Accepted Abstracts

Oral Presentation

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Abdoulaye Djire—Invited Speaker
Assistant Professor, Dept. of Chemical Engineering
Texas A&M University
USA

Day 2, August 6, 2024, 9:45 AM, Mitchell Auditorium

Title: Operando Spectroelectrochemical Techniques for Elucidating the Mars-van Krevelen Cycle for Green Ammonia Production on Nitride MXene
Co-Authors: Denis Johnson

The electrochemical nitrogen reduction reaction (NRR) provides an opportunity to convert nitrogen (N2) to ammonia (NH3) at ambient conditions. Protons (H+), which stem from water oxidation, are necessary for this process, but result in the hydrogen evolution reaction (HER) reducing overall selectivity. Another cause for low selectivity in the NRR is the high energy required to activate the NN bond during typical adsorption-desorption mechanisms. An avenue to mitigate these challenges altogether is available on transition metal nitride materials through the Mars-van Krevelen (MvK) mechanism, where sub-lattice nitrogen atoms are protonated to form NH3, which then desorb to form nitrogen vacancies that require less energy to weaken the NN. Recently, we have provided preliminary evidence that the Ti2NTx MXene operates through this MvK mechanism. To further corroborate this mechanism, a series of electrochemical and in-situ spectroscopic techniques, such as X-ray absorption spectroscopy (XAS) and Raman spectroscopy were utilized. We use XAS to track the Ti oxidation state shift as a function of applied potential to understand the role of the Ti in the MvK mechanism and to understand the dynamic change in the Ti-N-Ti bond network. Raman spectroscopy displayed a stable cycle of vacancy creation and replenishment after long-term NRR experiments in inert atmosphere. Finally, we use DFT to corroborate the experimental work and further enhance our understanding of the mechanisms of NRR. These findings serve as the foundation to produce green ammonia using earth abundant resources.

Açelya Yılmazer—Invited Speaker
Associate Professor, Biomedical Engineering Department
Ankara University
Turkey

Day 3, August 7, 2024, 10:45 AM, Mitchell Auditorium
Title: From cancer research to anti-virals: a journey with MXenes and 2D materials
Co-Authors:

Since their discovery, MXenes and 2D materials have attracted a lot of attention in biomedical applications, especially in cancer research. Thanks to their extraordinary properties, we have been using them to diagnose cancer, deliver chemotherapeutics or exert anti-tumor activities through various different mechanisms. The COVID-19 pandemic has shown the success of nanotechnology in combating with viruses in different applications including the development of vaccines or personal protective equipment (PPE). Among these nanotechnology-based systems, MXenes have been shown to efficiently favor anti-viral activity and maintain a safer environment to protect people against pathogens. During this presentation, starting from anti-cancer applications, the anti-viral studies performed using MXenes and other 2D materials will be discussed in detail. Our group has also used various omic approaches to reveal the mechanisms behind these anti-cancer and anti-viral properties. The talk will underscore the importance of harnessing omic biology to propel nanotherapeutics forward, for combating cancer or global infectious diseases in the future.

Aleksandra Vojvodic – Invited Speaker
Associate Professor, Department of Chemical and Biomolecular Engineering
University of Pennsylvania
USA

Day 1, August 5, 2024, 4:05 PM, Mitchell Auditorium

Title: Hydrogen Production and Storage enabled by MXenes
Co-Authors:

As part of the endeavor towards alternative energy sources, there is a resurgence in research activities on materials for hydrogen production and hydrogen storage. In this presentation, I will provide a discussion of the potential that MXenes offer for different hydrogen chemistries. I will start by describing our efforts since the first discovery in 2016 of active MXenes for electrochemical hydrogen production. Next, I will discuss our recent efforts to establish a framework to evaluate hydrogen storage in MXenes. We propose a framework for hydrogen storage in 2D MXenes where it is assumed that the total hydrogen storage has multiple contributions with two dominating scenarios: (i) direct bond formation between the hydrogen and the basal plane or inside of a single MXene sheet (intra-layer); or (ii) stored in-between two MXene sheets. A systematic evaluation both of molecular and atomic hydrogen uptake and storage by stoichiometric and non-stoichiometric functionalized MXenes is discussed. Throughout the presentation, I will emphasize the power of having a close combined computation-experiment feedback loop. With the many opportunities that MXenes offer for different chemistries including hydrogen production and storage, it is imperative that careful and prudent measurements are made, and these measurements are accompanied, supported, or driven by computational modeling that closely resembles real materials and physical conditions.
Ammanda Sfeir  
PhD student  
Université de Lille - CNRS  
France

Day 2, August 6, 2024, 5:00 PM, Mitchell Auditorium

Title: Unlocking the potential of MXenes in H related catalytic reactions  
Co-Authors:

**Introduction:** With aiming to decrease CO2 emissions and searching for clean energy sources, H2 related reactions (ammonia synthesis, ammonia decomposition, CO2 methanation,...) are of high importance and the search of optimal catalysts is vital. MXenes' tunable surface chemistry, as well as scalable synthesis, give the potential for use as catalysts or supports for various catalytic reactions. Thus, it is crucial to unfold the potential of these materials in heterogeneous catalysis. The objective of this work is to study a variety of MXenes on model reactions and asses their behavior and activity. **Ammonia Synthesis:** Figure 1 shows the results of Co decorated MXenes for ammonia synthesis. EDS confirms the 2D morphology of the catalyst with homogeneously dispersed Co (Fig 1-a) and the accordion-like structure (fig 1-e) with an interlayer spacing between the Mo2CTx layers (Fig 1-b). The shift in [0002] peak to lower 2 confirms the successful etching (Fig 1-d). The developed catalyst was highly active for ammonia synthesis (Fig 1-c,e), demonstrating a high rate up to 9500 µmol g^{-1}active phase h^{-1} at 400 °C under ambient pressure in steady state conditions, and did not suffer from any deactivation after 15 days of reaction.

**HDO of m-cresol:** Table 1 reports the HDO reaction rate, distribution of products, and selectivity at low conversion using m-cresol as a model molecule. 5-Ni-Mo2CTx-MI exhibited the highest deoxygenation activity,16-fold higher than that for Mo2CTx. The selectivity to toluene followed the order: Mo1.33CTx (100) = Mo2Ti2C3Tx (100) > 5Ni-Mo2CTx-MI (95) > Mo2CTx (90) > 5Ni-Mo2CTx-WT (65).

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Ana Primo  
Tenured Scientist  
Instituto de Tecnología Química (UPV-CSIC)  
Spain

Day 2, August 6, 2024, 4:40 PM, Mitchell Auditorium

Title: MXenes dots as photocatalysts for CO2 hydrogenation  
Co-Authors: Hermenegildo García

Four MXene dots (MDs) (Ti3C2, Ti2C, V2C and Nb2C) have been prepared by laser ablation of the corresponding MAX phases in aqueous medium and subsequent separation by double centrifugation. These MDs were characterized by atomic force and transmission electron microscopy that show, respectively, thickness between 3 and 7.5 nm corresponding to few-layer nanoparticles and homogeneous lateral dimensions between 2.5 and 5 nm with high crystallinity. IR
spectroscopy indicates that Ti3C2 and Ti2C contain OH as surface terminal groups, while XPS indicates the presence of O on the surface for the four samples. MDs present the most intense absorption band in the UV region with onset below 400 nm. These samples exhibit photocatalytic activity for CO2 hydrogenation to CO and methane, following the order Ti3C2>Nb2C>Ti2C>V2C. Isotopic label experiments confirm CO2 as the origin of the photo products. Most of the photoresponse derives from the UV photons, the photocatalytic activity increasing with the temperature in the range from 200 to 300 °C. These results show the possibility of tuning the composition, surface terminal groups, and other structural parameters of MXenes to produce semiconducting materials exhibiting important photocatalytic activity. Considering their versatility, flexible composition, and tunability, MXenes appear as promising 2D materials with intrinsic photoresponse to develop highly efficient photocatalysts.

Andreas Rosenkranz – Invited Speaker
Professor, Department of Chemical Engineering, Biotechnology and Materials
University of Chile
Chile

Day 2, August 6, 2024, 1:30 PM, Mitchell Auditorium

Title: Tunable Mechanical and Tribological Properties - Underlying Mechanisms and Kinetics
Co-Authors:

MXenes, a new class of early transition metal carbide, nitrides and carbonitrides, have gained tremendous attention in the scientific community due to their interesting property combination. Applied as solid lubricant coatings, MXenes have shown an outstanding performance resulting in an excellent durability and longevity (ultra-high wear resistance), which even outperformed state-of-the-art solid lubricant including graphene and MoS2. This contribution presents the latest findings regarding MXenes’ ability to form beneficial tribolayers depending on MXenes’ number of layers (few- versus multi-layer systems), coatings thickness (amount of lubricious material), applied load (thermomechanical) and sliding velocity (kinetics). Based upon the experiments conducted, we verify thermomechanical and kinetic aspects of the involved tribolayer formation, which align well with the respective temporal evolution of the coefficient of friction. When exceeding a critical value of the applied normal load (Hertzian contact pressure), the formation of a stable tribolayer with beneficial friction and wear properties is not possible. More importantly, the same conclusion can be drawn when exceeding a critical sliding velocity, which clearly shows the kinetic aspect of the involved layer formation. We also verify that increasing the respective thickness of the MXene coatings does not necessarily result in more beneficial effects (low friction, low wear, and long-lasting effects). This contribution also sheds some light on this open question, thus giving some important guidelines and recommendation for future tribological experiments using MXenes.

André Taylor – Invited Speaker
Professor, Dept. of Chemical and Biomolecular Engineering
New York University
USA
Recent advancements in cadmium telluride (CdTe) photovoltaic technology have significantly improved efficiency and commercial viability, but the development of an optimal back contact layer remains a challenge. Our research addresses this by leveraging the unique properties of MXenes. We present a hierarchical transparent back contact design that integrates an AlGaOx passivating layer with Ti3C2Tx MXene and a transparent cracked film lithography (CFL) templated nanogrid on copper-free CdTe devices. The AlGaOx layer enhances open-circuit voltage but initially reduces the fill factor, which is mitigated by the Ti3C2Tx interlayer. This interlayer improves the fill factor, reduces Schottky barriers, and facilitates transverse conduction into the nanogrid. Evaluating the bifacial performance of the AlGaOx/Ti3C2Tx/CFL gold contact, we achieve 19.5% frontside efficiency and 2.8% backside efficiency under 1-sun illumination. Under dual illumination, the device generates 200 W/m² with 0.1 sun backside illumination. Additionally, Ti3C2Tx MXene films, processed from an aqueous colloidal dispersion, demonstrate high metallic conductivity and work function, making them efficient hole contact materials for CdTe solar cells. We analyze Schottky barrier formation in Ti3C2Tx-contacted CdTe devices, offering insights for future development. The versatility of the MXene family presents a promising strategy for next-generation hole contacts, potentially overcoming current limitations and driving further advancements in CdTe solar cell technology.

Andrew Rappe -Invited Speaker
Professor, Dept. of Chemistry and Dept. of Materials Science and Engineering
University of Pennsylvania
USA

MXenes are promising 2D materials exhibiting a broad range of applications from energy storage, catalysis, and sensing devices, all the way to biomedical applications. With a combination of conductivity and tunable surface chemistry, they make major contributions to the family of 2D materials, most of which are semimetals, dielectrics, or semiconductors. In this talk, we showcase our efforts exploring the design, synthesis, and characterization of MXenes and demonstrate the role of theory and computational tools, in particular, DFT, as the guiding compass in deciphering MXenes’ characteristics at the atomic and electronic levels. Such understanding will provide insights that allow for fine-tuning and designing novel compositions and structures with tailored properties. As part of an NSF future manufacturing center, we address, through first-principles calculations, one of the ongoing challenges: MXene stability against oxidation under high temperature. We unravel that water molecules are more likely to be trapped between the MXene flakes, which can be removed merely through vacuum annealing at high temperatures. Furthermore,
by calculating the electrical and optical conductivity and comparing the calculated extinction coefficient spectrum to the experiments, we identify the prominent surface terminations of Ti3C2T2. We further show that the peak in the extinction coefficient spectrum will red-shift, due to the presence of intercalated water, consistent with our collaborators’ experimental observations. Throughout our ongoing work, we display the synergistic interplay between theory and experiment by utilizing the predictive power of computation and modeling along with experiments in exploring the phase space of MXenes, advancing them toward nanomaterial applications.

Andrii Boichuk  
Postdoctoral Researcher  
University of Valencia  
Spain  

Day 2, August 6, 2024, 2:45 PM, Hill Conference Room

Title: Pseudocapacity mechanisms in delaminated and non-delaminated MXenes: electrochemical studies  
Co-authors: Tetiana Boichuk, Marie Krečmarová, Mahesh Eledath Changarath, Saïd Agouram, Rafael Abargues, Juan Francisco Sánchez Royo

Since 2D MXene materials have lot of unique properties, they have found their way into a wide variety of applications, including that of electrochemical devices. There are several advantages to these methods, one of which is their ability to form ultra-thin electrodes that can be used in the charge-discharge reaction in order to reduce the mass of parts that are not involved in the electrochemical reaction. This is why it is essential to obtain high-quality MAX and MXene materials capable of delaminating completely in this case. However, often together with single flakes, we have multilayered MXenes particles that also participate in the electrochemical reaction. In this study, we demonstrate the electrochemical behavior of Ti3C2 in lithium electrolytes as well as sodium electrolytes upon different steps of the delamination process. MAX phase was obtained by the traditional method using a stainless-steel vacuum jar. Electrodes were formed from different fractions of MXenes in the process of their gradual centrifugation during delamination. Electrochemical measurements were carried out using a three-electrode cell with a Pt counter electrode and a Ag/AgCl reference electrode. Based on the results of cyclic voltammetry, impedance spectroscopy and XPS and Raman ex situ studies, it was established that there is a difference in charge accumulation for delaminated and non-delaminated materials. In particular, it is shown that non-delaminated Ti3C2 can provide higher values of capacity at low currents, however, during cycling, a lower value of Coulombic efficiency and lower capacity retention during cycling is observed.

