrations. Finally, TEM imaging confirmed the high crystallinity and 2D morphology of Nb_2C, revealing large sheets with lateral dimensions exceeding 1 μm.

Aniline coupling into azobenzene and azoxybenzene was performed in a 7 mL autoclave at 800 rpm by reacting of 1 mmole of aniline with 50 mg MXene, in toluene, under autogenous pressure. Then, it was followed by a 10-hours hydrogenation step at 140 °C under 5 bars of H_2. Nb_2C MXene exhibit activity as hydrogenation catalyst even in the absence of metal nanoparticles for the oxidative coupling of aniline, resulting in high selectivity toward azo- (61.5%) and azoxybenzene (38.5%) at 140 °C and 24 h for a conversion of 11.6%. Theoretical calculations indicated a required cooperation of two neighboring O

vacancies. In terms of stability, a small decrease in the conversion was observed while the selectivities towards azobenzene and azoxybenzene remained almost unchanged (64.5% and 35.5%, respectively) with unaltered XRD, Raman and XPS. A maximum azobenzene selectivity of 98.4% was achieved by incorporating a second hydrogenation step to reduce azoxybenzene into the desired product.

Acknowledgments
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#19

NiAl-Ti_3C_2 MXene: A Robust and Versatile Platform for High-Performance Fine Chemical Synthesis

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Since their ground-breaking discovery by the Gogotsi's group in 2011, MXenes have emerged as a focal point in the materials science serving as a versatile family of 2D early transition metal carbides and carbonitrides.[1] Their unique structural and electronic properties have spurred intensive research across an wide spectrum of applications, most notably in heterogeneous catalysis and energy storage (batteries), and also supercapacitors. On the other hand, by ensuring the production of compounds with purity levels exceeding 99%, the fine chemical industry acted as a vital enabler for the development of essential everyday products, including from advanced electronics to the life-saving medicines. Thus, starting from this state of the art, this study aims to evaluate the thermal heterogeneous catalytic performance of 2D MXene NiAl-Ti3C2 across three complex chemical transformations: (i) the Biginelli reaction, (ii) the Claisen-Schmidt condensation of benzaldehyde with cyclohexanone, and (iii) the hydroamination of phenyl alkyne by diverse amines.

The 2D MXene NiAl-Ti3C2 was prepared by from Ti3AlC2 by molten salt followed by exhaustive acid washings. In a typical procedure, the Biginelli reaction was conducted in a batch reactor under reflux for 4 h. The reaction mixture consisted of benzaldehyde, ethyl acetoacetate, and urea/thiourea in a 1:1:1.5 molar ratio, using 3 mL of ethanol as the solvent and 80 mg of catalyst. The Claisen-Schmidt condensation was performed by stirring benzaldehyde (0.002 mol) and cyclohexanone (0.001 mol) with 20 mg catalyst at 120 °C for 2 h under solvent-free conditions. The hydroamination reactions were conducted in an autoclave under a nitrogen atmosphere at 150 °C for 24 h. Typically, an alkyne-to-amine molar ratio of 1:2 was employed in 2 mL of toluene, using 5 mg of catalyst. After the etching process, new XRD diffraction lines characteristic of the Ti3C2 phase, were observed. Then, the absence of the Ni-related diffraction lines suggested a highly uniform dispersion of the nickel across the catalyst surface. Also, the XRD analysis confirmed that the crystalline structure of the catalyst remained intact preserving the robustness of the solid framework after the catalytic reactions. Then, the DRIFT spectra of the spent catalyst revealed signals corresponding to the Biginelli product, also evidencing a strong chemisorption. This behavior also suggests a more intense interaction between the active sites and the oxygen of the –N–CO–N– bridge, rather than the sulfur atom of the –N–CS–N– moiety. Further, Raman spectra shown characteristic D and G lines, typical of carbonaceous materials alongside the reflections attributed to the out-of-plane vibrations of the Ti and C atoms. The NH_3/CO_2 chemisorption confirmed a acid-base character of the fresh solid. In addition, the material demonstrated significant hydrogen adsorption capabilities (3.53 $mmol \cdot g^{-1}$), that confirmed the presence of a pronounced metallic character. Finally, the XPS analysis indicates a strong adsorption affinity of NiAl-Ti3C2 for the pyrimidine derivative. This was evidenced by the carbon content of the spent catalyst, where the atomic percentage of C=O and O-C=O bonds was nearly doubled, indicating an intense surface interaction with the carboxylate and the oxo groups.

The catalytic efficiency of the system in the Biginelli reaction was confirmed by a sharp increase in

the yield during the initial hour, then stabilizing at 92–95% after 4 hours. This performance reflected a high catalytic productivity, with TONs in the range of 361.2 to 371.9 for both urea and thiourea as precursors. In the Claisen-Schmidt condensation, NiAl-Ti_3C_2 afforded a conversion of 24.7% and a significant shift in the selectivity generating the di-condensed product with 93.29%, the MXene-catalyzed process redirected the reaction toward the mono-condensed product with a selectivity of 91.3%. However, for the hydroamination of phenyl-alkyne, only the reaction of n-butylamine yielded the desired product with a limited selectivity of 9.9%. Conversely, all other investigated amines promoted homo-coupling pathways, resulting in dimer and trimers formation with selectivities ranging from 43% to 57%.

Acknowledgments

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#20

The study of surface terminations and single atoms addition in $Ti_3C_2T_x$ Mxenes with electrochemical method

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MXenes represent a new class of two-dimensional (2D) materials, first introduced in 2011 with the synthesis of $Ti_3C_2T_x$ at Drexel University. Since then, more than 50 structures have been successfully synthesized, with over 100 predicted theoretically. This diversity in composition and structure has enabled applications in multiple fields, including catalysis, renewable energy, sensing, and biomedicine.[1] The methods to obtain MXenes are varied but in general involve a process of chemical etching with strong oxidating agent followed by delamination of the 3D precursor called MAX phase. To further expand the field, developing innovative synthesis methods (CVD and ampoule-based growth), and post- synthesis treatments that modify morphology, enhance crystallinity, and incorporate new elements into the structure are key trends for the following years. Our work focuses on the challenges of obtaining high-quality Mxenes, starting from the synthesis of MAX phases and studying methods to add additional functionalities by incorporating transition metals single atoms (Ex. Pt, Cr, V) and changing the surface chemistry. We have begun by the synthesis of $Ti_3C_2T_x$ in two different methods, the HF/HCl, [3] one and the LiF/HCl, [4] comparing crystallinity and optical response with UV-Vis analysis and HRTEM imaging, as well as the phase stability in water, which is directly correlated with the number of defects in the structure. Both methods led to the synthesis of the 2D Mxenes phase, but differences in morphology, composition and optic response were observed with a clear increase in flake quality for the LiF/HCl synthesis, but less synthetic yield and stability as compared to the HF/HCl one. The results are shown in **Figure 1**.

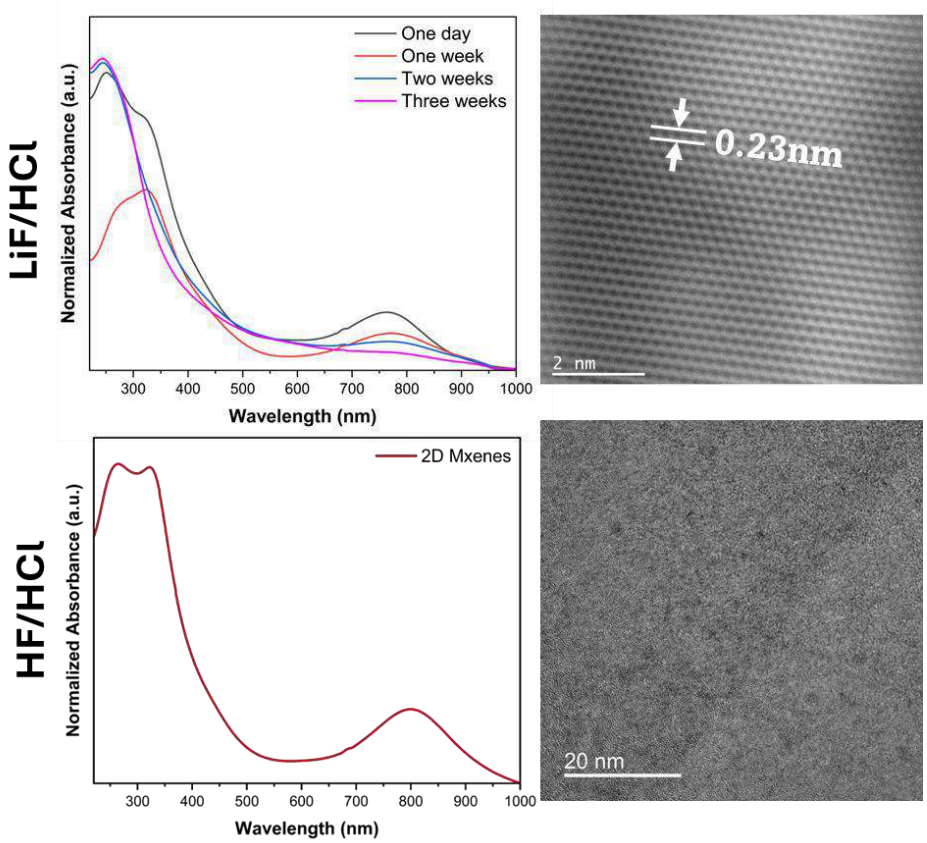

Figure 1. Comparison between Ti3C2Tx synthesis methods, with UV-Vis and HRTEM analyses for both samples.