Anirudha Sumant- Invited Speaker  
Group Leader, Center for Nanoscale Materials  
Argonne National laboratory  
USA  

Day 3, August 7, 2024, 1:25 PM, Mitchell Auditorium
Over the past decade, tribological research has been revolutionized by the exceptional lubricant properties of graphene and other 2D materials, along with their synergies with various nanomaterials [1-5]. These advanced nanolubricants have shown unparalleled performance in reducing wear and friction across diverse systems. Their remarkable capability to achieve near-zero levels of friction and wear, known as superlubricity, extends even to macroscopic scales under various environments and moderate to high contact pressures. This positions them as a promising alternative to traditional oil-based lubricants. Despite their impressive performance, the sustained and long-term reliability of these solid nanolubricants under more complex tribological conditions remains an area of ongoing investigation. In this context, MXenes offer a promising solution due to their layered structure, easy shearability, and robust mechanical properties [6-7]. However, their chemical stability, a critical factor for long-term reliable lubrication remains a concern, constraining their full application potential in the lubrication industry. In our recent collaborative work, we investigate an ordered double transition metal MXene (Mo$_2$TiC$_2$Tx) and demonstrate its exceptional tribological performance in a dry nitrogen atmosphere using macro-scale pin-on-disc tribo-testing. We demonstrate sustained superlubricity with a friction coefficient as low as 0.005, persisting over an extensive sliding distance of 86 kilometers, with no signs of failure and minimal wear rates. This remarkable tribological performance surpasses all previous records of sustained superlubricity demonstrated by any 2D materials as solid lubricant. The exceptional durability and ultralow friction exhibited by multi-layer Mo$_2$TiC$_2$Tx underscores the potential for further development and exploration of new MXenes in diverse tribological applications.

Anju Gupta
Associate Professor
The University of Toledo
USA

Day 2, August 6, 2024, 4:45 PM, Hill Conference Room

Title: Mxene for Thermal Management
Co-authors: Saketh Merugu

This study explores the pool boiling performance of 2D titanium carbide (Ti3C2Tx) MXene nanofluids under atmospheric pressure conditions. The results show that Ti3C2Tx MXene nanofluids exhibit high critical heat flux (CHF) and heat transfer coefficient (HTC) values at low wall superheat (WS), outperforming deionized water and Ag/ZnO nanofluids. The enhanced pool boiling performance is attributed to a combined mechanism involving thermophoretic and Brownian motion of the thermally conductive Ti3C2Tx MXene flakes, which facilitates circulation and improved surface wettability. The findings highlight the potential of MXene nanofluids with tunable rheological properties for various thermal and electric applications.

Anupma Thakur
Post-doctoral Research Associate
Purdue University
Title: **Theory-driven synthesis of tungsten titanium carbide MXene for hydrogen evolution electrocatalysis**


Tungsten (W) based-MXenes are of particular interest as they are predicted to have overpotentials close to Pt-based catalysts in hydrogen evolution reaction (HER), making them candidates for a more sustainable clean energy application. However, the incorporation of W into the MXene structure has proven difficult due to the calculated instability of its hypothetical precursor Mn+1AXn phases (W2AC and W3AC2). In this study, we present the theory-driven synthesis of a tungsten titanium carbide, W2TiC2Tx, derived from a modified covalently bonded nanolaminated double transition metal carbide ternary carbide (W,Ti)4C4-y precursor. We confirm the atomistic out-of-plane ordering of W and Ti, using density functional theory, Rietveld refinement, and electron microscopy methods. Our results indicate the importance of W and Ti ordering and defects in the successful synthesis of W2TiC2Tx. Additionally, the W-rich basal plane endows W2TiC2Tx MXene with a remarkable electrocatalytic HER performance with the lowest HER overpotential (~144 mV at 10 mA/cm2) for a MXene under acidic conditions over other W1.33CTx MXenes (~320 mV) and Mo2CTx MXenes (~190 mV). In this direction, more efforts on the continuous exploration of W-containing MXenes with low overpotentials are noteworthy toward the clean energy applications due to their highly active basal plane.

Babak Anasori—**Invited Speaker**
Reilly Rising Star Associate Professor, Dept. of Materials and Mechanical Engineering
Purdue University
USA

Day 1, August 5, 2024, 9:45 AM, Mitchell Auditorium

Title: **Defect Engineering of 2D MXenes at ambient and elevated temperatures**

Co-Authors:

MXenes are a large family of 2D transition metal carbides, nitrides, and carbonitrides with more than fifty compositions synthesized to date. In addition to the compositional and structural tunability of MXenes, defects, specifically basal plane point defects, provide us with opportunities (and challenges) in controlling MXene stability and properties. In parallel, interactions of MXene flake basal planes with cations and molecules are key in MXene processing (intercalation and delamination) and many of their applications. In this talk, we will present how MXene synthesis
conditions control the basal plane metal vacancy concentrations, ranging from less than 1 at.% vacancy to above 16 at.%. The optimized Ti3C2Tx single flakes with < 1 at.% vacancies show remarkable stability in air up to 600 ºC before oxidation and stability in an inert environment up to 1000 ºC before transformation to 3D bulk carbide. We will also present atomic-layer resolution secondary ion mass spectrometry (SIMS) results showing alkali cations can either decorate the surface or occupy the metal vacancy sites, depending on the vacancy concentration of the basal planes. When defect sites are occupied by alkali cations, defective MXene flakes can be stabilized and approach the stability of pristine MXene flakes. Understanding and controlling defects demonstrates an important way to tune MXenes' behavior and properties and represent a potential new atomic-scale tool for designing and achieving ideal phase-property relationships of carbides for extreme environment applications.

Bahram Nahbet—Invited Speaker
Professor, Dept. of Electrical and Computer Engineering
Affiliated Professor, Dept. Materials Science and Engineering
Drexel University
USA

Day 1, August 5, 2024, 2:55 PM, Mitchell Auditorium

Title: Co-optimization of van der Waals (vdW) MXene heterojunctions with two-dimensional electron gas (2DEG) for ultra high speed optoelectronics
Co-Authors: Kian Montazeri, Michel Barsoum, Marc Currie

An electric contact is necessary in order to extract every single bit of information within electronic circuits or for contacting the external world, hence understanding the physics of (metal) contacts to semiconductors has been fundamental since the time of triodes. MXenes with their in-plane large conductivity have long been known as a replacement for metals, but the physics of inter-plane charge transport to semiconductor, the rectifying Schottky contacts is less studied even though such contacts are ubiquitously present as gates of field-effect transistors (FETs), or in Schottky diodes that may operate up to THz speed. Here we report on a simple room-temperature process of depositing MXene on a III-V structure with embedded 2D electron gas (2DEG), which results in a large area photodetector (PD) device that greatly outperforms vacuum deposited Ti/Au metal-semiconductor-metal (MSM) PD’s. By co-optimizing properties of 2D MXene contacts and the III-V material heterojunctions, this device sets new operating records with responsivity up to 1.04 A W⁻¹ at low optical powers, corresponding to >230% internal quantum efficiency, dark current of 50 fA μm⁻², greater than 105.6-dB dynamic range, and 25–150 ps response time, which improves our previously reported MXene-Semiconductor-MXene device responsivity by nearly a factor of 3, and is ~ 10³ -10⁶ times faster compared to other MXene-based PDs. This is achieved by enhancing the Schottky barrier height by forming a Van der Waals (vdW) heterojunction between a wide bandgap AlGaAs surface layer and spin coated Ti3C2Tz electrodes. A layered architecture transports the optically generated electrons to a 2DEG channel at the GaAs/AlGaAs heterointerface, where they are rapidly collected. The landscaped electric field pushes the slow holes to an underlying low temperature-grown GaAs (LT-GaAs) region where they recombine. The proposed Schottky-2DEG Photoconductor-Schottky model for device operation shows how this device circumvents the canonical limitations of gain-bandwidth
product, and carrier transit time, while replacing the need for vacuum deposition of gold or other precious metals.

Bhoj Gautam
Associate Professor
Fayetteville State University
USA

Day 2, August 6, 2024, 5:00 PM, Hill Conference Room

Title: \textbf{Investigation of structural properties of Nb2CTx MXenes at elevated temperature}
Co-Authors: Angelina K. Locke, Nisha Hiralal Patel Makani, Joshua Abbott

The 2D material Nb-based MXene is known for its high conductivity, outstanding electrochemical properties, hydrophilicity, and excellent chemical and mechanical features. We synthesized Nb2CTx MXenes from the Nb2AlC MAX phase using the LiF/HCl solution method. After that, prepared MXenes were annealed in a nitrogen environment from 30 to 950°C. We have used X-ray diffraction (XRD) and Raman spectroscopy to characterize the structural and vibrational properties of the prepared samples. Upon comparing the XRD patterns of the pristine and annealed samples, a shift in the etching peak to a higher angle is observed, indicating a change in the lattice parameter. This alteration is caused by the elimination of water molecules linked with interlayer functional groups, like –O and –OH, at higher temperatures. A higher shift in basal planes is due to surface terminations on MXene and the removal of Al from the MAX phase. The spacing between the nanosheets was investigated using scanning electron microscopy. Additionally, the chemical stability and microstructure of Nb2CTx were examined using a differential scanning calorimeter. Our findings offer insights into the alterations in structural properties observed at elevated temperatures in Nb2CTx MXenes. This information can be utilized to optimize the Nb-based MXene’s properties and functionality in real-world applications.

Brian Wyatt
PhD student
Purdue University
USA

Day 2, August 6, 2024, 4:30 PM, Hill Conference Room

Title: \textbf{Alkali cation defect stabilization of MXenes at elevated temperatures}
Co-authors: Matthew G. Boebinger, Zachary D. Hood, Shiba Adhikari, Pawel P. Michalowski, Srinivasa Kartik Nemani, Murali Gopal Muraleedharan, Annabelle Bedford, Wyatt J. Highland, Paul R. C. Kent, Raymond R. Unocic, Babak Anasori

The chemically diverse family of 2D MXenes have been widely adopted in areas such as energy storage, conversion, and electronics. For these applications, fundamental understanding of the interaction of alkali cations with surface defects is critical to know 1) the interaction site of alkali cations with MXenes and 2) the overall effect on the stability of MXenes. In this presentation, we demonstrate that alkali cations preferentially occupy vacancy sites in the surface transition metal
layers on Ti3C2Tx and Mo2TiC2Tx MXenes. Further, we show that this stabilizes the structure and restrains the phase transition of Ti3C2Tx, Mo2TiC2Tx, and Mo2Ti2C3Tx MXenes at elevated temperatures. To do so, we use a combination of in situ x-ray diffraction and scanning transmission electron microscopy paired with ex situ secondary ion mass spectrometry (SIMS) with other ex situ and simulation techniques. Overall, this cation-based engineering of defects shows potential for improvements in MXene’s stability and further develops the available tools to apply MXenes as a diverse and tunable family of nanoceramics for high temperature applications.

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Chong Min Koo – Invited Speaker
Professor, School of Advanced Materials Science and Engineering
Sungkyunkwan University
South Korea

Day 2, August 6, 2024, 11:05 AM, Mitchell Auditorium

Title: MXenes for Multispectral Electromagnetic Shielding
Co-authors:

The rapid advancement of electronics, telecommunications, mobility solutions, and medical devices operating across a broad spectrum of electromagnetic (EM) waves, ranging from ultralow kHz levels to high THz frequencies, underscores the need for EMI shielding materials that can operate effectively across multispectral EM bands. MXenes, a class of two-dimensional materials consisting of transition metal carbides, nitrides, and carbonitrides, have emerged as state-of-the-art functional EMI shielding materials since their initial report in 2016. This is due to their exceptional metallic conductivity, large surface area, diverse surface terminations, and excellent solution processability. This presentation aims to showcase MXenes' remarkable capabilities in providing multispectral EMI shielding against radio-frequency (RF) waves, GHz-range microwaves, and THz/infrared (IR)-frequency waves, all achieved with minimal thickness and in various structural forms. Pristine MXene films with nanometer-scale thickness effectively interact with EM waves across the RF, GHz, and THz frequency ranges, while also exhibiting remarkably low IR emissivity. This low IR emissivity is particularly crucial for applications such as selective thermal management, IR camouflage, stealth, and anti-counterfeiting measures. Through this exploration, we aim to underscore the versatility and effectiveness of MXenes in meeting the evolving demands of EM wave shielding across a wide range of electromagnetic frequencies and applications.

Christopher Shuck – Invited Speaker
Assistant Professor, Dept. of Chemistry and Chemical Biology
Rutgers University
USA

Day 1, August 5, 2024, 1:35 PM, Mitchell Auditorium

Title: Using Multiple M-Elements To Understand the Chemistry and Structure of MXenes
Co-authors:

MXenes are potentially the largest class of 2D materials discovered so far. With a general formula of Mn+1XnTx, M is an early transition metal (Ti, V, Nb, Ta, etc.), X is C and/or N, Tx represents the surface groups (-O, -OH, -F, -Cl), and n = 1–4, over 30 stoichiometric phases have already been discovered, with many more predicted computationally. This class of materials has been widely studied owing to their exceptional properties, including hydrophilicity, scalability, mechanical strength, thermal stability, redox capability, and ease of processing. Because MXenes inherit their structure from Mn+1AXn (MAX) phase precursors, understanding MAX phase synthesis leads to control over flake size, defect density, and chemical composition of the resultant MXene. One understudied, yet important class of MXenes are solid-solution MXenes, where multiple elements are randomly distributed within the M layers. Herein, a set of multi-M chemistries (Mo, V, Ti, Nb, Ta) are used to study the effect of structure and chemistry on MXenes. While solid-solution MXenes have unique and tunable chemical, optical, and electronic properties, they also enable the formation of novel MXenes that cannot exist otherwise. By choosing specific chemistries, we can then begin to understand fundamental aspects of MXene chemistry and structure.