We have also performed a series of electrochemical treatments in acidic media (H2SO4), applying 1000 cycles between (0 and -0,6V RHE) with a counter electrode of platinum [5] to deposit single platinum atoms in the Mxenes structure. For that experiment we have started with the MXene done using HF/HCl which has more defects and lower crystallinity, facilitating the aggregation of platinum. The results showed an increase in catalytic performance, with overpotential-η8 going from 583 to 395 mV (**Figure 2a**) as the cycles were done, and Tafel plot decreasing in half (**Figure 2c**). With the XPS it was possible to observe the appearance of a Pt4f doublet after treatment, and a change on the surface terminations, replacing Cl atoms with S atoms because of the electrolyte used. X-Ray absorption (XAS) of the Ti L2,3 border also shows significant differences, specifically related to the oxidation of Ti, as evidenced by the different ratios of eg/t2g on the L2 edge, with the bigger ratio after electrochemical method indicating an increase in oxidation of Titanium. Interestingly, the MAX phase Ti3AlC2 also shows signs of oxidation of Titanium, indicating that the precursor for MXenes can have a influence on the quality of the final flakes.

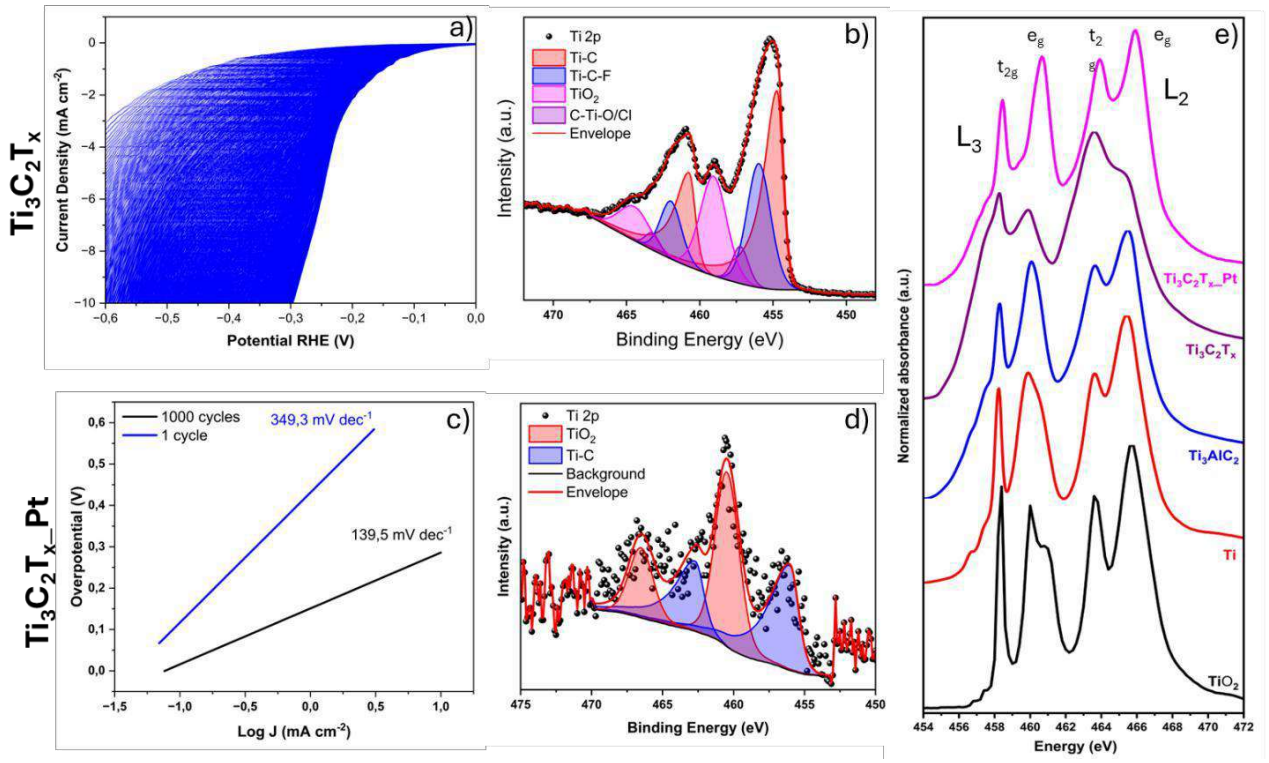

Figure 2. LSV and Tafel plot of the electrochemical voltammetry sweep performed on the Ti3C2Tx MXenes flake. XPS and XAS analyses of the sample before (Ti3C2Tx) and after the electrochemical treatment.

The next steps of this work involve testing the main differences in the catalytic performances for the Hydrogen Evolution Reaction (HER) using pure and modified Ti3C2Tx Mxenes, comparing the differences in results with the presence of defects and degree of crystallinity.

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#21

Deconvoluting the electronic state of MXene using operando UV-Vis spectroscopy

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Understanding the charge storage processes in MXene-based electrochemical energy storage (EES) devices is necessary for improving electrochemical performance through optimization of their physical properties. While electrochemical techniques are sufficient to distinguish between double-layer capacitance, pseudocapacitance and battery type charge storage,[1,2] many MXene-based systems exhibit mixed charge storage mechanisms that require deeper investigation.[3–5]

A powerful approach is using operando characterization techniques, connecting electrochemical behavior to real-time changes in structure, chemical environment or electronic state. As such, operando UV-Vis spectroscopy was recently demonstrated as an accessible and cost-effective technique to probe the real-time electronic state of $Ti_3C_2T_x$ MXene.[6] Herein, absorbance changes are directly linked to charge insertion in the electrode, enabling clear distinction between double-layer capacitance, pseudocapacitance and battery type charge storage, and even mixed mechanisms that cannot be inferred from the electrochemistry alone. Operando UV-Vis has since been used to monitor the inner workings of counterintuitive systems.[4,7,8]

However, the fundamentals behind the absorbance changes of MXene are poorly understood. Besides, the current approach fails to consider different types of electron regions that contribute to the overall electronic state and absorbance patterns of MXene. As a result, the absorbance changes are tracked at arbitrary wavelengths and the true physical meaning behind operando UV-Vis data remains unclear. To fully understand what the data represents, we must gain a deeper understanding of the electron regions in MXene and their interaction with photons.

In this work, we deconvolute the operando UV-Vis spectra into three separate regions, consisting of an interband transition (IBT), transversal surface plasmon resonance (TSPR), and longitudinal surface plasmon resonance (LSPR).[9] We then cycle $Ti_3C_2T_x$ under partially irreversible conditions, and monitor the respective evolution of each region while MXene is undergoing gradual irreversible change. Preliminary results indicate that every region represents different physical properties of MXene, such as electronic conductivity, interlayer spacing and surface redox activity. Spectral changes reflect changes in these properties. This lets us distinguish reversible from irreversible redox reactions, and tell apart different types of pseudocapacitance.

This study enables new possibilities for using operando UV-Vis spectroscopy on MXene, providing a deeper understanding of electrochemically induced absorbance changes, leading to more accurate insights into the charge storage mechanisms of MXene-based EES systems.

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#22

MXene-Based Electrochemical Platforms for Enhanced Sensing of Bisphenol A and Propofol

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2D nanomaterials have become key components in the design of advanced electrochemical sensors, as they provide remarkable improvements in electrocatalytic performance, sensitivity, and selectivity toward a variety of target compounds. Their outstanding properties arise mainly from their surface-dominated nature, characterized by a large specific surface area and a high surface-to-volume ratio. These features make them particularly attractive for electrochemical sensing platforms, which offer advantages such as portability, low cost, mass production capability, and *in situ* analytical measurements. The integration of nanomaterials into these devices further enhances charge transfer and analyte-electrode interactions, resulting in superior analytical responses.

Among the 2D nanomaterials, MXenes emerge as highly promising materials for next-generation electrochemical sensors with enhanced analytical performance due to the unique combination of metallic conductivity, hydrophilicity, and tunable surface chemistry. MXenes such as Ti_3C_2 are commonly produced through top-down chemical exfoliation of MAX phases (e.g., Ti_3AlC_2) using wet etching with hydrofluoric acid or alternative *in situ* acid generation methods. These treatments remove the A element, while simultaneously functionalizing the surface with terminations such as O, OH, F, and Cl, enabling the formation of stable aqueous dispersions.

In this work, we present two different electrochemical sensors based on 2D MXenes synthesized either by: i) a fluoride etching procedure, or ii) an *in situ* generated fluoride etching procedure. After electrochemical and morphological characterization by scanning electron microscopy and atomic force microscopy, we show an enhanced electrochemical response toward two different analytes of relevance in the environmental and clinical fields, bisphenol A and propofol.

Bisphenol A, a widely used component in the manufacture of plastics and consumer products, is an endocrine-disrupting compound that can be easily released into the environment from polymers such as polycarbonates, posing significant risks to human health and other organisms, particularly during early stages of development. Propofol is a widely used intravenous anesthetic with rapid onset and short half-life, making it suitable for anesthesia induction and maintenance. Despite its favorable pharmacokinetics, propofol misuse has been reported, leading to addiction and severe adverse effects, including fatal respiratory depression.

The developed electrochemical sensors exhibit an enhanced analytical response compared to

the unmodified electrode toward both analytes, leading to excellent detection limits, as well as improved accuracy, precision, and stability. Their applicability to the determination of the analytes in real samples has also been demonstrated.

#23

Synergistic Effect of Integrating MXenes and Diamond Nanoparticles for High-Performance Electrochemical Sensing

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The integration of low-dimensional materials into nanostructured electrochemical sensors has emerged as a powerful strategy to enhance electrocatalytic performance, as well as analytical sensitivity and selectivity. While graphene and transition metal chalcogenides have been widely studied, growing attention has turned toward other nanomaterials, such as MXenes and diamond nanoparticles (DNPs). MXenes, with the general formula $M_{n+1}X_nT_x$ (where M is an early transition metal, X is carbon and/or nitrogen, and T represents surface terminations such as –OH, –O, or –F), combine a large specific surface area with metallic conductivity and a hydrophilic, functionalized surface. Their excellent biocompatibility and resistance to passivation and fouling further contribute to operational stability. Diamond nanoparticles consist of a sp^3-hybridized carbon core, characteristic of pure diamond, and are inherently insulating. However, surface defects and sp^2 carbon regions, functionalized with groups such as oxygen or carboxylic acids, increase the electronic density of states, thereby enhancing conductivity. In addition to the intrinsic properties of diamond—high thermal conductivity, rigidity, and hardness—DNPs offer a large surface area, hydrophilicity, high adsorption capacity, biocompatibility, and electrocatalytic activity. Together, these features make DNPs highly promising for technological, biomedical, and electrochemical applications.

In this work, we explore the synergistic integration of MXenes and diamond nanoparticles in electrochemical sensors, revealing how their complementary properties boost analytical performance. To optimize the sensor design, among other parameters, we evaluate the impact of different MXene synthesis routes, including conventional fluoride etching, *in situ* fluoride generation, and an electrochemical fluoride-free approach. The resulting sensing platforms were comprehensively characterized by cyclic voltammetry, scanning electron microscopy, and atomic force microscopy. Based on these results, we selected the most suitable approach according to the specific target, focusing on two distinct analytes: fenitrothion and tanshinol. Fenitrothion is a widely used organophosphorus insecticide, that may cause environmental contamination of soil and water, posing potential risks to the human nervous system. Tanshinol is a water-soluble compound extracted from the roots of *Salvia miltiorrhiza*, known for its strong antioxidant and anti-inflammatory activities, with potential therapeutic applications, especially in cardiovascular and neuroprotective treatments.

The proposed hybrid approaches enable highly sensitive and selective detection of fenitrothion

and tanshinol, demonstrating the potential of combining 2D and 0D nanomaterials for next-generation sensing platforms.

#24

On the C(1s) core level binding energies of MXene flakes

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Abstract

The C(1s) core-level binding energies (CLBEs) of all C atoms in finite pristine $(M_2C)_{18}$ and O-terminated $(M_2CO_2)_{18}$ MXene flakes (with M = Sc, Y, Ti, Zr, Hf, V, Nb, and Ta) were computed explicitly accounting for final state effects through the ΔSCF approach[1] using density functional theory with the PBE and PBE0 functionals. For each flake, we obtained the distribution of C(1s) CLBE values, which we represent by reporting the maximum and minimum values, together with the value corresponding to the central C atom (Fig. 1). The latter is expected to be more relevant in larger flakes, and in the comparison with periodic and experimental studies. The range of CLBEs originates in structural defects[2] and low coordination sites of the flakes, and should be representative of the width of measured XPS peaks.

The CLBEs increase along periods, in line with radii reduction and increase of electronegativity of the metals, whereas variations along groups resemble ionization potential trends. All $(M_2CO_2)_{18}$ flakes exhibit the same tendency as the $(M_2C)_{18}$ flakes, however, their CLBEs are shifted to higher energies and display a broader distribution (Fig. 1). This is due to (i) the charge transfer and (ii) larger structural distortions caused by the terminal O atoms. Results comparing CLBEs shifts, ΔCLBEs, are in line with the literature,[3] confirming the trends observed for central carbons, with minor quantitative differences. Initial and final state approaches correlate well across different pristine flakes, although deviations arise when comparing C atoms within a given flake. On the other hand, $(M_2CO_2)_{18}$ flakes deviate from this trend due to structural deformations induced by the presence of O terminations. Noteworthy, a linear correlation is found between PBE and hybrid PBE0 functional computed CLBEs, showing that reliable trends can be obtained with the computationally less demanding PBE functional. Moreover, the size effect of MXene flakes was evaluated for larger $(Ti_2C)_n$ flakes (with n = 18, 36, 60, 90, 126, 168, and 216) without significantly modifying the CLBE of the central C atoms, enabling the extrapolation of the present results for XPS peak positioning of larger MXene flakes.

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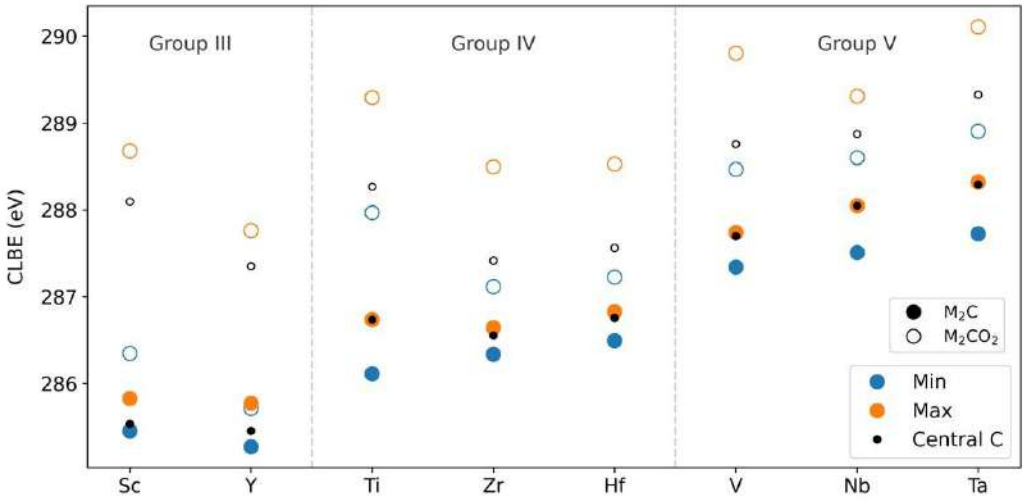

Fig. 1. Calculated C(1s) CLBE for all C atoms in $(M_2C)_{18}$ and $(M_2CO_2)_{18}$ MXenes, ordered by groups according to their transition metal. The minimum and maximum values for each flake are shown in blue and orange, respectively, while the CLBE of the central carbon is shown in black. Filled and open circles correspond to $(M_2C)_{18}$ and $(M_2CO_2)_{18}$ MXenes, respectively.

#25

Assessing the environmental sustainability of V_2CT_x MXenes: a comparative life cycle assessment with $Ti_3C_2T_x$ MXenes

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The rapid expansion of the MXene family has been accompanied by limited research on their environmental sustainability, with most assessments focused on titanium-based systems such as $Ti_3C_2T_x$. This study presents the cradle-to-gate Life Cycle Assessment (LCA) of vanadium-based MXenes, specifically V_2CT_x, and compares its environmental performances with those associated with obtaining $Ti_3C_2T_x$ MXenes evaluated in previous studies. V_2CT_x was prepared through HF-etching of the corresponding V_2CT_x MAX phase, according to previously reported procedures.

The environmental profile of V_2CT_x highlights electricity demand, MAX phase synthesis, hazardous waste from etching, and intercalation reagents as major hotspots in V_2CT_x production. To understand the influence of the nature of transition metals, the corresponding MAX phases were first compared. Although V_2AlC synthesis shows higher burdens on most impact categories than Ti_3AlC_2 pathways, the overall environmental burdens of the resulting MXenes strongly depend on the preparation strategy. Notably, V_2CT_x can exhibit lower impacts than several $Ti_3C_2T_x$ preparation methods despite the contributions associated with the upstream processes producing vanadium precursors, indicating that process-related energy requirements frequently outweigh the environmental burdens attributed to raw-material production.

These findings emphasize the role of synthesis optimization in shaping MXene sustainability and show that vanadium-based MXenes can perform competitively with commonly studied titanium-based analogues in terms of environmental performances.

#26

Electrochemical Impact of MXene Content on $NiFeO_x@V_2CT_x$ for Alkaline OER

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Water electrolysis is a key technology for producing green hydrogen and decarbonizing industrial processes. However, the oxygen evolution reaction (OER) remains the kinetically limiting step, requiring highly active and stable catalysts under alkaline conditions [1]. NiFe-based systems are among the most promising non-noble OER catalysts, showing competitive activities compared with noble-metal oxides such as RuO_2 and IrO_2 [2].

Nevertheless, their performance can be further improved by employing nanostructured conductive supports that optimize catalyst-layer architecture and charge-transfer interfaces [3]. MXenes, a class of 2D materials derived from MAX phases, offer high conductivity, hydrophilicity, and a large electrochemically active surface area, making them attractive supports for NiFe-based catalysts [4].