De-en Jiang – Invited Speaker
Professor, Dept. of Chemical and Biomolecular Engineering & Dept. Chemistry
Vanderbilt University
USA
Day 1, August 5, 2024, 12:30 PM, Mitchell Auditorium

Title: Understanding ligand chemistry on MXene surfaces from simulations
Co-authors:

Hybrid MXenes with organic terminal groups are a new derivative class of MXenes that provide new opportunities to probe the organic-inorganic interfaces and the ligand chemistry on MXene surfaces. In this talk, we will address the stability and dynamics of amine-derived ligands on the Ti3C2 surfaces from density functional theory based geometry optimization, molecular dynamics, and transition-state searches. Key questions to address include the ideal coverage, the interconversion amino-amido-imido groups, the proton shuffling, and the denticity effect.

Di Wang
Graduate student
University of Chicago
USA
Day 1, August 5, 2024, 4:20 PM, Hill Conference Room
MXenes are a large family of two-dimensional (2D) transition metal carbides and nitrides. MXenes are typically synthesized from a series of non-van der Waals precursors (MAX phases, where A is typically Al) by selectively extracting A atoms with hydrofluoric acid-containing solutions. This process is relatively time-consuming and generates hazardous waste, both of which may limit the scalability of MXene manufacture. We demonstrated two direct ways, bypassing the MAX phase intermediates, to prepare one of the most widely used MXenes, Ti2CCl2. One is based on the high-temperature reaction of a stoichiometric mixture of precursors. The other uses chemical vapor deposition (CVD), where gaseous reagents flow through a heated substrate to form a thin film of product. We even pushed MXene bottom-up synthesis to a new level by expanding the scope of MXene available through direct synthesis, tuning the morphology of MXene products from stacks to spheres. The direct synthesis routes save time and minimize hazardous waste production. Besides, these new routes offer synthetic modalities not compatible with traditional methods, especially in cases where corresponding MAX phases are not available.

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**Dhriti Nepal** – *Invited Speaker*
Sr. Research Materials Engineer, Polymer Composite Branch
Air Force Research Laboratory
USA

Day 2, August 6, 2024, 10:45 AM, Mitchell Auditorium

**Title:** Vitrimers Nanocomposites: Thermomechanical and Self-Healing Properties
**Co-authors:**

Vitrimers, an emerging class of materials, are cross-linked by dynamic covalent bonds that change their topology at elevated temperatures. In addition to a traditional glass transition temperature (Tg), vitrimers have a second topology freezing temperature (Tv) above which dynamic covalent bonds allow for rapid stress relaxation, self-healing, and shape reprogramming. In this study, we showcase the development of vitrimer nanocomposite with fillers such as gold nanoparticles, graphene, and MXene with different architectures and study the influence of fillers on thermomechanical and self-healing properties. Our findings reveal that the Tv increases with nanofiller concentration, while nanofiller composition minimally impacts Tv, offering a promising avenue for future research and development. In addition, we demonstrate the photo-thermal self-healing response of the hybrid materials allows for shape memory and shape reconfigurable applications, promising for many aerospace, automobile, and electronics applications.

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**Dmitri Talapin** – *Invited Speaker*
Ernest DeWitt Burton Distinguished Service Professor, Department of Chemistry, James Franck Institute, and Pritzker School of Molecular Engineering
Two-dimensional (2D) transition-metal carbides and nitrides (MXenes) show impressive performance in supercapacitors, batteries, electromagnetic interference shielding, and electrocatalysts. These materials combine the electronic and mechanical properties of 2D inorganic crystals with chemically modifiable surfaces, and surface-engineered MXenes represent an ideal platform for fundamental and applied studies of interfaces in 2D functional materials. The comprehensive understanding of MXene surfaces is required for prescriptive engineering of their physical and chemical properties. We discuss general strategies to install and remove surface groups by performing topotactic substitution and reductive elimination reactions. Successful synthesis of MXenes with halido-, oxo-, imido-, thio-, seleno-, or telluro- terminations, as well as bare MXenes (no surface termination) can be synthesized both by traditionally (from MAX phases) and directly synthesized MXenes. We also successfully synthesized a series of hybrid organic-inorganic MXenes by covalently attaching dense carpets of organic surface groups. Since organic and inorganic materials are, in many aspects, complimentary to each other, organic-inorganic MXenes open a pathway to merging the benefits of both worlds into a hybrid matter that combines engineerability of molecules with the electronic, thermal, and mechanical properties of inorganic 2D materials. The description of MXene surface structure and reactivity requires a mix of concepts from the fields of coordination chemistry, self-assembled monolayers, and surface science. MXene surface groups control biaxial lattice strain, phonon frequencies, electrochemical performance, and strength of the electron-phonon coupling, making MXene surfaces not spectators but active contributors to conductivity, superconductivity, and catalytic activity.
controlled nickel nanoparticles. The PVDF/MXene/Ni composites demonstrate exceptional absorption coefficients and shielding effectiveness against unwanted THz EM waves. This is attributed to the synergistic interaction between electrically conductive Ti₃C₂Tx MXene and magnetic nickel nanoparticles. By controlling the external magnetic field during synthesis, we produced flower-like Ni nanoparticles with enhanced magnetic properties, outperforming spherical counterparts. A 20-µm thick PVDF/MXene/Ni composite film, containing a 10 wt.% loading of flower-like Ni nanoparticles, achieved an impressive THz SE of 34 dB at 1 THz, surpassing previous materials. In addition, we successfully developed a novel ultrathin and flexible MXene-coated Nickel film using a simple one-step synthesis method. Nickel particles were uniformly deposited onto one side of the MXene surface, significantly enhancing the magnetic properties of the resulting films. The distribution of Nickel coating was precisely controlled by adjusting the reaction time. These thin films exhibit outstanding EMI shielding performance within the X-band frequency range, markedly improving both the absorption characteristics of the MXene film and the overall EMI shielding effectiveness. The Janus MXene film achieved EMI SE values of 79 dB, 89 dB, and 106 dB for thicknesses of 15 µm, 25 µm, and 35 µm, respectively. At equivalent thicknesses, the non-magnetic films exhibited EMI SE values of 71 dB, 80 dB, and 91 dB, respectively. These findings highlight effective approaches to tailoring the shielding properties of polymer composites and thin films by modifying the composition and morphology of conductive and magnetic fillers.

Francesca Urban
Post Doctoral Researcher, A. J. Drexel Nanomaterials Institute
Drexel University
USA

Day 3, August 7, 2024, 1:20 PM, Hill Conference Room

Title: **Fundamental investigation of the charge transport mechanisms in Ti3C2Tx single-flake devices**

Co-authors: Dr. Stefano Ippolito, Jane Frostad, Prof. Paolo Samori, Prof. Steven J. May, Prof. Yury Gogotsi

Ti3C2Tx is the most investigated MXene thus far. Yet, despite the great interest for its electronic applications, there is a little understanding on the fundamental electronic properties. Most of today's research focuses on studying and developing possible application of thin films, leaving aside single-flake investigation, which could provide a deeper understanding of MXene properties. In this work, we investigate the electrical characterization and charge transport mechanisms of Ti3C2Tx single-flake devices. Pristine and vacuum annealed devices are compared to understand the effects of MXene surface terminations as well. Ti3C2Tx is widely reported having a metallic conductivity in both theoretical and experimental studies, however for annealed samples the material resistivity is not entirely consistent with Ti3C2Tx metallic character. A low-temperature upturn of the resistivity is usually reported, but rarely explained along with the effect of surface terminations. By monitoring the flake resistance as a function of temperature (T), we observe a metallic behavior of the pristine sample, with an upturn of the resistivity at low temperature, which can be ascribed to weak-location phenomena occurring for T < 70 K, as confirmed by magnetoresistance analysis. Upon 600 °C annealing, a metal-to-insulator transition occurs (proved to be independent on flake thickness), with
the material resistivity decreasing when the temperature increases (dρ/dT < 0). Such a semiconducting-like behavior (commonly reported in literature for annealed Ti3C2Tx films and other Ti-based MXenes) is actually due to a metal to glassy-metal transition, which might be related to defect density and their propagation during the annealing steps.

G

Goknur Cambaz Buke  
Professor, Department of Materials Science and Nanotechnology Engineering  
Tobb University of Economics and Technology  
Turkey

Day 1, August 5, 2024, 4:50 PM, Hill Conference Room

Title: Growth of 1D and 2D MoC Through Chemical Vapor Deposition  
Co-authors:  
Transition metal carbides (TMCs) are popular for their exceptional mechanical and electrical properties, which make them key candidates for advanced nanoelectronics including sensors, electron emitters, and catalytic systems such as those used in hydrogen evolution reactions. However, the controlled synthesis of these nanomaterials with large area, high quality, reproducibility, and homogeneity through scalable processes, remains challenging. In this study we explore the controlled synthesis of 1D and 2D Mo2C nanostructures using an unconventional chemical vapor deposition (CVD) technique. This presentation will discuss the mechanisms for the formation of self-aligned 1D Mo2C nanorods with high surface area and high quality 2D Mo2C crystals. The formation mechanisms will be explained using comprehensive characterization techniques including electron microscopy (SEM) with EDS, transmission electron microscopy (TEM), X-ray diffraction (XRD) and Raman spectroscopy. Our discussion will highlight the correlations between growth mechanisms and critical processing parameters aiming to understand the causation behind the diverse morphologies observed, including their heterostructures with graphene. This study not only advances our understanding of Mo2C growth but also contributes to the broader field of low-dimensional materials synthesis, offering new possibilities for improved performance and miniaturization. (This material is based on the work supported by the Air Force Office of Scientific Research; award numbers: FA9550- 19-1-7048, FA9550-22-1-0358).

H

Hendrik Heinz  
Professor  
University of Colorado Boulder  
USA

Day 1, August 5, 2024, 4:25 PM, Mitchell Auditorium

Title: Simulation of MXenes and Related 2D Hybrid Materials Up to the Micrometer Scale in High Accuracy
MXene based materials are finding a huge application space in functional materials for structural composites, catalysts, batteries, electromagnetic shielding, radiation damage, and in many other fields. One of the challenges regarding modeling and simulation of such materials at a scale from atoms to micrometers has been the lack of a physics and chemistry inspired model with interpretable parameters, validated results, and compatibility with widely used force fields such as CHARMM, AMBER, IFF, CVFF, PCFF, and others. In this talk, we will describe a parameterization of the INTERFACE force field (IFF) for MXenes and some initial applications that characterize the role of surface functional groups on surface properties, cohesion, shear, and binding to polymers in composites. The bonding in MXenes can be described as predominantly covalent between Ti and C and significantly ionic between Ti and outer layers of OH and F groups, which we compare to a few other 2D substrates such as MoS2 and graphite. Besides lattice parameters, surface energies, contact angles with various liquids and mechanical properties are obtained in outstanding agreement with experimental data. The model is also suitable to investigate interfaces with complex electrolytes, proteins, and DNA without additional fit parameters, as is the case for other compounds included in IFF as well. Challenges in the prediction of thermal conductive properties are discussed. Finally, some opportunities for the use of AI-enhanced methods towards accelerated automated discovery of functional MXene based materials will be described.

Hesam Jafarian
PhD student
The University of Alabama
USA

Day 3, August 7, 2024, 11:00 AM, Hill Conference Room

Title: MXene Membranes for Water Treatment: From State of the Art Lab-scale to Large Scale Fabrications
Co-authors: Hesam Jafarian, Anupma Thakur, Annabelle Bedford, Reza Behzadnia, Mohsen Pilevar, Mark Elliott, Babak Anasori, Mostafa Dadashi Firouzjaei

The quest for efficient water treatment solutions has led to the exploration of novel materials and techniques in membrane technology. This research presents a study on integrating MXene, a two-dimensional transition metal carbide, into nanofiltration (NF) and ultrafiltration (UF) membranes, showcasing advancements from lab to large-scale fabrications. For NF, we developed polyamide (PA) mixed matrix membranes incorporating MXene and Holey-MXene (H-MXene) onto a polyethersulfone support. H-MXene, with perforations created through chemical etching, enhances water permeability. Membranes were fabricated using interfacial polymerization, employing both dip-coating and spin-coating methods. An evaluation revealed that MXene and H-MXene membranes significantly improved water permeance and salt rejection over conventional NF membranes. Specifically, spin-coated membranes showed sodium sulfate rejection rates of 95.7% (MXene) and 94.4% (H-MXene), with permeate fluxes of 64.4 and 60.8 LMH, representing a 32% and 25% enhancement over traditional PIP-TMC membranes. In UF, we ventured into large-scale fabrications with a polysulfone-MXene nanoparticle composite membrane. SEM, FTIR, and contact angle measurements indicated improved hydrophilicity and mechanical strength, enhancing flux and rejection efficiency. A comprehensive Life Cycle Assessment (LCA) showed this membrane has
a lower environmental footprint than conventional UF membranes, highlighting its potential for sustainable applications. This study underscores MXene's versatility in advancing membrane technologies for water treatment and sets a precedent for scalable high-performance membrane production. Further research should optimize fabrication processes and explore membrane stability in various water treatment scenarios.

Hirotaka Ooi  
Japan Material Technologies Corporation  
Japan

Day 1, August 5, 2024, 2:45 PM, Hill Conference Room

Title: **Non-contact evaluation method for concentration and dispersion stability of delaminated MXene in water using X-ray transmittance measurements**  
Co-authors: Kosei Sasaki, Manato Un, Tomoyuki Yokota, Yuma Shimbori, Kiyoshi kanamura

Delaminated Ti3C2Tx MXene (d-MXene) exhibits outstanding electrical properties and solvent dispersibility, making it promising for various applications such as energy storage, and transparent electrodes. However, the difficulty in quantitatively evaluating dispersion stability has been a challenge in managing the manufacturing process in coatings and composites. In this study, d-MXene dispersion was prepared, and its concentration and dispersion stability were evaluated by measuring the X-ray transmittance without diluting the solution. The X-ray transmittance of the dispersion relative to water decreased from 98% to 84% with the increase in concentration from 0.11wt% to 3.59wt%. Additionally, even after standing for 16 days, the X-ray transmittance of the dispersion showed almost no change. This indicates that there is minimal sedimentation in the dispersion while it is left standing. Using this dispersion, lithium-ion batteries and photodiodes were fabricated.