Here, we present the first stage of a systematic study in which TMAOH-intercalated V_2CT_x MXene is used as a conductive support to anchor $NiFeO_x$, which can evolve into NiFe (oxy)hydroxide phases under polarization, forming $NiFeO_x@V_2CT_x$ heterostructures. A compositional series is investigated by varying the MXene content to 1, 10, 20, 30, and 50 wt%, while keeping the catalyst loading per geometric area constant through a reproducible electrode-preparation protocol. The heterostructures are characterized by X-ray diffraction (XRD) and FE-SEM/EDS. OER performance is evaluated in 1 M KOH in a half-cell configuration using cyclic voltammetry (CV), linear sweep voltammetry (LSV), electrochemical impedance spectroscopy (EIS), and chronoamperometry (CA), as a screening step prior to testing in AEM-type architectures. Interfacial kinetics are assessed from the charge-transfer resistance (Rct) estimated by EIS, and stability is evaluated by 48 h CA.

Overall, this study identifies the MXene content in $NiFeO_x@V_2CT_x$ that best balances OER activity, charge transfer, and durability, providing design criteria for MXene-based anodes targeting AEM water electrolysis.

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#27

Thermal Properties of Pristine and Functionalised $Ti_3C_2T_x$ Printed Thin Films

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The high conductivity, solution processability and rich chemistry of MXenes make them very attractive for applications requiring flexible substrates and thermal functionality with minimal thickness and mass [1] There are currently many theoretical studies on the thermal properties of MXene thin films, but very few experimental results. [2-5] Here we study the thermal properties of pristine and ligand-functionalised $Ti_3C_2T_x$ printed films. MXene nanosheets were obtained from Nanoplexus Ltd, dispersed into a water-based and printable solvent [6] and subsequently inkjet-printed onto SiN membranes. A thin film analyser (TFA) operating under vacuum and at temperatures between –170°C to 250°C was used to extract their thermal and electrical properties as a function of temperature in a single measurement.

The results show that annealing of the $Ti_3C_2T_x$ film before the measurements enable a thermal conductivity of ~14 W/m·K to be achieved at 30°C, [7] which is higher than the thermal conductivity reported in [5]. While the thermal conductivity remains stable after exposure to air of the film for at least 14 days, the sheet resistance increases and saturates to 30 Ω/sq. The ligand functionalisation enables lowering of the thermal conductivity to ~3.5 W m^{-1} K^{-1} at 30°C, but also improves the electrical conductivity, enabling a sheet resistance below 15 Ω/sq to be reached in air, stable for at least 14 days. Due to the improvement in electrical properties, this functionalization is expected to facilitate charge transfer between the nanoflakes. [8,9] Our results show that the thermal conductivity in $Ti_3C_2T_x$ is stable in air and can be decreased *via* ligand functionalization. However, since the electrical conductivity is also affected by the ligand-functionalization, all the $Ti_3C_2T_x$ films show a similar Seebeck coefficient of -10 W μV/K at 30°C, which is in good agreement with [10]. In conclusion, this work demonstrates the ability to tune thermal and electrical conductivity in printed $Ti_3C_2T_x$ films, stable in air for at least 14 days, hence opening up their applications for multifunctional conductive films.

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#28

Synergistic engineering and sintering-induced tuning of Al–Sn co-doped Zn/Co ferrites for integrated hydroelectric and Supercapacitive energy systems.

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Abstract:

The growing demand for sustainable energy technologies has prompted intensive research into multifunctional materials capable of both energy generation and storage. In this study, nanostructured spinel ferrites $ZnAl_{0.1}Sn_{0.1}Fe_{1.8}O_4$ (ZASFO) and $CoAl_{0.1}Sn_{0.1}Fe_{1.8}O_4$ (CASFO) were synthesized via a sol–gel auto-combustion method and sintered at 800 ◦C, 1000 ◦C, and 1200 ◦C to investigate their structural, electrochemical, and hydroelectric properties. Structural analyses using X-ray diffraction, scanning electron microscopy, Fourier trans form infrared spectroscopy, and X-ray photoelectron spectroscopy confirmed single-phase cubic spinel formation with thermally induced grain growth, cation redistribution, and strain relaxation. Electrochemical performance was assessed via cyclic voltammetry and galvanostatic charge–discharge, revealing superior pseudocapacitive behaviour in CASFO sample sintered at 1000 ◦C (CASFO1000), driven by Co2+/Co3+and Fe2+/Fe3+redox transitions, high conductivity, and optimized mesoporosity. CASFO1000 achieved a specific capacitance of 756.57 F/g at 1 mV/s and retained >90 % capacity after prolonged cycling. Concurrently, hydroelectric cell evaluations demonstrated enhanced water dissociation and energy conversion in CASFO1000, yielding an open-cell voltage of 1.05 V and maximum power output of 31.74 mW. These findings underscore the synergistic role of Co substitution, Al and Sn co-doping, and optimized sintering in tailoring spinel ferrite frameworks for integrated green energy applications. This study offers a comprehensive pathway for the design of high-performance oxide-based materials for concurrent energy harvesting and storage systems.

Keywords: Hydroelectric cell, Cationic substitution, Supercapacitor, Defect engineering.

#29

Sustainable MXene synthesis via Lewis-Acid Molten Slats and Tellurium-Assisted approaches for Lithium-Sulfur Batteries

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Abstract:
Lithium-Sulfur batteries (LSBs) are promising next-generation energy storage devices due to their high theoretical energy density, low cost, and environmental friendliness. However, their practical application is limited by challenges such as the insulating nature of sulfur, volumetric expansion during cycling, and the polysulfide shuttle effect, which leads to capacity fading and reduces cycle life. These challenges require the development of advanced host materials that can improve conductivity, accommodate structural changes, and interact effectively with polysulfides. MXenes, 2D transition metal carbides and nitrides, are promising for LSBs due to their conductivity, layered structure, and tunable surface chemistry. Their properties depend on Al-layer etching, which controls interlayer spacing, surface terminations, and structural quality. In this study, we systematically compared four etching elements, CuCl2, ZnCl2, PbCl2, and tellurium (Te), for the preparation of Ti-, V-, Nb-, and Mo-based MXenes. Each method was applied under controlled conditions to selectively remove Al layers and achieve well-delaminated MXene sheets. Structural and surface characterisation using X-ray diffraction, scanning and transmission electron microscopy, and X-ray photoelectron spectroscopy revealed significant differences in etching efficiency, enhanced interlayer spacing, and surface functionalization. Among the four etching components, Te-assisted etching proved superior, enabling simultaneous selective Al removal and in situ Te functionalization. This one-step approach eliminates additional surface functionalization steps, producing MXenes with uniform and abundant surface terminations, expanded interlayer spacing, minimal structural defects, and distinct accordion-like morphologies. In contrast,
MXenes etched with $CuCl_2$, $ZnCl_2$, or $PbCl_2$ required additional processing steps to achieve delamination and surface functionalization. These samples showed agglomerated sheets and the presence of unreacted MAX phase, indicating less controlled etching compared to the Te-assisted route. The effectiveness of Te arises from its mild yet selective etching mechanism, which preserves the MXene lattice while optimising surface chemistry. This work highlights the critical role of etching chemistry in defining MXene structure and surface properties. By demonstrating that Te is the most effective agent for preparing MXenes with optimised interlayer spacing and surface terminations, this study provides practical guidance for designing MXene-based cathode hosts for LSBs. These findings emphasise that careful selection of the etching method can significantly enhance MXene functionality, offering pathways to improved electrochemical performance and long-term stability in LSBs and other applications.

Key Words: MXenes, Lewis-acid molten salts(LAMS), Surface functionalization, Interlayer spacing, Lithium-sulfur batteries (LSBs).

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#30

Nitrogen-to-ammonia conversion on sulphur-terminated molybdenum carbide MXenes

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Ammonia (NH_3) is an essential feedstock for fertilizers and industry, and a promising hydrogen carrier. However, its large-scale production through the Haber-Bosch process remains energy-intensive, requiring harsh conditions to cleave the N≡N bond. This process contributes significantly to global energy consumption and greenhouse gas emissions, urging scientists to find more effective and greener catalysts to N_2 reduction to NH_3.

MXenes have emerged as versatile materials for many important applications, including catalysis, either as the active component, due to its high conductivity and high specific surface area, or as a support for single-atom catalysts (SACs), enhancing their properties. Other applications include energy storage, electromagnetic shielding, sensing, water purification, and electronics [1].

In this communication, we present the results of a computational study, based on density-functional theory, using the PBE-D3 approach, on sulphur-terminated molybdenum carbide (Mo_2CS_2), both in its pristine form and with metallic atoms as SACs for N_2 reduction to NH_3. In particular, we analyse the thermodynamics and kinetics of nitrogen adsorption, activation and hydrogenation, assessing the potential of this MXene as a sustainable catalyst for ammonia production.

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#31

Surface Stability of $Ti_3C_2T_x$ MXenes: A Time-Resolved XPS Study

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Two-dimensional (2D) materials exhibit exceptional physical and chemical properties arising from their atomic-scale layered structure and tuneable composition, making them attractive for both fundamental studies and technological applications. Among them, MXenes have recently emerged as a versatile family of materials with the general formula $M_{n+1}X_nT_x$, where M is a transition metal, X is carbon and/or nitrogen, and T_x represents surface terminations (e.g., F, O, OH). MXenes are typically obtained by selective etching of the corresponding $M_{n+1}AX_n$ (MAX) phases using fluoride-containing solutions. In this work, we focus on Ti-based MXenes.

We introduce a transfer approach that enables wet chemically etched MXenes to be introduced into ultra-high vacuum (UHV). The method involves drop-casting onto a pre-cleaned conductive substrate in vacuo followed by rapid vacuum drying to preserve the surface state. The primary aim is to investigate oxidation pathways under ambient exposure and assess the long-term stability of the material.

In situ characterization was performed using X-ray photoelectron spectroscopy (XPS) complemented by atomic force microscopy (AFM). Samples were subsequently exposed to air for controlled durations (1 h, 24 h, 10 days, 1 month, and 2 months), and the evolution of their surface composition was systematically monitored. This study provides fundamental insight into the environmental stability of MXenes and establishes guidelines for engineering their surface chemistry and optimizing device performance.

#32

Multi-Route Etching of $Mo_2Ti_2C_3T_x$ MXene with tuned surface terminations for Sodium Metal Anodes

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Abstract

Metal batteries have attracted substantial attention for next-generation high-energy storage systems because of their ultrahigh theoretical energy densities and low redox potentials. However, their practical implementation remains limited by uncontrolled dendritic nucleation, unstable solid-electrolyte interphase formation, large nucleation overpotentials, and poor cycling stability. Conventional MXene synthesis predominantly relies on concentrated hydrofluoric acid (HF) etching of MAX precursors. Although HF etching is widely adopted due to its high efficiency and strong selectivity for A-layer removal, it suffers from severe drawbacks including hazardous handling, excessive –F terminations, structural over-etching, and significant environmental concerns. These limitations necessitate the exploration of sustainable etching strategies that can precisely tailor surface terminations while minimizing structural damage. Herein, we comparatively investigate the synthesis of $Mo_2Ti_2C_3T_x$ via multiple etching pathways: *(i)* concentrated HF etching (fast kinetics; F-rich surfaces), *(ii)* mild HF-containing etching (controlled reaction; reduced defects and balanced terminations), *(iii)* Lewis acidic molten salt (LAMS) etching (fluorine-minimized route; alternative halide terminations), and *(iv)* Te-assisted etching (chalcogen-mediated modification; expanded interlayers with possible impurity incorporation). Each strategy induces distinct surface chemistries (–F, –O, –Cl, –Te), defect densities, and interlayer architectures, thereby modulating metal binding energies, ion diffusion pathways, and interfacial stability. During nucleation, the optimized MXene host enables homogeneous metal deposition and reversible stripping with suppressed dendrite growth and low polarization. Among the investigated routes, the mild etching strategy yields $Mo_2Ti_2C_3T_x$ with favourable NaF rich surface terminations, enlarged interlayer spacing, and preserved structural integrity, resulting Coulombic efficiency of 99.2% at high current density (3 mA cm^{-2}) a fixed cutoff capacity of 3 mA h cm^{-2}. Thus, this study highlights the decisive role of synthesis-route engineering in tailoring $Mo_2Ti_2C_3T_x$ surface terminations and structural properties by unlocking the full potential of $Mo_2Ti_2C_3T_x$ MXene by correlating etching chemistry with nucleation thermodynamics and plating/stripping kinetics.

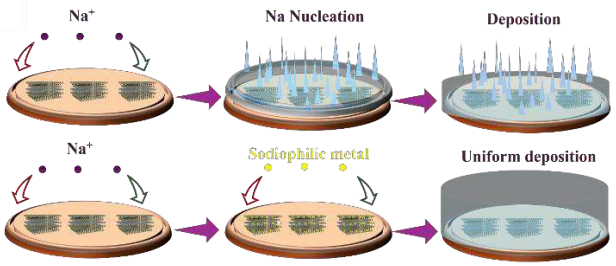

Figure1: Schematic mechanism for nucleation behaviour of $Mo_2Ti_2C_3T_x$ based Na metal anode

Keywords: $Mo_2Ti_2C_3T_x$; Multi-route etching; Na^+ diffusion; High current density; Na-metal anode

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#33

SYNERGISTIC ELECTROCHEMICAL PERFORMANCE OF $Ti_2VC_2T_x$ MXENE AND CARBON CONFINED METAL PHOSPHIDE HETEROSTRUCTURES FOR ADVANCED ENERGY STORAGE

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Abstract:

The rapid expansion of portable electronics and electric vehicles has intensified the demand for advanced energy storage systems that simultaneously deliver high power density, large charge storage capacity, and long-term cycling stability. Two-dimensional (2D) transition metal carbides and nitrides, known as MXenes, have emerged as highly promising electrode materials owing to their metallic conductivity, hydrophilic surfaces, tuneable surface terminations, and dominant surface-controlled charge storage mechanisms. Among the MXene family, $Ti_2VC_2T_x$, belonging to the M_3X_2 structural class, represents an advanced material platform in which the incorporation of vanadium into the titanium carbide lattice enables change of electronic structure and redox activity. This bimetallic configuration has been shown to enhance electrochemical reactivity compared to monometallic MXenes, however, the practical capacity of pristine MXenes remains constrained by nanosheet restacking, which limits ion accessibility and active surface area.

In this work, we explore a composite electrode strategy that integrates $Ti_2VC_2T_x$ MXene with carbon confined copper phosphide (Cu3P@C), derived from copper-based metal organic framework (MOF) via pyrolysis, to address these limitations and enable enhanced electrochemical performance. A series of $Ti_2VC_2T_x$/Cu3P@C composites with varying component ratios were systematically investigated to identify optimal compositions that balance the high electrical conductivity and pseudocapacitive behaviour of the MXene matrix with the high specific capacity associated with the metal phosphide. In the composite architecture, the MXene sheets serve a dual function. The MXene sheets form a continuous conductive network that enables rapid electron transport and buffer the volume changes of Cu_3P during repeated ion insertion and extraction, while the Cu_3P@C phase provides additional redox-active sites, leading to enhanced overall charge storage capacity.

Preliminary electrochemical characterization using cyclic voltammetry, galvanostatic charge–discharge measurements, and electrochemical impedance spectroscopy indicates that the formation of a $Ti_2VC_2T_x$/ Cu3P@C heterostructure effectively suppresses MXene restacking, thereby increasing the density of electrochemically accessible active sites. The resulting interfacial coupling enhances charge transfer kinetics and promotes a synergistic charge storage mechanism combining surface-dominated pseudocapacitance from the MXene with faradaic redox reactions associated with the Cu3P phase. Furthermore, the presence of multiple redox-active transition metals (Ti, V, and Cu) introduces a richer and more flexible redox chemistry, contributing to increased charge storage capacity and an expanded operational potential window.

Overall, this study demonstrates that the rational integration of bimetallic MXenes with carbon confined metal phosphides provides an effective pathway for overcoming intrinsic limitations associated with individual electrode components. By highlighting the critical role of interface engineering and ion-accessible surface design, this work positions $Ti_2VC_2T_x$-based composite electrodes as promising candidates for high-rate pseudocapacitive energy storage and next-generation battery technologies, in line with the emerging directions of MXene-enabled electrochemical systems.

Keywords: $Ti_2VC_2T_x$, MXene, MOF mediated structures, Copper Phosphide, Energy Storage, Heterostructures, Bimetallic MXenes.

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#34

Self-assembled Moiré superstructure of MXene

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The atomically reconstructed Moiré superlattice and its impact on the microscopic electronic structure remains absent. In this investigation, we meticulously inspect and compare the self-assembled Moiré superlattices of MXene. Employing a combination of experimental scanning tunneling microscopy/spectroscopy observations and ab initio simulations, we investigated three distinct self-assembled Moiré patterns characterized by wavelengths approximately around 2.32 nm, 2.17 nm, and 1.12 nm. Our results illuminate a non-monotonic behavior in the Moiré potential concerning periods on the conductance band side. This research not only contributes to a detailed comprehension of MXene's Moiré phenomena but also establishes a fresh foundation for further exploration into unique correlated phases.

#35

Title: Precision Lamellar Engineering of MXene–Lignin Nanocomposites for Tunable GHz Electromagnetic Metasurfaces and Modulators

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Abstract

The integration of 2D transition metal carbides ($Ti_3C_2T_x$ MXenes) into high-frequency electronic and photonic systems remains constrained by their intrinsic structural instability and the difficulty of precisely modulating interlayer spacing to achieve targeted electromagnetic (EM) responses.Here, we present a sustainable design strategy that employs fractionated lignin—an abundant, bio-derived industrial byproduct—as a structure-directing agent and intercalant, enabling sub-nanometer tunable control over MXene lamellar architecture.

Unlike conventional small-molecule dispersants or synthetic polymers, fractionated lignin enables continuous and fine control of MXene interlayer spacing across the colloidal-to-solid-state transition. This lamellar tunability governs interlayer coupling and charge-transport pathways, thereby dictating the macroscopic electrical properties of the resulting films. High-resolution X-ray scattering combined with mesoscale structural analysis establishes a direct correlation between lignin-mediated assembly and the emergent lamellar architecture.

Through controlled lamellar engineering, the resulting MXene-based films exhibit tailored conductivity and permittivity in the GHz regime. The scalability of this approach is demonstrated through integration into patterned metasurfaces and high-speed modulators. Precise regulation of interlayer spacing enables deterministic modulation of EM-wave interactions, while preserving the mechanical integrity and high electrical conductivity of the MXene framework.

This work establishes lamellar spacing engineering as a powerful design lever for 2D material systems. Using sustainable lignin as a structure-directing additive provides a general, environmentally benign toolbox that bridges molecular-scale assembly and device-level electromagnetic functionality. Beyond addressing the structural instability of $Ti_3C_2T_x$ MXene, this strategy offers a scalable pathway toward next-generation GHz-band electronic and photonic devices.