Husam Alshareef – *Invited Speaker*  
Professor, Materials Science and Engineering  
King Abdullah University of Science and Technology (KAUST)  
Saudi Arabia

Day 1, August 5, 2024, 11:00 AM, Mitchell Auditorium

Title: **Recent Developments in MXetronics**  
Co-authors:

The integration of MXenes in electronic devices (MXetronics) is a newly emerging field in which MXenes have shown promising potential. MXenes are essentially 2D metal contacts with a tunable work function, suggesting they can be used in a variety of electronic devices. Our group has been developing deposition processes, transfer techniques, interface engineering, surface functionalization, photolithographic patterning, and wet and plasma etching of MXenes to demonstrate and improve the performance of electronic devices using MXenes. In fact, MXenes have been successfully integrated with oxide semiconductors, 2D semiconductors, quantum dot semiconductors, and wide band-gap semiconductors at the wafer scale. The data so far indicates
that the quality of MXene Ohmic contacts is generally inferior to those of traditional metal contacts, leading to lower device mobility. However, for devices that require Schottky contacts (e.g., HEMTs), MXenes perform much better. In this talk, the benefits and challenges of using MXenes in various electronic devices will be discussed, with a particular focus on the role of the interface. Strategies to improve the MXene/semiconductor interfaces and to improve the wafer-scale fabrication processes will be summarized. In addition, using MXene thin films as active layers in electronic devices will be discussed.

Hui Fang
Postdoctoral Researcher
University of Pennsylvania
USA

Day 3, August 7, 2024, 1:05 PM, Hill Conference Room

Title: Investigating the Mechanisms of Oxidation and Charge Transport in Ti3C2Tx MXenes
Co-authors: Anupma Thakur, Zhenyao Fang, Amirhossein Zahmatkeshsaredorahi, Vahid Rad, Ahmad Arabi Shamsabadi, Masoud Sorouch, Xiaoji G. Xu, Andrew M. Rappe, Babak Anasori, Zahra Fakhraai

Two-dimensional MXenes have demonstrated potential in applications such as optoelectronic devices, supercapacitors, sensors, and biomedicine. However, their oxidation and charge transport mechanisms remain elusive, impeding the exploration for new applications. Here, we investigate the oxidation and charge transport mechanisms via resistivity measurements using spectroscopic ellipsometry. We demonstrated the higher thermal stability of mono-flake Ti3C2Tx, compared to their multi-flake counterparts. The readily oxidation of multi-flake MXenes are due to the inter-flake trapped confined water, which can be removed in high temperature vacuum annealing. The removal of confined water also affects the inter-flake charge hopping transport. These findings provide fundamental insights into the kinetics of confined water and its role in both oxidation and charge transport in Ti3C2Tx MXenes.

Hyunho Kim
Postdoctoral Researcher, A. J Drexel Nanomaterials Institute
Drexel University
USA

Day 2, August 6, 2024, 4:15 PM, Hill Conference Room

Title: Understanding Light-Matter Interactions of MXenes
Co-authors: Danzhen Zhang, Teng Zhang, Yury Gogotsi

The MXene materials family has been the subject of extensive research activities for the past decade. Recent developments in the molten-salt route have enabled the full control of MXenes’ surface termination groups. For example, Ti3C2Cl2 is found to have a vis-NIR absorption band centered at ~880 nm, which is red-shifted from the acid route prepared Ti3C2Tx counterparts with O, OH, and F terminations (770~800 nm). The origin of this vis-NIR absorption band is yet to be understood, and the redshift with the chlorine group makes a contradiction to the surface plasmon
concept using free carrier density. Here we adapt an interband transition mechanism considering light polarization to explain both UV and vis-NIR absorption bands of MXenes. The light-matter interactions of MXenes will be discussed based on in-situ UV-vis and Raman spectroscopy under electrochemical modulations. The important relationships between photons, electrons, and phonons in MXene, which are important for numerous applications of those materials, will be discussed.

Ian Kinloch – Invited Speaker
Morgan Advanced Materials/Royal Academy of Engineering Research Chair in Carbon Materials,
Dept. of Materials
University of Manchester
UK

Day 1, August 5, 2024, 1:55 PM, Mitchell Auditorium

Title: Electrochemical Exfoliation of MXenes and Their Use in Energy Storage and Composites
Co-authors: Kai Chio Chan, Mufeng Lin, Pei Yang, Yuling Zhuo, Vildan Bayram, Xiang Guan, Kailing Lin, Yi He Huang, Lingshu Lei, Yiannis Georgantas, Chris Shuck, Philip J. Withers, Robert J. Young, Suelen Barg, Yury Gogotsi, Mark A. Bissett

MXenes show considerable promise in electrochemical energy storage and as reinforcements in polymer composites. However, an obstacle to their uptake is the use of hazardous hydrofluoric acid (HF) during their synthesis. We have developed an electrochemical etching process for the synthesis of Ti3C2 and Ti3CN MXenes by using aqueous tetrafluoroboric acid as the electrolyte, thus only involving a very low concentration of HF. The MXene flakes from the electrochemical etching process have larger lateral dimensions compared to chemically etched MXene flakes as a result of the suppression of the HF decomposition and rapid etching rate. The electrodes of lithium-ion supercapacitors made from electrochemically etched Ti3C2 and Ti3CN exhibited cyclic performance and rate capabilities comparable to HF-etched MXenes. High aspect ratio flakes are also important for reinforcing polymer composites; we have previously shown that 2D materials follow the shear lag model for reinforcement where a minimum flake length is required in order to get good mechanical properties. We have used Raman mapping to study the strain distribution within a single MXene flake under tension and hence show that ideally MXene flakes need to be longer than 10 mm for good reinforcement. Significant we also show that, unlike for van der Waal 2D materials, the modulus of MXenes is virtually independent of flake thickness. Hence, large MXene flakes which are 10’s of nanometres thick can be successful used in composites compared to an ideal flake thickness of just 2.1 nm for graphene.

Jeffrey Simon
PhD student
Title: **Nonlinear Optical Properties of 2D Transition Metal Carbides and Nitrides**
Co-authors: Benjamin Reigle, Colton Fruhling, Dazheng Zhang, Stefano Ippolito, Hyunho Kim, Vladimir Shalaev, Yury Gogotsi, Alexandra Boltasseva

Two-dimensional (2D) transition metal carbides, nitrides and carbonitrides (also known as MXenes) are a large class of materials with very attractive but underexplored optical characteristics. MXenes have a chemical formula of Mn+1XnTx (where n ranges from 1 to 4) consisting of transition metal atoms (M), carbon and/or nitrogen atoms (X), as well as surface termination groups (Tx, typically =O, -OH, -F). Various MXenes find utility in nonlinear optics and are used for all-optical switching and as a saturable absorber (SA) element for passive mode-locked or q-switched in fiber lasers. Recent work indicates that both the thickness and surface termination affect the intensity-dependent optical properties of Ti3C2Tx. While Ti3C2Tx is electrically conductive and has metallic optical properties in the infrared spectrum, some MXenes have dielectric characteristics suggesting variations in the nonlinear mechanisms and effects. We explored the nonlinear optical properties of various MXenes using the intensity-scan (I-scan) measurement technique to monitor both the transmission and reflection of light from the sample with an incident femtosecond-pulsed laser. Our results show a significant intensity-dependent reflection change, which was previously overlooked. Recognizing this property could change how MXenes are used in fiber lasers and lead to novel MXene optical devices.

Jizhen Zhang  
Postdoctoral Research Fellow  
Deakin University  
Australia

Title: **Understanding the Orientation Transform of Two-Dimensional MXene Nanosheets in Fluids**
Co-authors: Ken A. S. Usman, Peter A. Lynch, Jozelito. M. Razal

Anisotropic nanomaterial orientation and alignment are critical for the mechanical or electrical performance of constructed macrostructures including fiber, film, and aerogel. It has been challenging to comprehend how nanomaterial orientation changes during solution processing under shear force. In this study, we use in-situ synchrotron small-angle X-ray scattering successfully observes the orientation change of MXene nanosheets in fluids at increasing shear rates. This allowed us to correlate the degree of orientation change with the change in shear rate and the creative data analysis helps identifying the shear rate threshold that initiates alignment. To get a deeper knowledge of the alignment of MXene sheets, we further investigated the effects of nanosheet size, concentration, and relaxing behavior. The findings of this study will serve as a theoretical guide for developing processing approaches for creating ordered structures out of MXene dispersions and an expanded class of anisotropic nanomaterials.
John S. Anderson—Invited Speaker
Associate Professor and Associate Chair, Dept. of Chemistry
University of Chicago
USA

Day 2, August 6, 2024, 11:30 AM, Hill Conference Room

Title: Catalytic Applications of Organometallic MXenes
Co-authors: Maia E. Czaikowski, Sophie W. Anferov

MXene surface functionalization is providing access to materials with tailored surfaces and functionalities. An exciting new direction is making MXenes with organometallic, i.e. C-based, capping groups. In this talk, I will discuss applications of new MXenes with surface organometallic groups to catalysis. Specifically, I will discuss how these materials can mediate both classic and novel transformations with olefins and amines. The relationship between MXene composition and surface structure with reactivity and selectivity will be discussed, as will mechanistic insights into catalytic turnover.

John Wang
Research Associate, A. J. Drexel Nanomaterial Institute
Drexel University
USA

Day 2, August 6, 2024, 2:15 PM, Hill Conference Room

Title: Stability of Pseudocapacitive Energy Storage in Ti3C2Tx MXene in a Wide Temperature Range
Co-authors: Mark Anayee, Muhammad Nihal Naseer, Teng Zhang, Yuan Zhang, Mikhail Shekhirev, Kateryna Shevchuk, Yong-Jie Hu, Yury Gogotsi

Pseudocapacitors have the potential to achieve high energy and high power density simultaneously, a holy grail for electrochemical energy storage. MXene-based pseudocapacitors have made major progress in the last decade, achieving better energy and power density than carbon supercapacitors using the double-layer charge storage mechanism. However, one obstacle facing pseudocapacitors is their shorter lifetime. In MXene-based pseudocapacitors, which showed up to 500,000 cycles lifetime in aqueous electrolyte at room temperature, this concern is pronounced particularly at high temperatures due to the limited stability of the active material in aqueous solutions. This work shows that Ti3C2Tx MXene electrodes in 5 M H2SO4 possess excellent rate capabilities from -50 °C to 100 °C but also a sufficient lifetime at 70 °C when using a float test holding at -0.9 V vs. Hg/Hg2SO4. Post-mortem characterization using X-ray photoelectron spectroscopy and Raman spectroscopy showed negligible signs of oxidation in the bulk of the film. This work suggests sufficient stability of Ti3C2Tx MXene as a negative electrode in protic aqueous electrolytes across a wide temperature range rooted in thermodynamics, making it promising for pseudocapacitor energy storage.

Joselito Razal—Invited Speaker
This talk will discuss how 2D MXenes are enabling the development of new fiber-based and textile-based materials. Of particular focus will be the recent advances in MXene liquid crystals and fibres, along with the development of analytical techniques required to advance the understanding of their structure-property relationship. It will be shown that this collective knowledge is key to better designing solution-based processing methods to fabricate architecture with the desired and tailored properties. It is believed that endless and exciting possibilities exist for MXene fibres, catering to applications beyond what is currently demonstrated in the present literature.

Joshua R. Uzarski -Invited Speaker
US Army, DEVCOM Soldier Center
USA

Day 3, August 7, 2024, 1:05 PM, Mitchell Auditorium

Title: MXenes and low-dimensional materials for US defense applications
Co-Authors:
The US Army and Joint Defense services are in constant need of novel material solutions with highly improved performance that are lightweight, require minimum power consumption, and are cost effective. Low dimensional materials, particularly MXenes, have shown great promise in obtaining these desired properties in multiple application spaces. These include electromagnetic shielding, thermal insulation, structural materials, electronic textiles, material diffusion barriers, catalytic chemical degradation, energy storage, and water filtration amongst others. This presentation will focus on providing an overview of these areas and highlight prior and on-going low-dimensional material work at Soldier Center and our Department of Defense partners. Special attention will be given to discussing existing fundamental and applied research gaps requiring novel solutions to facilitate future transition to deployable products.

Joshua Little
PhD student
University of Maryland
USA

Day 3, August 7, 2024, 11:15 AM, Hill Conference Room
Title: Morphology Controlled Synthesis of Catalytic Metal Nanocrystals within 2D Material Nanoconfinements
Co-authors: Amy Chen, Ali Kamali, Tanmay Akash, Chan-Soo Park, Dongxia Liu, Siddhartha Das, Taylor J. Woehl, Po-Yen Chen

The synthesis of products within confined nanoscale regions, termed nano-confined synthesis, has led to a new generation of heterostructured materials. Within the Van der Waals (VdW) gaps of 2D nanomaterials (2DM), a variety of products can be formed generating unique sizes, geometries, crystallinities, and even catalytic properties. However, there remains a gap in knowledge in how to precisely control the complexation of metal ions and strategically guide the in-plane crystallization/growth of metals. Herein, a noble metal ion-complexed assembly of graphene oxide (GO) and Ti3C2Tx (MXene) nanosheets was developed generating nano-confined films with adjustable noble metal loadings using tetraammineplatinum(II) nitrate (TPtN). To understand how water removal processes influence the redistribution of noble metal ions on 2DM substrates, two different solvent drying processes were evaluated in 2DM VdW gaps 1) Air drying and 2) Freeze drying. The TPtN–2DM multilayers were then thermally reduced to synthesize Pt–2DM heterostructures. Then, Pt particle size and morphology were evaluated using HAADF-STEM imaging for all samples. To understand the observed Pt morphologies, molecular dynamic (MD) modeling was performed using the LAMMPS software to confirm the drying influence on TPtN precursor movement between 2DM sheets by determining equilibrium states of TPtN–2DM systems with and without water. Lastly, the Pt–2DM heterostructures were applied towards the hydrogenation of phenylacetylene. Pt–MXene heterostructures demonstrated a very high substrate dependent activity (2617 molPA molPt-1 h-1) with an average styrene selectivity (82.4%) while Pt–rGO demonstrated a lower activity (1070 molPA molPt-1 h-1) but improved styrene selectivity (85%).

Jouan Yu
Undergraduate Student
Rutgers University
USA

Day 1, August 5, 2024, 2:15 PM, Hill Conference Room

Title: Self-Limiting Electrospray Deposition of MXene Composites via Sub-percolation Assembly
Co-authors: Michael J. Grzenda, Jouan Yu, Maria Atzampou, Jonathan M. Blisko, Rachel M. Vladimirsky, Kelly Hughes, Christopher Shuck, Xin Yong, Jeffrey Zahn, Jonathan P. Singer

Electrospray deposition (ESD) uses strong electric fields to produce monodisperse droplets from dispersions and solutions that are driven toward grounded targets. Self-limiting electrospray deposition (SLED) is a regime of ESD that achieves controlled targeted coatings by trapping charge in the growing film and redirecting incoming droplets to uncoated areas of the substrate. However, when conductive nanoparticles are added to self-limiting (SL) sprays, the buildup of charge required to repel incoming material becomes disrupted as particle loading increases. The goal of this work is to maximally deliver MXene flakes and other nanoparticles in the controlled SL regime. Methylcellulose (MC) was chosen as the SL binder due to its ability to form high aspect ratio nanowires, which should increase the interparticle spacing and prevent percolation. MC was sprayed with MXene particles of two different sizes along with a variety of other nanoparticles. The SL behavior was characterized by measuring the growth of films on 2D patterned gratings as well as
on flat wafers. It was shown that smaller MXene flakes could achieve a higher loading before reaching the percolation threshold and exiting the SL regime when compared to larger flakes. A MXene nanoflake composite was deposited on an interdigitated electrode with 50 μm features using this maskless technique, and the device showed an enormous change in capacitance compared to the unfunctionalized device.

Julian Thomas Müller
Faculty III Process Sciences, Institute of Material Science and Technology
Technische Universität Berlin
Germany

Day 1, August 5, 2024, 4:35 PM, Hill Conference Room

Title: Molten salt etching beyond chlorine salts
Co-authors: Maged F. Bekheet, Aleksander Gurło

Surface terminations play a pivotal role in shaping the character of MXenes, essentially determining their properties and applicative potential in fields such as batteries, catalysis or gas sensing. For batteries, the surface terminations crucially influence the interlayer spacing, diffusion kinetics and electrode wettability directly impacting their feasibility. These terminations, initially acquired during the MXene's formation through the etching process from its parent MAX phase, are a critical aspect. Among the various etching methodologies proposed, molten salt etching emerges as a promising avenue, allowing for a higher degree of control over surface terminations through the strategic selection of halogen salts. While fluorine and chlorine salts have been commonly employed, resulting in corresponding terminations with the addition of oxygen ones from the washing process, our study ventures into new territory beyond these halogens. With a clever twist on molten salt etching we introduce a straightforward technique aimed at producing bromine-terminated Ti-based MXenes, presenting a fresh array of terminations. Taking the exploration a step further, we are currently trying to utilize this approach to generate MXenes with iodine terminations. The significance lies in their lower binding energies compared to chlorine, fluorine, or oxygen terminations, hinting at broader possibilities for surface modification and increasing the horizon of terminations. For optimization, the etching process will be followed by in situ synchrotron XRD experiments.

K

Ken Aldren Usman
Associate Research Fellow, Institute for Frontier Materials
Deakin University
Australia

Day 2, August 6, 2024, 2:10 PM, Mitchell Auditorium

Title: MXene Liquid Crystals for Multifunctional Architectures
Co-authors: Ken Aldren Usman, Jizhen Zhang and Joselito Razal
The recent development in liquid crystalline (LC) dispersions of two-dimensional (2D) transition metal carbides (MXenes) has elevated this distinct nanomaterial into a domain of cutting-edge structural designs, including films, coating, and fibers. Moreover, when compared to structures formed using conventional non-LC dispersions, those derived from LC MXenes can be easily tuned to achieve unique properties such as tuneable ion transport, boosted conductivity, as well as improved physical attributes. This underscores their potential across various applications, including, but not limited to electronic displays, smart eyewear, and thermal camouflage technology. Here, we provide an overview of the recent efforts in producing and processing LC MXenes, along with crucial discussions on how to satisfy the conditions for LC formation. We also highlight how LC dispersions expanded the current manufacturing paradigm of MXene-based materials, leading to unparalleled performance improvements in their traditional applications such as energy, storage, electromagnetic interference shielding, and strain sensing, as well as their emerging applications like tribology. Lastly, we also discuss the opportunities for innovation and foreseen challenges, providing insights into future research avenues aimed at maximizing the promising potential of LC MXenes.
Koshuke Kawai Razal—Invited Speaker
Assistant Professor
Waseda University
Japan

Day 2, August 6, 2024, 11:45 AM, Mitchell Auditorium

Title: Strain-free MXene anodes for all-solid-state batteries
Co-Authors:

All-solid-state batteries with non-flammable inorganic solid electrolytes are a key technology to address the safety issues of lithium-ion batteries with flammable organic liquid electrolytes. However, conventional electrode materials suffer from substantial volume change during lithium-ion (de)intercalation, leading to the failure of the interface between the electrode materials and solid electrolytes and then severe performance degradation. In this work, we report strain-free charge storage via an interface between a transition-metal carbide nanosheet (MXene) and solid electrolytes, where MXene shows negligible structural change during lithium-ion (de)intercalation. Our multiscale analyses confirm MXene’s ability to maintain a robust interface with the solid electrolyte and visualize Li+ intercalation in MXene. A strain-free all-solid-state battery, which consists of Ti3C2Tx anode and disordered rocksalt Li8/7Ti2/7V4/7O2 cathode, demonstrates a long-term operation owing to the strain-free nature of both electrode materials.

Krutarth Kamath
PhD Student
Purdue University
USA

Day 1, August 5, 2024, 2:30 PM, Hill Conference Room

Title: Time-dependent colloidal stability of Ti3C2Tx MXene: effect of Ti3AlC2MAX phase purity, synthesis protocol, and storage conditions
Co-authors: Anupma Thakur, Nithin Chandran B S, Lia Stanciu, Babak Anasori

Ti3 C 2 T x is the most studied MXene with high electrical conductivity (up to 24000 S/cm), remarkable stiffness (up to 484 GPa), and negative zeta potential (-50 mV), tunable surface functionality, and scalable synthesis. While several studies have looked into the degradation of Ti3 C 2 T x in water, many parameters such as flake-level defects, non-stoichiometry in precursor MAX, solution concentration, and light exposure contribute to susceptibility to electron acceptors O2 and H2 O attack and MXene deterioration. In this study, we conducted a systematic investigation of the factors controlling the in-water stability of Ti3 C 2 T x MXenes, including Ti3 AlC2 MAX phase purity, etching/delamination synthesis approach, and storage conditions. We compared Ti3 C 2 T X MXenes made from three sources of Ti3 AlC2 MAX: oxycarbide MAX, optimized MAX, and commercially available MAX powders and two etching conditions: mixed acid etching (HF-HCl/LiCl) and minimally intensive layered delamination (MILD, HCl/LiF) methods. Further, we examined the effect of solution concentrations under both dark and light conditions over varying time intervals for a total of 200 days. Our results show the most stable Ti3 C 2 T x MXene can be made from the optimized MAX etched with mixed acid. Light exposure accelerated degradation, while higher concentrations
extended shelf-life. This study’s time-scale degradation analysis pinpoints areas that need attention to enhance the quality and stability of MXenes.

Lyubov Titova
Professor
Worcester Polytechnic Institute
USA

Day 1, August 5, 2024, 2:35 PM, Mitchell Auditorium

Title: **Ultrafast Photoexcitations in 2D MXenes**

Co-Authors:

MXenes are 2D transition metal carbides and nitrides with electronic properties that can be tuned by their chemistry and structure. Metallic-like conductivity, flexibility, high optical damage threshold and ease of processing owing to their hydrophilicity, make MXenes candidates for a host of electronic and optical applications. We use ultrafast optical and THz spectroscopic techniques to investigate the nature and behavior of photoexcitations in MXenes of different chemistries. We show that electronic and optical properties of MXenes can be engineered by choices of the transition metals and their order as well as by controlling the intercalants in the interlayer gaps [1,2]. Furthermore, we demonstrate that MXenes with high free carrier density show promise as polarizers and tunable electromagnetic interference shields in the THz range [3,4].


Majid Beidaghi- **Invited Speaker**
Associate Professor, Aerospace and Mechanical Engineering
University of Arizona
USA

Day 2, August 6, 2024, 4:00 PM, Mitchell Auditorium

Title: **Tailoring Mechanical and Electrochemical Properties of MXenes Through Defect Engineering and Assembly**

Co-Authors:

Recent advances in two-dimensional (2D) MXenes have opened new avenues in engineering materials for various applications due to the unique physical, chemical, and electrochemical properties of this family of materials. This presentation will delve into our group's research focused on optimizing the synthesis process and assembly techniques to maximize the performance of MXenes in various applications. MXenes, characterized by their exceptional electrical conductivity and electrochemical properties, have shown great potential as electrode materials for energy storage devices. Our research shows that the synthesis conditions crucially affect MXenes' morphology, defect concentrations, and surface chemistry, which in turn impact their electrical, electrochemical, and mechanical performance. This talk will highlight the effects of defects on the properties of MXenes and how the introduction of defects during synthesis can be manipulated to enhance the mechanical properties and the capacitive performance of MXene electrodes. Moreover, cation-assisted assembly of MXene flakes into heterostructures is shown to significantly improve their capacitive performance. Our recent studies suggest that standardized synthesis protocols are essential to achieve consistent MXene properties and facilitate reliable performance reporting across different applications. The presentation will also discuss the development of new strategies for MXene synthesis and assembly that are aimed at enhancing the performance of MXene-based devices.

Maksym Pogorielov - **Invited Speaker**

Senior Researcher
University of Latvia
Latvia

Day 3, August 7, 2024, 11:45 AM, Mitchell Auditorium

Title: **Novel concept of MXene-assisted targeted photo-thermal therapy of melanoma**


Photothermal therapy (PTT) is a cutting-edge approach to specifically eradicate cancerous tissues by employing photothermal agents and photosensitizing materials. Among these agents, MXenes are being actively explored due to their ability to act as photosensitizers in PTT. Nonetheless, enhancing the specificity of MXenes to tumor cells is a pivotal challenge. This specificity can be amplified by attaching specific antibodies (Abs) that target tumor antigens directly to the photosensitizers. In this context, Polydopamine (PDA), a biosourced compound, emerges as a viable solution for creating robust binding to diverse substrates. In our research, we introduce a novel method for the targeted ablation of melanoma cells using a composite of MXene-PDA and antiCEACAM1 antibodies. We successfully coated Ti3C2Tx MXene with PDA and then attached the anti-CEACAM1 antibody to it. Our findings demonstrate the biocompatibility of both Ti3C2Tx-PDA
and its antibody-conjugated form across a range of cell types. Additionally, we have developed a protocol for the targeted ablation of CEACAM1-expressing melanoma cells using near-infrared (NIR) light. The resulting complexes show remarkable selectivity and potency in eradicating CEACAM1-positive melanoma cells, without affecting CEACAM1-negative ones. This indicates the immense promise of MXene-PDA-Ab composites as a highly selective and potent cancer therapy modality. It also highlights the importance of targeted treatments in oncology, representing a hopeful path for the accurate and benign eradication of melanoma and potentially other cancers with specific markers. Our future endeavors will focus on refining these complexes for clinical application, which could revolutionize cancer treatment strategies.

Mark Anayee  
NRC Postdoctoral Fellow  
Air Force Research Laboratory  
USA

Day 2, August 6, 2024, 11:15 AM, Hill Conference Room

Title: **Surface and diffusion limited layer-by-layer etching of MAX phases for MXene synthesis**  
Co-authors: John Wang, Marley Downes, Stefano Ippolito, Yury Gogotsi

MXenes are the fastest-growing family of two-dimensional materials with great potential for various applications from energy storage to biomedicine, sensing, shielding, and others. MXenes are also commercially viable and can now be produced in kilogram-scale batches through selective chemical etching of atomic layers from precursor layered MAX phases. Although MXene synthesis has progressed to such large scales, the fundamental mechanism and kinetics of the etching reaction are not well understood, which hinders the rational optimization of the synthesis process. In this work, we monitored the etching process of MAX phase particles to produce MXenes, using a combination of in-situ and ex-situ techniques at single-particle levels. Our work shows that although Ti$_3$AlC$_2$ MAX phase particles are tens of microns thick, initial etching the outermost few tens of nanometer-thick layers accounts for more than a quarter of the total etching time. The etching process is well described through a JMAK model where nucleation occurs instantaneously and etching proceeds in one dimension along the out-of-plane direction of the MAX platelets, which is confirmed through crosssectional cutting of partially etched Ti$_3$AlC$_2$/Ti$_3$C$_2$Tx particles that reveals a layer-by-layer etching behavior. Further, the etching reaction is diffusion-limited for V$_2$AlC whereas Ti$_2$AIC and Ti$_3$AIC$_2$ are reaction-interface limited with an additional surface reaction limitation for Ti$_3$AIC$_2$. Overall, our work provides significant knowledge of the etching mechanism and kinetics, as well as an overview of the tools and techniques available to further investigate etchable materials.