#36

Plasma-Assisted Surface Modification of Ti_2C MXene for Supercapacitor Applications

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The growing demand for clean and sustainable energy solutions, fueled by rapid industrialization and rapid consumption of fossil fuels, has intensified the search to develop more efficient energy storage systems (ESS). Supercapacitors (SCs) have attracted considerable attention due to their high-power density, fast charge-discharge cycles, low self-discharge, and stable performance. However, their large-scale application remains limited by low energy density, which is largely determined by the electrode material properties. Recently, MXenes – a new category of two-dimensional transition metal carbides and nitrides – have gained considerable attention due to their high electrical conductivity, chemical tunability, and mechanical strength, making them promising candidates for electrode materials in SCs.[1] In this work, Ti_2C MXene was synthesized from the underexplored Ti_2AlC MAX phase using an in-situ HF etching method based on ammonium bifluoride. Compared with traditional HF etching methods, this route offers a much safer approach, minimizing the formation of toxic byproducts while improving the surface quality of Ti_2C MXene. The successful formation of MXene was confirmed by observing its typical accordion-like layered structure. Later, the Ti_2C MXene was functionalized via sulfur and oxygen plasma treatments to effectively replace fluorine groups on the surface of the MXene with sulfur and oxygen-containing groups. The introduction of sulfur and oxygen on the surface of the MXene creates additional redox-active sites, thereby improving pseudocapacitive behavior, facilitating stronger electrode-electrolyte interactions, and reducing charge transfer resistance.[2][3] Electrodes prepared from sulfur and oxygen-functionalized MXenes were tested for SC performance, demonstrating a remarkable improvement in performance, delivering a high specific capacitance of 733 F g^{-1} and 205 F g^{-1} at 1 A g^{-1} for sulfur and oxygen-treated Ti_2C MXene, respectively, while maintaining excellent electrochemical stability over 10.000 cycles. Finally, the asymmetric device testing further demonstrated the potential of these plasma-engineered materials, highlighting their suitability for long-term use. Employing such plasma-based techniques for the surface engineering of MXene underscores the practical potential of plasma-based modifications for advanced electrode materials to enhance the performance of SCs.

Key Words: MXenes, plasma-assisted synthesis, energy storage, supercapacitors.

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#37

Exploring the Annealing Effect of Ultra-Thin $Ti_3C_2T_x$ MXene Coated Cu-Substrate Towards Anode-Free Lithium Metal Batteries.

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Abstract

Anode-free or anode-less concept is gaining more attraction in the research community. These types of systems poised deliver much higher energy density and better manufacturability than conventional lithium metal models. Apart from the performance advantage, the increasing cost of Lithium propels more innovative solutions like Anode-free designs for the market balance. If it can be achieved, these systems can effectively reduce the cost of modern batteries. Similar to all the high-concept technologies, anode-free also has huge challenges ahead in terms of shorter cycle life, dendrite formation, cathode dependency and high sensitivity to coulombic efficiency changes. Many of these challenges are closely related to the Li inventory loss. Researchers are working on many aspects of the cell design to overcome these challenges. Substrate/current collector modification is one such approach that we are focusing. Cu, the established current collector faces severe lithium wettability issues which leads to uneven solid-electrolyte interface and dead lithium or dendrite formation. MXene have emerged as material with multitude of properties and applications in the last decade. In this work, an ultra-thin layer of $Ti_3C_2T_x$ MXene coating on Cu foil has been explored to improve the litholphilicity and cyclability of the electrode. We explored annealing effects of the MXene coated electrodes in H_2/Ar atmosphere in multiple temperatures (200, 400 and 600°C) to improve the conductivity and Lithium plating/striping performance. The symmetric cell configuration study shows the annealed samples performed better than pristine MXene sample and bare Cu foil during the cyclic study with 100% coulombic efficiency. The annealing treatment has improved the lithophilicity of MXene and reduced the dendrite formation. Also, the modified surface terminations in MXene after annealing provides a stable and regulated solid-electrolyte interphase that controls the Li^+ transfer and slows down the dendrite growth. To evaluate the performance of these electrode in full-cell configuration they were paired with conventional LFP cathodes. The annealed electrode delivered a considerable capacity retention of 75% after 100 cycles at 1 A/g with good coulombic efficiency. This approach can be a stepping stone to accelerate the anode-free lithium metal battery concepts in much larger scale.

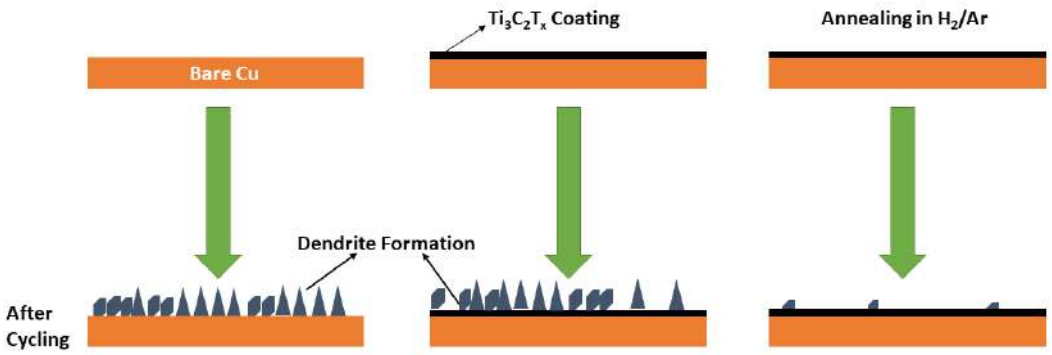

Figure 1: Schematic illustration of the bare Cu, MXene coated Cu and annealed MXene coated Cu electrodes after the cycling.

#38

Toward Multicomponent 2D Carbides: Synthesis and Insights into High-Entropy MXenes

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MXenes are an emerging class of 2D materials with significant potential in various technological applications, particularly in energy conversion and storage [1]. The introduction of high-entropy MXenes presents a novel approach to tailoring nanolaminate carbides microstructure and chemical composition [1]. High-entropy MXenes are distinguished by their excellent electrical conductivity and stability, making them highly suitable for applications in electrolysis and catalysis as co-catalysts [2]. In this study, the multi-elemental single-phase (TiNbTaMo)C_3T_x MXene was synthesized through etching with HF and HCl, enabling the delamination and exfoliation of the respective MAX phase precursor. Various techniques were employed to characterize their structural, morphological, and electrochemical properties, including X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS), X-ray, transmission electron microscopy (TEM), electrochemical impedance spectroscopy (EIS), and cyclic voltammetry (CV).

Acknowledgements

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#39

Laser-Assisted Synthesis of $Ti_3C_2T_x$ MXene decorated with Platinum Nanoparticles for Enhanced Hydrogen Evolution

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The global demand for sustainable energy carriers has established hydrogen as a pivotal alternative to fossil fuels. While water electrolysis is the leading method for green hydrogen production, its efficiency depends on electrocatalysts capable of overcoming the kinetic barriers of the Hydrogen Evolution Reaction (HER). Platinum (Pt) remains the benchmark catalyst due to its optimal Gibbs free energy for hydrogen adsorption [1]. However, its high cost and scarcity necessitate strategies to maximize atomic efficiency, such as dispersing nanoparticles onto conductive 2D supports [2]. MXenes have emerged as exceptional support due to their metallic conductivity, hydrophilic surface, and ease of functionalization.

Usual synthesis routes for these MXene-based hybrids often rely on thermal reduction, which presents significant technical challenges, such as the requirement for furnaces with controlled inert atmospheres to prevent oxidation and prolonged synthesis times [3]. In contrast, recent studies have successfully explored laser-induced techniques for reducing metals onto graphene oxide, offering a more efficient alternative for 2D material processing [4]. Inspired by these advancements, we propose a novel method using a 450 nm laser to reduce Pt precursors onto $Ti_3C_2T_x$. This approach provides a significantly simpler and faster synthesis route, enabling reduction without the need for complex experimental setups.

TEM analysis confirmed the successful formation of finely dispersed Pt nanoparticles, with diameters below 2 nm. This localized laser-induced reduction effectively did not show nanoparticle agglomeration. Electrochemical evaluations via Linear Sweep Voltammetry reveal that the laser- assisted Pt decoration significantly lowers the overpotentials of pristine MXenes (from -344 mV to -89 mV at -10 mA/cm^2). Notably, the decorated hybrids demonstrated superior mass activity when compared to commercial Pt/C benchmarks. This confirms that the synergy between the $Ti_3C_2T_x$ and the nanoparticles creates a highly efficient electrocatalytic system. This study marks a significant step toward the development of low-loading, high-activity electrocatalysts, providing a cost-effective manufacturing route for sustainable hydrogen production.

Acknowledgments

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#40

Rapid Molten Salt Synthesis of $Ti_3C_2T_x$ MXene for Neuromorphic Memristive Devices

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MXenes high electrical conductivity alongside straightforward solution-processable thin-film deposition make them attractive for electronic applications, particularly for low power artificial intelligence (AI) hardware.
The rapid expansion of AI infrastructure is placing unprecedented demands on the global energy supply. Globally, data centres consumed around 415 TWh in 2024 and the International Energy Agency projects this will more than double by 2030, driven primarily by AI [1].

Developing hardware that minimises energy consumption is therefore critical, and MXenes offer a promising route toward this goal. Neuromorphic computing is a new paradigm that rethinks computing architecture for enabling AI at a large scale. It mimics how neurons and synapses in the brain process and store information simultaneously. Memristors, the core building blocks of neuromorphic computing, are resistive switching devices with programmable conductance states. The ability to tune MXene conductivity and surface chemistry makes them strong candidates for the active element within a memristor. In this work, $Ti_3C_2T_x$ MXene was prepared via an optimised molten salt synthesis route using
ammonium bifluoride (NH_4HF_2) [2], for memristor applications. In our approach, the MAX phase and the corresponding salts are ball-milled prior to etching.

This maximises interfacial contact and accelerates reaction kinetics to complete etching in under 5 minutes. Additionally, this technique poses much lower hazard, avoiding the acute toxicity risks associated with concentrated HF. Successful MXene exfoliation was confirmed using various characterisation tools. The scanning electron microscopy image in Figure 1(a) shows well-exfoliated $Ti_3C_2T_x$ sheets with a distinct accordion-like layered structure, indicative of successful etching and delamination. The XRD pattern in Figure 1(b) reveals a (002) peak at 6.46°, significantly lower than the 6.96° reported in the original method. This confirms successful etching of MAX phase and expansion of the interlayer spacing between the exfoliated MXene sheets

An increased interlayer spacing enhances ion migration channels within the MXene layers, leading to more uniform filament formation and improved switching stability of the memristor devices. Thin film memristor devices were fabricated by sandwiching MXene between two conductive electrodes, namely Ag and Pt. Electrical characterisation revealed reproducible hysteretic IV characteristics, consistent with resistive switching behaviour within the MXene layer. Resistance states were reproducibly maintained across successive sweeps, with devices remaining stable over one month, indicating stable, non-volatile switching behaviour. In summary, these findings highlight the molten salt route as a promising, scalable pathway for producing MXenes tailored for next-generation neuromorphic computing architecture.

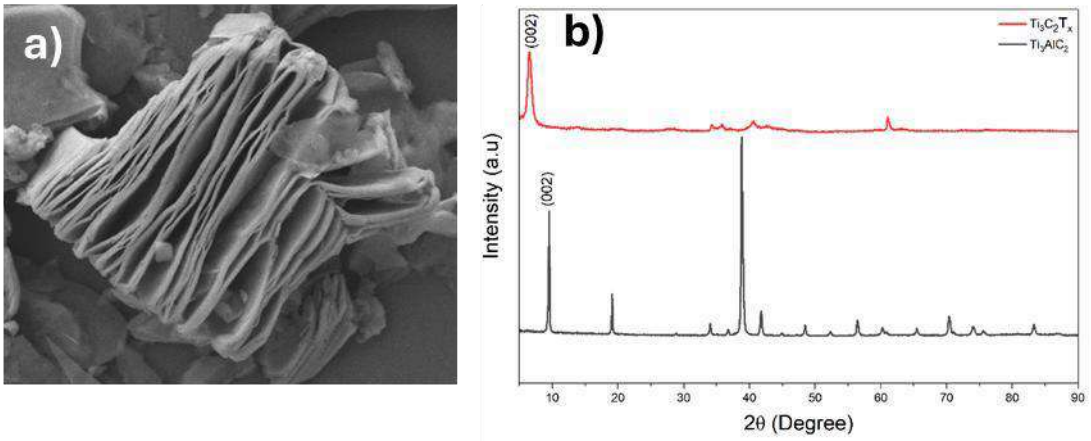

Figure 1. Characterisation of $Ti_3C_2T_x$ MXene and memristor device performance. (a) XRD patterns of Ti_3AlC_2 MAX phase and $Ti_3C_2T_x$ MXene (b) SEM image of $Ti_3C_2T_x$

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#41

Ti_3C_2 MXene/Human Hair Activated Carbon Engineered Composites for High-Performance Supercapacitor Applications

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This study reports the synthesis of Ti_3C_2 MXene and its composites with human hair– derived activated carbon (HH-AC) for enhanced supercapacitor performance. Ti_3C_2 MXene was prepared via hydrofluoric acid etching of Ti_3AlC_2 (MAX phase), followed by a sonication-assisted incorporation of HH-AC at different mass ratios (1:0.5, 1:1, and 1:2) to form Ti_3C_2:HH-AC composites. The structural and textural properties of the as-synthesized materials were investigated using TEM, SEM, XRD, Raman spectroscopy, and BET surface area analysis. Electrochemical evaluation in a three-electrode configuration revealed that the Ti_3C_2:HH-AC (1:1) composite delivered the highest specific capacitance of 215.8 F g^{-1} in 1 M H_2SO_4, significantly surpassing that of pristine Ti_3C_2 (74.2 F g^{-1}). The composite electrode also exhibited a high coulombic efficiency of 106.6% and excellent cycling stability, retaining 82.1% of its initial capacitance after 5,000 charge–discharge cycles. The enhanced electrochemical performance is attributed to the porous HH-AC framework, which effectively suppresses MXene restacking and improves ion accessibility, thereby promoting higher charge storage capability.

Keywords*:* Ti_3C_2 MXene, HH-AC, porous, layers, electrochemical properties, specific capacitance, supercapacitor.

#42

Impact of $Ti_3C_2T_x$ MXene Form and Loading on FTO/Cu_2O Photocathodes for Selective PEC CO_2 Reduction to Ethanol

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Photo-electrocatalytic CO_2 reduction (PEC CO_2RR) is emerging as a promising route to convert CO_2, which, rather than being treated solely as a problematic greenhouse gas, can be reconsidered as an alternative carbon feedstock. Among the various semiconductors explored as photocathodes, Cu_2O stands
out due to its suitable bandgap of about 2.2 eV, which enables efficient harvesting of visible light, unlike wide-bandgap oxides such as TiO_2 that require UV illumination.
However, Cu_2O suffers from fast charge recombination and photocorrosion, which severely restrict its long-term operation as a photocathode. To mitigate these issues, Cu_2O is typically coupled with an additional phase that forms a heterojunction. It promotes rapid charge separation and extraction from the Cu_2O surface, and reduces the probability that photogenerated electrons will be consumed in $Cu_2O \rightarrow Cu$ reduction instead of driving CO_2 conversion. MXenes are particularly attractive for this role because (i) their
metallic-like conductivity provides an efficient pathway for electron transport, (ii) their high volumetric capacitance supports charge buffering at the Cu_2O/MXene interface, (iii) their 2D layered morphology ensures intimate interfacial contact and large effective area, and (iv) their surface terminations can be tailored to optimize band alignment and interfacial chemistry with Cu_2O.
In our previous study1, we systematically examined how tailoring the $Ti_3C_2T_x$ surface impacts the behaviour
of Cu_2O–MXene photocathodes in CO_2RR with highly selective ethanol formation. This work revealed that achieving a continuous MXene overlayer is crucial for long-term electrode stability. Building on these findings, the present work focuses on how different forms of $Ti_3C_2T_x$ and their deposition routes control the coverage of Cu_2O and, consequently, dictate the photocathode's activity and durability in PEC CO_2RR.
Cu_2O photocathodes were fabricated by electrodeposition on FTO, followed by spraying an aqueous $Ti_3C_2T_x$ dispersion to form the MXene overlayer. Four distinct $Ti_3C_2T_x$ batches were used: (i) multilayer $Ti_3C_2T_x$ obtained via conventional HF etching of the Ti_3AlC_2 MAX phase, (ii) the same multilayer $Ti_3C_2T_x$ further downsized by ball-milling, (iii) colloidal $Ti_3C_2T_x$ produced by tetramethylammonium hydroxide intercalation and subsequent exfoliation, and (iv) colloidal $Ti_3C_2T_x$ prepared via the MILD route. For each MXene type, at least two loadings (10 and 50 wt% $Ti_3C_2T_x$ with respect to Cu_2O) were deposited. The resulting FTO/Cu_2O/MXene electrodes were characterized by XRD, SEM-EDX, linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS), and their photo-electrocatalytic CO_2 reduction performance was assessed chronoamperometrically at 0.24 V vs. RHE for 2 and 6 h under CO_2-saturated conditions.

Preliminary results reveal a pronounced enhancement of long-term photocathode stability when colloidal $Ti_3C_2T_x$ dispersions are employed, as they enable more homogeneous Cu_2O coverage and effectively suppress direct contact between Cu_2O and the aqueous electrolyte, thus mitigating self-reduction. In this contribution, we elucidate how the specific MXene synthesis route and deposition conditions onto FTO/Cu_2O govern interfacial architecture, durability, and CO_2-reduction performance over extended operation. Together, these insights provide practical guidelines for rationally engineering Cu_2O/MXene architectures that combine high activity with robust stability in photo-electrochemical CO_2 conversion.

1 Luis A.M. Carrascosa, Magdaléna Linková, Monika Remzová, Tomáš Hrbek and Pavla Eliášová; Surface- engineered Ti3C2Tx MXene/Cu2O Photocathodes for Highly Selective Photoelectrocatalytic CO2 Reduction to Ethanol; under revision in Advanced Energy Materials, 2026.

#43

PDA-Functionalised MXene Hydrogels as Injectable Bioadhesives

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Abstract

Damage to electrically active tissue, specifically heart, disrupts signal transmission and can lead to several functional impairment. Conductive biomaterials have emerged as promising approach in tissue engineering to restore the electrical continuity and promote regeneration [1]. However, most existing materials require invasive implantation and often exhibit trade-offs among electrical conductivity, wet adhesion, and mechanical integrity, limiting their overall performance in dynamic cardiac environments.