Marley Downes  
PhD student  
University of Chicago  
USA

Day 1, August 5, 2024, 3:50 PM, Hill Conference Room
Title: Synthesis of (Mo2/3V1/3)n+1CnTx (n = 1, 2, 3): Exploring MXene Structure-Property Relationships
Co-authors: Christopher E. Shuck, Ruocun (John) Wang, Raul Arenal, Paweł Michałowski, Danzhen Zhang, Yizhou Yang, Mike Shekhirev, Steven J. May, Yury Gogotsi

The MXene family has rapidly expanded since their discovery in 2011 to include nearly 50 unique MXenes. However, a question that has been raised since their discovery has been: What is the effect of n? In other words, how does the number of layers affect MXene properties? Herein, we synthesize a system of MXenes with identical chemical composition spanning n: the (Mo2/3V1/3)n+1CnTx (n = 1, 2, 3) system. This allows, for the first time, the study of MXene structure-property relationships across n. We study the optical, electronic, electrochemical, colloidal, and magnetic properties of this system to determine trends with respect to n.

Masoud Sorosh - Invited Speaker
Professor, Dept. Chemical and Biological Engineering
Drexel University
USA

Day 2, August 6, 2024, 11:45 AM, Mitchell Auditorium

Title: Enhanced CO2 Membrane Separation Performance Caused by Strong Interactions between Functionalized Ti3C2Tx and Matrimid
Co-Authors: Mohammad Mozafari, Saeed Khoshhal Salestan, Manushree Tanwar, Kritika Jha, Ahmad Arabi Shamsabadi, Hyehyun Kim, and Zahra Fakhraai

Strong interfacial interactions between a filler and a continuous phase in a mixed-matrix membrane (MMM) allow for overcoming the tradeoff between permeability and selectivity in membrane gas separation. Two-dimensional nanomaterials with adjustable surface terminations permit controlling the interfacial interactions. In this work, we study two types of free-standing MMMs, one composed of pristine Ti3C2Tx MXene and Matrimid and the other consisting of a surface-modified Ti3C2Tx and Matrimid, for CO2/CH4 gas separation. Compared to pristine Ti3C2Tx membranes, the MMMs have higher CO2 solubility and higher tortuosity. Characterization results reveal that –OH termination groups on Ti3C2Tx surface form hydrogen bonds with carbonyl groups in Matrimid. The MMMs composed of Ti3C2Tx surface-functionalized with [3-(2-aminoethylamino)propyl]trimethoxysilane (AEAPTMS) show improved CO2 permeability and CO2/CH4 selectivity of about 140% and 130%, respectively, compared to pristine Matrimid membranes. Molecular dynamics simulations show that due to its AEAPTMS amine groups, the modified MXene has stronger interfacial interactions with Matrimid chains compared to the pristine Ti3C2Tx, causing improved affinity of the modified MXene toward condensable CO2 molecules. The elongation of gas pathways, disruption of polymer chains, and the existence of Ti3C2Tx interlayer nanogalleries and surface terminations positively contribute to the CO2 separation performance of the MMMs. These insights enable addressing current challenges in membrane gas separation and offer new prospects in membrane design for environmentally friendly CO2 separation.

Mawethu Pascoe Bilibana
Senior Lecturer
North-West University
South Africa

Day 2, August 6, 2024, 3:00 PM, Hill Conference Room

Title: X-ray diffraction profile and electrochemical analysis of green synthesized Mxene nanoparticles
Co-authors:

The research involved creating Mxene nanoparticles through plant-extract-mediated hydrothermal synthesis. The nanoparticles were then analyzed using X-ray diffraction (XRD) to determine their crystalline nature and phase characteristics. Further evaluation was carried out using XRD profile models such as Williamson-Hall analysis, size-strain plot, and Rietveld analysis to determine their microstructural parameters. The results showed that the calculated particle size using all models was consistent, ranging from 33.82-41.9 nm for Mxene. The microstrain varied based on the model, while the stress in the nanoparticles was evaluated at 13.7 MPa for Mxene. Mxene had a high energy density of $8.96 \times 10^{-8}$ KJ/m3. The Mxene layer was electrochemically deposited on the electrode at 100 mVs−1/Ag–AgCl. Two different redox peaks were observed during cyclic voltammetric characterization of the Mxene film in 1M H2SO4, indicating that the film was electroactive and displayed rapid reversible electrochemistry. Predicted values for the adsorbed electroactive species’ surface concentration and film thickness were $1.85 \times 10^{-7}$ mol/cm−2 and around 16 nm, respectively.

Micah Green - Invited Speaker
Professor and Associate Department Head, Dept. Chemical Engineering
Texas A&M University
USA

Day 2, August 6, 2024, 1:50 PM, Mitchell Auditorium

Title: MXenes at Interfaces: Pickering Emulsions and Structured Composites
Co-Authors: Huaixuan Cao, Jodie L. Lutkenhaus, Miladin Radovic, Emily B. Pentzer

The fabrication and design of structured polymer composites are still challenging and the common methods (e.g., solution casting, melt blending) have limited control over the internal filler structures. Pickering emulsion templating, in contrast, is an attractive approach to creating structured composites due to their well-defined interfaces, manageable structure and dimensions, and ease of scale-up. MXenes are of great interest as Pickering stabilizers as they have the ability to not only stabilize emulsions but also introduce functional properties into structures, such as high electrical conductivity, high EMI shielding, and rapid radio frequency (RF) heating. Here, we focus on the development of MXene Ti3C2 Pickering emulsions in fluid-fluid systems (e.g., oil-water, oil-oil) and their use as templates for functional structured MXene-polymer composites. Pickering emulsions drive nanosheets to the fluid-fluid interfaces and subsequent localized polymerization creates diverse structured polymer composites (e.g., capsules, armored particles, and porous monoliths). The ability to access both aqueous and non-aqueous emulsion systems largely expands the possible polymer compositions. The nanosheets are organized in these composites instead of being randomly distributed throughout. For instance, polymerization of the emulsion interfaces gives
polymer shells with nanosheets embedded, polymerization of the dispersed phase gives polymer particles armored with nanosheets, and polymerization of the continuous phase gives porous monoliths with polymer struts and nanosheets coated pores. The incorporation of MXenes imparts functional properties into their structures for additional applications. The work provides a simple platform to produce diverse structured MXene-polymer composites with well-controlled filler distribution, versatile compositions, and functional properties for advanced applications.

Michael Barsoum
Distinguished Professor, Materials Science and Engineering dept.
Drexel University
USA

Day 1, August 5, 2024, 1:15 PM, Mitchell Auditorium

Title: MAX phases
Co-Authors:

Michael Naguib - Invited Speaker
Associate Professor, Dept. of Physics and Engineering Physics
Tulane University
USA

Day 3, August 7, 2024, 2:50 PM, Mitchell Auditorium

Title: MXene Nano- and Atomic-Scale Engineering for Electrochemical Energy Storage and Conversion
Co-Authors:
MXenes form an extensive family of 2D transition metal carbides/nitrides, identified by the formula Mn+1XnTx (where M signifies an early transition metal, X represents carbon or nitrogen, n varies from 1 to 4, and Tx denotes surface terminations). Their outstanding electrical conductivity and ability to host ions position them as promising options for electrode materials in electrochemical energy storage. While intercalation is crucial in MXene applications for ion storage, understanding the effects of pre-intercalation on MXene’s electrochemical performance is limited. Here, we explore instances where pre-intercalation has notably altered MXene’s electrochemical behavior. By engineering MXene multilayers through pre-intercalation, an unprecedented areal capacitance of up to 5.7 F/cm2 has been achieved—a record in MXene performance. Pre-intercalated MXene, with an interlayer spacing of around 2.2 nm, has demonstrated a capacitance of 257 F/g—ten times higher than pristine MXene—over a voltage range exceeding 3V in pure EMIMTFSI electrolyte, resulting in a high-energy density comparable to batteries without sacrificing impressive power density. By forming nitrogen-doped graphene-like carbon confined between Ti3C2Tx layers to form a heterostructure, the capacity and stability of sodium-ion and lithium-ion batteries are significantly enhanced, with the specific capacity doubling. Additionally, we delve into other atomic-scale engineering approaches for MXenes, covering electrochemical energy storage and the hydrogen evolution reaction. Moreover, we introduce the recent discovery of 2D transition metal carbon-chalcogenides (TMCC), akin to MXenes but with chalcogen terminations, produced via scalable solid-state synthesis, offering new pathways for MXenes synthesis.
Mohammad Hossein Zarif - Invited Speaker
Associate Professor, School of Engineering
University of British Columbia
Canada

Day 3, August 7, 2024, 9:45 AM, Mitchell Auditorium

Title: MXene Guides Electromagnetic Waves in Communications and Shielding
Co-Authors:

MXene, a two-dimensional material, emerges as a strong candidate against traditional metals due to its comparable electrical conductivity and outstanding mechanical and thermal properties. MXene has also gained attention for its applications in electromagnetic shielding and absorber designs, showcasing its potential in advanced material applications. However, its use in sophisticated microwave components like filters, radiators, oscillators, and waveguides has not been fully realized. In this study, we explore the capabilities of MXene in these critical applications by detailing the fabrication methods employed and evaluating the resulting microwave performance characteristics. Our analysis focuses on the dielectric properties, conductivity, and compatibility of MXene with other materials used in microwave device fabrication. Additionally, our research employs numerical methods and lumped circuit modeling to highlight the potential of MXene in additive manufacturing processes, particularly for the development of low-cost but efficient electromagnetic components. These simulation techniques allow us to precisely predict the interactions between MXene and other polymers within various microwave components, assessing parameters such as transmission power, reflection power, and impedance matching under different manufacturing scenarios. By integrating MXene into 3D printing processes, we can innovatively create light weight, and low-cost electromagnetic components that maintain high performance while reducing production complexity. This approach not only demonstrates MXene’s adaptability and efficiency in component fabrication but also paves the way for its widespread application in producing complex electromagnetic structures with enhanced functionality and reduced material waste towards IoT applications in Beyond 5G (B5G) platforms.

Mohsen Beladi Mousavi
Faculty of Physics
Ludwig-Maximilians-Universität München
Germany

Day 2, August 6, 2024, 2:00 PM, Hill Conference Room

Title: Ion Transport Dynamics in Single MXene Nanoparticles Revealed by Interferometric Scattering Microscopy
Co-authors: Franz Gröbmeyer, Christoph Gruber, Kyle Matthews, Kateryna Shevchuk, Alex Inman, John Wang, Yury Gogotsi, Emiliano Cortes

MXene, a novel class of two-dimensional materials, holds significant potential in revolutionizing energy storage systems due to its exceptional electrical conductivity, large surface area, and ability
to accommodate various ions, enhancing the performance of batteries and supercapacitors.[1-2] In this pioneering study, state-of-the-art operando microscopy, i.e., interferometric scattering microscopy (iSCAT) reveals the intricacies of ion diffusion within MXene nanostructures at the scale of individual nanoparticles (Fig. 1). The research delivers an in-depth analysis of the dynamics of ion transport and charge transfer, shaped by variables such as ion size, hydrophilicity, and the nature of the solvent used. The deployment of non-invasive operando microscopy for live tracking has shed light on the influence of these variables on ion mobility within MXene frameworks. Notably, the research has identified how ion diffusion contributes to power density at the nanoparticle level, thus enhancing our ability to precisely measure the boundaries of charge transport in MXene films. These breakthroughs are vital for the advancement of energy storage technologies, providing a clearer understanding of ion movement at the nanoscale and its implications for the efficacy of high-performance materials. This investigation lays the groundwork for future enhancements in energy storage devices, suggesting that finetuning ion transport could markedly elevate power density and efficiency.

Moses Abraham Bokinala
Fulbright Post-doctoral fellow
Drexel University
USA

Title: When MXenes Meet Machine Learning: A Promising Initiative Towards Data-Intensive Scientific Revolution
Co-Authors:

Advancing sustainable technologies such as water-splitting devices, fuel cells and rechargeable batteries require cost-effective and eco-friendly materials, but discovering these innovative technologies is hindered by complex trade-offs and optimization challenges. Artificial intelligence, employing data mining and machine learning (ML) tools revolutionizes material discovery by accelerating the screening process through efficient exploration of vast chemical space. Particularly, investigation of recently developed transition metal carbides/nitrides (MXenes), distinguished by their distinctive physical and chemical characteristics has gathered widespread attention of material scientists. Given the practical constraints of synthesizing the vast array of possible MXenes, a holistic approach that combines experimental and computational methods with ML gains prominence. This presentation highlights the pivotal role of ML in extracting knowledge from existing MXenes by using implicit data patterns and intricate correlations, providing intelligent guidance for purposeful MXene’s development. Emphasizing the importance of SMART (specific, measurable, attainable, relevant, and timely) targets, the presentation illustrates how these objectives strategically shape the selection and transformation of data. Subsequently, our recent work is showcased, featuring a versatile multistep procedure employing various supervised ML algorithms to develop well-trained data-driven models capable of predicting the hydrogen evolution reaction (HER) activity across a dataset comprising 4,500 MXenes configurations. A notable achievement in this exploration of ML modelling is the outstanding performance of Gradient Boosting Regressor, demonstrating accurate prediction of the Gibbs free energy associated with hydrogen adsorption. Feature importance sheds light on key descriptors influencing HER
performance, including d-band center variance, electron affinity and number of valence electrons in terminating groups.

Naresh Osti - **Invited Speaker**  
R&D Staff/Beamline scientist, Backscattering Silicon Spectrometer (BASIS)  
Oak Ridge National Laboratory  
USA  

Day 2, August 6, 2024, 3:10 PM, Mitchell Auditorium  

**Title:** Dynamics of Confined Fluids in MXenes - A Neutron-based Approach  
**Co-Authors:**  
The interactions between MXene surfaces and electrolyte molecules affect the mobility and properties of the electrolytes at the interface, differing from their bulk properties. Understanding the structure and dynamics of the confined molecules at the interface is crucial for optimizing electrochemical performance when using MXenes as electrodes in energy storage applications. Since electrolytes are rich in hydrogen and hydrogen has a high incoherent neutron scattering cross-section, we have used neutron scattering techniques (elastic, quasielastic, and inelastic) to study the MXene-fluid interfaces. Here, we present the contribution of neutron scattering techniques to gain a fundamental understanding of the dynamics of confined fluids in MXenes.

Paul S. Weiss - **Invited Speaker**  
UC Presidential Chair and is a distinguished professor, Dept. of Chemistry, Bioengineering, and Materials science  
University of California, Los Angeles  
USA  

Day 1, August 5, 2024, 12:30 PM, Mitchell Auditorium  

**Title:** Identifying, Characterizing, and Leveraging Local Structure in Functionalized MXenes  
**Co-Authors:**  
We measure the local structure in functionalized MXenes that have been proposed for hydrogen storage and many other applications. The specific interactions at and near vacancies, adsorbates, and defects can vary substantially from the pristine material. By using combinations of scanning probe microscopies and spectroscopies, closely coupled to theory, we are able to determine local electronic and structural effects, as we build a comprehensive picture of how to optimize these materials for hydrogen storage and other chemistries.
Title: **Secondary ion mass spectrometry - a new tool in the toolbox for the characterization of MXenes**

Co-Authors:

MXenes properties can be finely tuned by precise engineering of each atomic layer. However, analyzing their elemental composition remains challenging because the techniques that offer atomic resolution (for example TEM) cannot identify light elements which are abundant in the MXene structure. On the other hand, the techniques that can readily detect them (for example XPS) cannot differentiate each atomic layer. The secondary ion mass spectrometry (SIMS) technique is capable to unambiguously identify each element with atomic precision. [1] The newly established protocol of deconvolution and calibration of the SIMS data enables layer-by-layer quantification of MXene/MAX phase samples with ±1% accuracy. [2] Such precision is particularly important for the detection of hydrogen and analysis of samples that consist of several different transition metals in their structure like high-entropy materials. Furthermore, it confirms that most MXenes contain a substantial amount of oxygen in the X layers, thus enabling the identification of oxycarbides, oxynitrides, and oxycarbonitrides subfamilies of MXenes. It can also be applied for under- and over-etched samples and to determine the exact composition of termination layers. Generally, the SIMS technique may provide invaluable support in the synthesis and optimization of the MAX phase and MXene studies.


Intercalated layered materials are usually produced by inserting guest species into the van der Waals (vdW) gaps of inherently layered materials such as graphite, hexagonal boron nitride (hBN), and transition metal dichalcogenides. The guest-host interaction alters the electronic structure and enables property tailoring for energy storage, catalysis, electronic, optical, and magnetic properties. Intercalation in non-van der Waals (non-vdW) nanolaminated materials and their two-dimensional (2D) derivatives is, however, rare and lacks understanding of the chemistry and structural tunability involved. Here, we show a structural editing protocol for non-vdW layered ternary carbides and nitrides (known as MAX phases) and their vdW multilayer derivatives (MXenes). Gap-opening and species-intercalating stages are separately mediated by chemical scissors and guest intercalants, respectively. A large family of 3D MAX phases with unconventional components and structures as well as 2D MXenes with versatile termination species, is accomplished. Moreover, a reverse transformation from 2D MXenes to 3D MAX phases is realized through knockout of surface termination species by metal scissors and stitching of ceramic slabs by zero-valence metal atoms. This scissor-mediated structural editing would enable structural and chemical tailoring in a broad class of layered ceramics. When delicately using Lewis acidic molten salts, two-dimensional rare earth metal carbides with chlorin termination can be obtained, showing promising magnetic and semiconductive behaviors.

References:
materials that trigger stiffness-related inflammatory and toxic reactions. Moreover, the large mechanical mismatch between the bioelectronic interfaces and the target tissues has been a bottleneck for wide clinical adoption. To overcome this challenge, biomimetic interfaces leveraging metal- and carbon-nanoparticle based hydrogels have been developed. However, they are limited by their electrochemical functionality, biocompatibility, and processability. Here we leverage liquid-phase processing of two-dimensional Ti3C2Tx MXene to fabricate MXene-based hydrogels for implantable soft bioelectronic interfaces. We directly crosslink individual MXene flakes using transition metal ions to achieve soft matrix-free hydrogels high electrical conductivity of up to 790 ± 150 S/m. The high capacitance and surface area of Ti3C2Tx MXene flakes allows us to fabricate electrodes that exhibit electrochemical impedance as low as 540 ± 130 Ω at 1 kHz, thus facilitating soft bioelectronics for electrophysiological recordings with high signal-to-noise ratio. Ti3C2Tx hydrogel electrodes further exhibit up to 50-fold greater high charge storage capacity and up to 7-fold greater charge injection capacity than conventional Pt-based rigid electrodes of the same size. This facilitates safe delivery of therapeutic electrical stimulation to the target tissues. Our results underscore the application of MXene-based soft hydrogel bioelectronics in studying neural function and disease pathologies, as well as developing therapeutic stimulation approaches.

Reagan Beers  
Graduate student  
University of Washington  
USA

Day 1, August 5, 2024, 4:05 PM, Hill Conference Room

Title: **Synthesis and Aqueous Stability Vanadium Carbide (V2C) MXene Films**
Co-authors: Jessica Ray

Vanadium carbide (V2C) MXene is 2-D nanomaterial that has been widely investigated for energy storage applications due to its multiple oxidation states, high gravimetric capacitance, and rapid electron transfer kinetics. However, V2C is unstable in aqueous environments (including within electrochemical cells)—particularly in its delaminated form—and quickly oxidizes and degrades in water which limits its performance and longevity in many applications. Furthermore, the relationship between V2C MXene synthesis parameters and aqueous stability is underexplored. In this study, we will determine the aqueous stability of V2C MXene films synthesized with different delaminating agents. V2AlC MAX phase precursors were produced through high temperature sintering of vanadium, aluminum, and graphite powders. V2C MXenes were etched from V2AlC then delaminated with tetraalkylammonium hydroxides of varying alkyl chain lengths (1–4). The delaminated V2C MXenes were formed into thin films and exposed to water under ambient conditions to assess relationships between the delaminating agent used and V2C degradation. Scanning electron microscopy, X-ray diffraction, and Raman spectroscopy were used to characterize the morphology, crystal structure, and degradation of MXenes films before and after water exposure. UV-visible light spectroscopy and inductively coupled mass spectrometry were used to quantify vanadium release from the films into water. Our results suggest that V2C MXene film morphology and aqueous stability depends on the delaminating agent. Our findings will benefit aqueous applications of V2C MXenes (e.g., electrochemical cells, water treatment) where material degradation and vanadium release need to be considered.
Sanjiv Dhigra—Invited Speaker
Professor and Associate Head of the Department, Dept. of Physiology and Pathophysiology
University of Manitoba
Canada

Day 3, August 7, 2024, 11:25 AM, Mitchell Auditorium

Title: MXene nanomaterials for cardiac regenerative medicine
Co-Authors:

Allogeneic (unrelated donor) mesenchymal stem cells (MSCs) and induced pluripotent stem cells (iPSCs) are being tested in animal studies and clinical trials for cardiac regeneration and repair. Outcome of initial studies was very encouraging and transplanted stem cells were safe after transplantation in the recipient heart. However, poor survival of transplanted stem cells in the infarcted heart has impaired the clinical translation of stem cells-based therapies. We have performed investigations to understand the mechanisms of poor survival of transplanted stem cells in the heart. We found that allogeneic stem cells after transplantation in the ischemic heart turned immunogenic and were subsequently rejected by host immune system. In our ongoing studies we are developing biomaterials-based strategies to prevent rejection of transplanted stem cells in the heart. We synthesized and characterized titanium carbide (Ti3C2) MXene quantum dots (MQDs). The immunomodulatory MQDs selectively reduce activation of CD4+IFN-γ+ T-lymphocytes and promote expansion of immunosuppressive CD4+CD25+FoxP3+ regulatory T-cells in an activated lymphocyte population. We also incorporated MQDs into a chitosan-based hydrogel to create a 3D platform for stem cell delivery to the heart. This composite immunomodulatory hydrogel-based platform improved survival of stem cells and mitigated allo-immune responses. We also found that MQDs have potential to mitigate allograft vasculopathy and prevent rejection of transplanted organs. These studies highlight the potential of MXene based next generation biomaterials for cardiac regenerative medicine.

Seong-Ju Hwang
Professor
Yonsei University
South Korea

Day 2, August 6, 2024, 5:15 PM, Hill Conference Room

Title: Conductive 2D inorganic nanosheets and their nanohybrids
Co-authors:

Conductive 2D inorganic nanosheets including MXene have evoked great deal of research activity because of their unique physicochemical properties and outstanding performances as functional materials. A great diversity in the chemical compositions, crystal structures, and defect structures of inorganic nanosheets provides this class of materials with a wide spectrum of physical properties
The conductive inorganic nanosheets can be used as powerful building blocks for exploring high performance hybrid electrodes and catalysts. Since the crystal defect and interfacial interaction have profound influence on the electrochemical and catalytic activity of hybrid materials, the energy functionalities of conductive 2D inorganic nanosheet-based hybrid materials can be greatly enhanced by defect- and interface-engineering. In this talk, several classes of 2D inorganic nanosheets (e.g. MXene, metal oxides, and metal chalcogenides) and their nanohybrids applicable for renewable energy technology will be presented together with the discussion about the relationship between chemical bonding nature and functionalities. The crucial role of interface/defect engineering in optimizing the energy performances of conductive 2D nanosheet-based materials will be highlighted.

Seon Joon Kim – Invited Speaker | Virtual |
Associate Professor and Sr. Researcher
Korea University of Science and Technology and Korea Institute of Science and Technology (KIST) South Korea

Day 2, August 6, 2024, 11:25 AM, Virtual

Title: Organic, Inorganic, and Organic-Inorganic Hybrid Surface Functionalization of MXenes for Gas Sensors
Co-Authors:

The demand for low-power gas sensing has been increasing due to the emergence of flexible, portable, and wearable devices. To achieve this, two-dimensional (2D) nanomaterials have drawn attention due to their high surface area, and high tunability, and room-temperature operation. Among them, MXenes especially show outstanding performance due to their simultaneous existence of high electrical conductivity and high-density surface functional groups. However, using MXenes solely as the active sensing material has shown limitations in sensitivity and selectivity between multiple target gases. Thus, it is necessary to hybridize MXenes with chemically active nanomaterials to overcome this limitation. Here, we introduce versatile methods to functionalize the surface of MXenes using organic, inorganic, or organic-inorganic hybrid techniques toward high-performance gas sensors. In the case of organic functionalization, ligands with tailored tail groups were grafted onto MXene to enhance selectivity. For inorganic functionalization, ultrafine metal/metal oxide nanoparticles of 1~3 nm size were densely anchored on individually delaminated MXene sheets. In addition, a combinatorial technique that employs both ligand functionalization and nanoparticle anchoring was utilized to synthesize highly selective gas sensors. Finally, we demonstrate the high dispersibility of all MXene hybrids toward solution-processable gas sensing devices.

Shayan Seyedin – Invited Speaker
Associate Professor Newcasle University
UK

Day 2, August 6, 2024, 11:45 AM, Mitchell Auditorium

Title: MXene Liquid Crystals for Multifunctional Fibers
Co-Author:

The development of liquid crystal (LC) phases in materials provides an opportunity to achieve highly ordered structural characteristics, which are highly desirable for fiber-based applications. By carefully tuning the aspect ratio of the MXene flakes and the concentration, additive-free Ti3C2 MXene dispersions are developed that exhibit nematic LC phases. The LC MXene formulations are then spun into pure MXene fibers using a wet spinning technique which involves extruding the aqueous LC MXene formulations into a coagulation bath. By carefully tuning the coagulation rate, Ti3C2 MXene fibers are developed with a high electrical conductivity of up to 7,750 S cm⁻¹, which is two orders of magnitude higher than the electrical conductivity of the LC graphene oxide-assisted MXene composite fibers developed previously. Moreover, when used as supercapacitor electrodes, the pure Ti3C2 MXene fibers exhibit a remarkable volumetric capacitance of 1,270 F cm⁻³ at the scan rate of 10 mV s⁻¹, comparable to the freestanding MXene film electrodes. This simple method is extended to other members of the MXene family such as Ti2C and Mo2Ti2C3. LC MXene fibers provide a novel platform to investigate MXene’s potential applications as energy storage electrodes in functional fabrics and heating elements in thermal comfort fabrics since they offer excellent electrical and electrochemical properties, surpassing other nanomaterial-based fibers. With application as electrical conductors, Joule heaters, and electrodes for energy storage devices, MXene fibers have accelerated the development of textile-based electronics that could be worn like everyday clothes.

Shiba Adhikari
Scientist
Argonne National Laboratory
USA

Day 3, August 7, 2024, 11:30 AM, Hill Conference Room

Title: Cu-based MXene electrocatalysts for selective CO2 reduction
Co-authors: Sixbert P. Muhoza, Zachary D. Hood

Addressing the rise in atmospheric CO2 levels requires proactive measures such as carbon capture and sequestration, alongside industrial decarbonization. While the CO2 reduction reaction (CO2RR) holds promise for converting industrial CO2, it grapples with challenges like complex catalyst preparation and selectivity control for desired C1 and C2 products. In this presentation, we demonstrate a recent breakthrough in introducing Cu-based MXene electrocatalysts, addressing these hurdles. These electrocatalysts are synthesized through the reductive adsorption of Cu ions onto hydroxy-terminated Ti3C2Tx, yielding unique metal-ceramic heterostructures with a tunable nanoscale hierarchy. This hierarchy significantly influences structure-property relationships critical for C1 and C2 production during CO2RR. Furthermore, these Cu-based MXene electrocatalysts exhibit enhanced selectivity towards electrocatalytic formaldehyde production, while also showing promise for C2 production like ethanol. These advancements pave the way for manipulating MXenes’ behavior to optimize characteristics for CO2RR, thus making substantial contributions to climate change mitigation efforts.