To overcome these limitations, we developed an injectable MXene-integrated hydrogel patch (PDA-MXene/SA-DA/GelMA) for minimally invasive delivery, integrating electrical conductivity, wet adhesion, and mechanical compliance within a single self-healing matrix. Sequential crosslinking via Ca^{2+} induced ionic assembly followed by spatially localised photo-crosslinking, establishing an asymmetric interpenetrating network that adheres conformally to tissue while forming a non-fouling outer surface [2]. The hydrogel formulation comprised 8 wt% GelMA, 5 wt% SA-DA (dopamine functionalised alginate), and 0.2 wt% N-(2-aminoethyl)-3-aminopropyltrimethoxysilane (AEAPTMS) or polydopamine (PDA) modified MXene, together with 3 wt% Ca^{2+}, 0.25 wt% lithium phenyl (2,4,6-trimethylbenzoyl) phosphinate (LAP), and 0.8 wt% poly (ethylene glycol) diacrylate (PEGDA). Three experimental groups were created to assess hydrogel performance: a control group without MXene, and two modified groups incorporating either AEAPTMS or PDA functionalised MXene. As pristine MXene ($Ti_3C_2T_x$) undergoes rapid oxidation and aggregation in gel environments (ionic condition), surface modification with PDA and AEAPTMS was employed to stabilise dispersion, enhance interfacial compatibility, and promote formation of a continuous conductive network [3, 4].

FTIR confirmed successful network formation and component incorporation across all groups, indicated by characteristic alginate/GelMA bands (COO^- at ~1600 and 1400 cm^{-1}, amide I/II near 1650 and 1540 cm^{-1}) and

additional aromatic/C–N signals from dopamine and MXene surface modifications in the 1500–1300 cm^{-1} region. Rheological characterisation revealed shear-thinning and gel-like behaviour ($G' > G''$) across all groups, with PDA-MXene displaying an enhanced storage modulus (~300 Pa) compared with the control (~85 Pa) and AEAPTMS -MXene (~92 Pa). Lap-shear tests on chicken tissue demonstrated superior adhesion strength for MXene-containing hydrogels, with PDA-MXene achieving 0.577 $N.mm^{-2}$ due to synergistic catechol-mediated crosslinking. Two-point probe measurements indicated increased electrical conductivity in MXene composites, with PDA-MXene exhibiting improved charge transport resulting from enhanced nanosheet dispersion and percolation. Swelling equilibrium was reached within 24 hours for all groups, with reduced swelling (~25 %) for MXene formulations compared with the control (40 %), reflecting higher network crosslinking density. Cytocompatibility assays using C3H10 fibroblasts confirmed > 85 % viability up to 72 hours across all group, with evidence of enhanced cell spreading and proliferation on MXene -modified hydrogels.

Taken together, these findings demonstrate that MXene functionalisation, particularly via PDA mediated surface chemistry, significantly enhances the electrical, mechanical, and adhesive performance of SA-DA/GelMA hydrogels while maintaining biocompatibility, establishing PDA MXene/SA-DA/GelMA as a promising minimally invasive platform for effective tissue repair.

Keywords: Bioadhesives, Conductive Hydrogel, PDA-MXene, Wet Adhesion

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#44

$Ti_3C_2T_x$ MXene in Metal Powders: A Step Toward 2D Material–Metal Composites for Energy Applications

Apostolos Koutsioukis, Siyuan Ruan, Dahnan Spurling, Rocco Lupoi, Valeria Nicolosi

Scalable fabrication of **2D** nanosheet-reinforced metal matrix composites (**2D**MMCs) remains a major challenge for advanced energy and thermal management applications. The rapid development of two-dimensional (2D) materials has opened new opportunities in this field, with MXenes emerging as particularly promising due to their excellent physicochemical properties and outstanding processability in liquid media. Here, we present a highly viscous MXene-based ink capable of uniformly coating a wide variety of metal powders used in additive manufacturing. This approach enables the formation of engineered MXene–metal matrix composites with potential for thermal management applications and compatibility with 3D printing technologies. The resulting $Ti_3C_2T_x$/MMCs are characterized using UV–Vis spectroscopy, TEM, and XRD to investigate their structural and chemical properties.

#45

Controlled Surface Termination Removal in MXenes via Transition Metal Substitution

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MXenes are two-dimensional materials composed of alternating layers of an early transition metal (M) and nitrogen or carbon (X), in a ratio of n+1 to n where n is an integer between 1 and 4. MXenes also contain an outermost termination layer (T), which derives from the chosen method of synthesis.[1] The first MXene, $Ti_3C_2T_x$, was synthesized by Gogotsi and coworkers in 2011 through Al exfoliation of the Ti_3AlC_2 MAX phase using hydrofluoric acid (HF).[2] MXenes have seen a significant development of the synthesis techniques over the past 15 years and found applications in an increasing number of fields.

The high customizability, conductivity and large surface areas of MXenes, among other properties, endow these materials with a noteworthy catalytic potential, which can be further improved through modification of their surface termination. The creation of vacancies at the surface of MXenes brings two advantages: i) it exposes the more reactive metal atoms, which then serve as catalytic sites; and ii) it disrupts the electronic environment of the neighbouring atoms, possibly encouraging the formation of more catalytic sites.[3]

This communication details the use of density functional theory (DFT) calculations to investigate the incorporation of single substitutional transition metal dopant atoms into the MXene metal layer and how these may influence the energetic cost for removal of the neighbouring surface termination. This effect is studied across various MXene structures and different surface termination compositions (T= O, F, S and Cl).

Acknowledgements
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#46

MXene-Based Transparent Conductive Thin Films Using Liquid-Liquid Interfacial Deposition

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Abstract

Two dimensional titanium carbides otherwise known as MXenes have attracted significant attention amongst the scientific research community due to their exceptional electrical and optical properties[1]. Previous studies have shown that the optoelectronic properties of solution- processed 2D material films are highly dependent on their morphology, where the tiling of nanosheets matters the most when creating connective pathways throughout the deposited monolayer[2]. Liquid-liquid interfacial deposition (LLID) has been reported as an effective and reproducible method to achieve this arrangement of nanosheets[3]. In this current research, we apply LLID to synthesise transparent conductive thin films (TCTFs) using MXene Ti_3C_2 dissolved in dimethylformamide (DMF), MXene Ti_3C_2 dissolved in Formamide (FA), and graphene dissolved in isopropanol (IPA) and examine their optical and electrical properties. We find that the absorption response increases with increasing layer number, as the samples absorb more light per unit thickness; showing that the film thickness can be carefully controlled and measured using LLID. Moreover, the sheet resistance decreases as film thickness increases. The conductivity of MXene FA thin films with a thickness of ≈ 8 nm was determined to be 4.5 × 10^5 S/m[4]. The electronic properties of both were compared to a model graphene system. This work demonstrates a promising route to deposit high-performing MXene thin-films for optoelectronic applications.

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#47

Anomalous microwave absorption hysteresis in ultrathin MXene films with confined water

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Abstract

MXenes, a family of two-dimensional (2D) transition-metal carbides, nitrides, and carbonitrides, are promising materials for electromagnetic interference (EMI) shielding due to their electronic conductivity, tunable surface functionalization, and adjustable interlayer spacing. In many practical environments, MXene films host water molecules between the carbide or nitride nanosheets. However, the influence of confined water on their microwave absorption remains unclear. Here, we demonstrate that water confinement is a major factor governing microwave absorption in $Ti_3C_2T_x$ MXene films. In situ humidity-dependent measurements reveal that protonated films exhibit a 56% increase in absorption even without measurable changes in interlayer spacing. In contrast, Li^+-intercalated films, which undergo interlayer swelling upon water uptake, show a 167% increase in absorption. Remarkably, the observed enhancement in microwave absorption upon water uptake is approximately four orders of magnitude larger than what would be expected from the increase in bulk water content alone. These anomalous changes indicate that water confined within MXene films produces microwave absorption behavior, unlike that of conventional microwave shielding materials where impedance matching is achieved by varying material thickness. The results provide new insight into the mechanism of EMI absorption in MXenes and identify water confinement as a tunable parameter for engineering high- performance EMI shielding materials.

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Defect-Enhanced Electrocatalytic and Energy Storage Performance of Mo_2CT_x MXene

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Mo-based MXenes have garnered significant interest for their applications in electronics, energy conversion, and storage, primarily due to their tunable surface chemistry[1,2,3]. However, the effects of realistic termination edges and point defects in these materials remain insufficiently explored. Edge and defect engineering in 2D materials is essential for uncovering emergent functional properties that may be absent in their pristine form [4]. In this study, we employ density functional theory (DFT) calculations to investigate how different surface terminations (-O, –OH, and –F) affect the electronic and transport properties of Mo_2C MXene. Alongside uniformly terminated structures, we consider a realistic mixed-termination model that better represents experimentally synthesized and etched MXenes. We evaluate the electrocatalytic activity toward the hydrogen evolution reaction (HER) through proton adsorption analysis and examine supercapacitor performance using various ions (Li^+, Na^+, K^+). Additionally, we investigate the effect of molybdenum (Mo) vacancies, which enhance proton and ion adsorption and facilitate significant charge transfer, ultimately improving the electrochemical activity of the system. Overall, the study demonstrates that both surface termination and defect engineering are effective strategies for designing the multifunctional properties of Mo_2C MXene for applications in nanoelectronics, electrocatalysis, and energy storage.

References

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