Acknowledgment: This material is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357.
Title: Advancing Sodium-Ion Batteries with Durable High-Capacity Electrodes Based on Customized MXenes
Co-authors: Shiba P. Adhikari, Zachary D. Hood

Abstract
While lithium-ion batteries have seen wide use in a range of applications from portable electronics to electric vehicles, the limited supply of lithium calls for alternative battery systems to meet the ever-increasing need for energy storage as the adoption of technologies such as electric vehicles and renewable energy continues to rise. Sodium-ion batteries are considered the most prominent alternatives to lithium-ion batteries as sodium has similar chemical properties, but a much higher abundance than lithium. Hence, in this work, we develop novel high-capacity sodium-ion battery electrodes comprising MXenes hybridized with high-capacity conversion-type electrodes: S, P, and Si. The resulting MXene/S, MXene/P, and MXene/Si electrodes deliver the high capacity intrinsic to S, P, and Si while limiting the volumetric changes that take place during their charge/discharge cycles to non-detrimental levels. This outcome arises from the two-dimensional MXenes dispersing, enveloping, and accommodating the expanding S, P, and Si moieties during sodium uptake, which preserves structural soundness of the electrodes. These results provide substantial insight as it pertains to developing novel high-capacity electrodes for next generation battery technologies.

Acknowledgements
This material is based upon work supported by Laboratory Directed Research and Development (LDRD) funding from Argonne National Laboratory, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC02-06CH11357. This research used resources of the Center for Nanoscale Materials; U.S. Department of Energy (DOE) Office of Science user facilities operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Stefano Ippolito
Post Doctoral Researcher, A. J. Drexel Nanomaterials Institute
Drexel University
USA

Title: Exotic Photothermal Properties in Ti-based MXenes for Optoelectronics
Co-authors: Francesca Urban, Jonathan E. Spanier, Paolo Samori, Yury Gogotsi

We delve into the analysis of photothermal and thermal properties of Ti-based MXenes, namely Ti3C2Tx and Ti2CTx, along with their potential use for optoelectronics. We compare their electrical response upon laser irradiation along with their photothermal behavior by changing the
environmental conditions, pressure and/or temperature. Comparing the current response at RT and ambient pressure (Air), we observe distinct behaviors: Ti3C2Tx shows a negative (photo)response upon laser irradiation (current decreases), while Ti2CTx exhibits a positive (photo)response (current increases). This is due to the different Resistance (R) vs. T trend recorded for the two systems, with Ti3C2Tx showing $dR/dT > 0$, unlike Ti2CTx with $dR/dT < 0$. Moreover, different kinetics are observed: while Ti3C2Tx exhibits a symmetric and fast current rise and decay ($\approx 10$ s), Ti2CTx presents a striking asymmetric and much slower kinetics during the current rise ($\approx 30$ s) and decay ($\approx 104$ s). By using Newton’s and Fourier’s laws, we estimate the ratio of the thermal conductivity for the two MXenes, with Ti3C2Tx showing a larger value by a factor $\approx 10$. Such exotic photothermal kinetics is strongly affected by the operating conditions and can be fine-tuned by exposing the devices to different atmospheres (Air vs. Ultra-High Vacuum) and T (from 100 K to 350 K). Our work highlights the dramatic effect of structure and composition in Ti-based MXenes on their optoelectronic properties, as well as photothermal and thermal characteristics. Particularly, the exotic photothermal kinetics recorded for Ti2CTx pave the way for its use in memory and neuromorphic devices.

Steven May – Invited Speaker
Professor and Department Head, Materials Science and Engineering
Drexel University
USA

Day 1, August 5, 2024, 2:15 PM, Mitchell Auditorium

Title: Magnetotransport and weak localization in Ti3C2Tx single flakes
Co-Authors:

The study of electronic transport in MXenes is complicated by the inherit complexity of these materials. Variations in surface terminations, sample degradation through oxidation and the challenges of distinguishing between inter- and intra-flake conduction mechanisms all create significant challenges in understanding and ultimately controlling electronic behavior. To probe intrinsic conduction, we have carried out temperature-dependent magnetotransport measurements on Ti3C2Tx single flakes. The samples exhibit metallic conduction with slight upturns in resistivity at low temperatures, the magnitude of which varies from sample to sample. At low temperatures, a negative magnetoresistance is observed that is strongly dependent on the angle between the applied magnetic field and the current direction. The magnitude of the magnetoresistance increases proportional to the temperature at which the resistivity transitions from negative to positive $dr/dT$, highlighting the role of disorder in the magnetoresistive mechanism. The angular and field-dependence of the magnetoresistance point to the presence of weak localization arising from quantum interference of the conduction electrons. The magnetoresistance is fit to models of weak localization to extract the temperature dependence of the phase coherence length, which follows a $T^{0.5}$ behavior from 20 to 80 K consistent with observations in other 2D materials. With this work, we conclusively elucidate the origin of the negative magnetoresistance in Ti3C2Tx and demonstrate that MXenes can exhibit quantum transport effects.

This work is performed in collaboration with Jane Frostad, Stefano Ippolito, Francesca Urban, and Yury Gogotsi. This research is supported by the U.S. Department of Energy, Office of Basic Energy Sciences, grant #DESC0018618
Susan Sanderman – Invited Speaker
PhD, Biomaterials and Tissue Engineering
University of Brighton
UK

Day 2, August 6, 2024, 11:45 AM, Mitchell Auditorium

Title: **MXenes at the biointerface: improving host response biology for medical device innovation**
Co-Authors:

Ti3C2Tx is the first described and most studied of the diverse, 2-dimensional family of MXenes. The growing breadth of biomedical device applications for this and other MXenes reflect the tunable properties of these materials for diverse applications from theranostics to neural guidance, medical imaging, cancer therapeutics, ophthalmic biomaterials and smart sensor devices within regenerative medicine. However, key challenges remain in understanding and optimizing the biological properties of MXenes at the bio-interface for sustained therapeutic benefit. This presentation will consider our work investigating the hypothesis that Ti3C2Tx may be used to repress the hyper-inflammatory and fibrotic response associated with loss of bioactive medical device function, particularly modelled in ophthalmic avascular and dermal vascular environment.

Tae Woo Lee – Invited Speaker
Professor, Materials Science and Engineering
Seoul National University
South Korea

Day 3, August 7, 2024, 1:45 PM, Mitchell Auditorium

Title: **Two-Dimensional Graphene and MXene for Flexible and Stretchable Displays**
Co-Authors:

Two-dimensional (2D) materials such as graphene and MXenes have great potential applications in a variety of flexible and wearable optoelectronic devices as a replacement of conventional brittle indium tin oxide (ITO) electrodes. However, the practical applications of such 2D electrodes have been limited due to the high injection barrier at the electrode/organic interfaces. Here the work function (WF) of the 2D electrode was modified using such as a post-fabrication treatment through overcoating of materials with electronwithdrawing or donating groups for charge transfer doping. Hence controlling the WF of electrode of graphene and MXene through surface engineering enables the significant improvement in electroluminescent efficiency with lowered injection barrier.
Furthermore, to tackle the charge injection problem occurred at the stretchable electrode interfaces, a graphene layer was introduced on top of silver nanowire percolation networks to form a complete two-dimensional contact stretchable electrode (TCSE). These works on 2D materials lay a solid platform for practical applications of 2D conductive materials as both electrodes for flexible and stretchable optoelectronics.

Tae Yun Ko
Nanoplexus
UK

Day 3, August 7, 2024, 2:05 PM, Mitchell Auditorium

Title: **Surface Functionalization of MXene for the Development of Electrically Conductive MXene/Polymer Composites**
Co-Authors:

Due to their unique electrochemical properties, the development of MXene framework is an attractive target in industry and of considerable importance. However, the pristine MXene based aqueous dispersion still suffers from one of the biggest challenges: organic solvent dispersion stability, making it difficult to composite with hydrophobic polymers. Surface functionalization with proper organic ligands on MXene surface is one of the powerful strategies to overcome this challenge. By modifying the surface of MXene from hydrophilic to hydrophobic, the composite process with a variety of hydrophobic polymers can be achieved more efficiently. Herein, we designed and conceptualized various organic ligands that can control chemical/physical bonding for efficient surface functionalization of MXene. Surface functionalized MXene with organic ligands has excellent dispersion stability in polar/non-polar organic solvents and high electrochemical properties even after producing MXene/polymer composites.

Vadym Mochalin– *Invited Speaker*
Associate Professor, Department of Chemistry and Materials Science & Engineering
Missouri University of Science & Technology
USA

Day 2, August 6, 2024, 2:50 PM, Mitchell Auditorium

Title: **Reactivity of 2D Transition Metal Carbides (MXenes)**
Co-Authors:
A large family of two-dimensional transition metal carbides and nitrides (MXenes) raises interest for many applications due to their high electrical conductivity, mechanical properties [1], potentially tunable electronic structure [2], nonlinear optical properties [3], and the ability to be manufactured in the thin film state [4]. However, their chemistry that is key to development of these applications, still remains poorly understood [5,6]. In this presentation we will discuss recent progress in understanding fundamental MXene chemistry and harnessing it for suppressing unwanted reactions and prolonging stability of these materials.

References
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technique highlights the promise of additive-free MXene inks for scalable fabrication of easy-to-integrate components of printable electronics.

Yasunori Hioki
Engineer
Murata Manufacturing Co., Ltd
Japan

Day 3, August 7, 2024, 2:05 PM, Mitchell Auditorium

Title: Development of Murata's MXene
Co-Authors: Mark Anayee, Mikhail Shekhirev, and Yury Gogotsi, Akari Seko, Shun Sakaida, Masashi Koyanagi, Yasuaki Okada, and Takeshi Torita

Murata Manufacturing Co., Ltd., a manufacturer of electronic components in Japan, is conducting material and application development for MXene. To apply MXene to electronic components, environmental reliability is important, and it is especially required to be stable under high temperatures and high humidity. Because of their hydrophilicity, MXene capture water from the surrounding environment, which may lead to swelling and degradation of the assembled multilayer films. Here we demonstrate that the intercalation of N-methylformamide (NMF) leads to MXene films with improved stability at high temperatures and high humidity through host–guest hydrogen bonding. Because of its strong interaction with the MXene surface and occupation of the interlayer spacing, NMF mitigates the intercalation of water and allows for better retention of electrical conductivity during prolonged use in hot and humid environments. Murata is also working on application development using various features of MXene. We have the technology to synthesize excellent MXene, so we are seeking partners to develop the application cooperatively.

Yasser Hassan
Assistant Professor, Department of Chemistry
Qatar University
Qatar

Day 2, August 6, 2024, 3:15 PM, Hill Conference Room

Title: Enhanced Energy Density in Sodium-Ion Batteries: The Synergistic Role of Mxene, and multielement doped-P2 Layered Oxides
Co-authors: Ahmed

Layered oxide materials for sodium-ion batteries have been extensively explored for their high energy density applications. However, the role of 3d cations, including Fe, Ni, and Mn,
in Cu-containing P2 layered oxides has not been examined in detail. In this work, we investigated the relationship between the stoichiometry of Fe, Ni, and Mn in Cu-containing P2-type layered oxides. Various stoichiometries were chosen to maintain a low pristine Mn redox state. The compositions were synthesized using a facile solid-state method. We observed varied responses to the interplay of Fe and Ni on the Mn valence redox state. The stoichiometry with a pristine Mn redox state of +3.75 exhibited the highest discharge capacity of 145 mAh/g and an energy density of 502 Wh/kg. The combined effect of Fe, Ni, and Cu in the stoichiometry with the lowest Mn redox state achieved the highest voltage of 3.61 V. Additionally, we studied the effect of incorporating MXene to enhance the conductivity of the cathodes. The combination of Cu, Ni, Fe, and Mn, along with MXene integration, offers a cost-effective and resource-friendly approach to developing high-energy sodium-ion batteries targeted toward electric vehicle applications.

Yuan Zhang
Post Doctoral Researcher, A. J. Drexel Nanomaterials Institute
Drexel University
USA

Day 3, August 7, 2024, 11:45 AM, Hill Conference Room

Title: Mechanical suppression of electron transfer in subnanometer confinement between MXene layers
Co-authors: Danzhen Zhang, Lingyi Bi, Ming Lei, De-en Jiang, Yury Gogotsi

Ion adsorption and electron transfer are the primary charge storage mechanisms in porous electrodes. Desolvation/solvation of ions in subnanometer confinement may alter the balance between those two processes. For 2D materials like MXenes, there is a continuous change in interlayer spacing as ions are transported and stored between the layers. However, little is known about the effect of the mechanical constraint (pressure) on electrochemistry in confinement. In this work, the ion transportation process in between mechanically constrained MXene layers is monitored by combining in-situ UV-vis spectroscopy, in-situ optical spectroscopy, and in-situ XRD characterization. Compared with spray-coated Ti3C2Tx films, physically constrained Ti3C2Tx film with a constant interlayer spacing exhibited exceptional capabilities in suppressing redox reactions. Notably, this property of faradaic suppression under mechanical strain led to the application of MXene-based electrochemical cells as high-pressure electrochemical sensors.

Yuemei Ye
Assistant Professor, Lehman College
City University of New York
USA

Day 1, August 5, 2024, 3:00 PM, Hill Conference Room

Title: Simple and Efficient Defluorination of PFAS in aquatic solution by V2C MXene and H2O2
Co-authors: Jessica R Ray

Per-and polyfluoroalkyl substances (PFAS) in wastewater has become widespread and attracted increasing attention due to its acutely toxic causing tumors, and kidney and liver diseases in humans as well as immunological effects in aquatic animals. Successful degradation of PFAS remains a key environmental challenge due to the extreme strength and stability of characteristic carbon-fluorine PFAS bonds. Therefore, developing an environmentally friendly, mild and convenient approach for PFAS degradation is highly desirable. Herein, a facile and green method is developed, which shows extremely efficient defluorination of PFAS in the presence of vanadium carbide (V$_2$C) nanosheets and H$_2$O$_2$ under room temperature. The as-prepared V$_2$C layered nanostructures were exfoliated into nanosheets resulting in a significant enlargement of V$_2$C surface area and reactive sites which facilitates the fast degradation of PFAS. Perfluorooctane sulfonate (PFOS) were selected as representative PFAS at initial concentrations of 50 µg/L. The V$_2$C-H$_2$O$_2$ defluorination mechanism is so effective, that over 96% PFOS removal was observed with 0.15 mg/mL V$_2$C within 4 h of reaction at circumneutral pH and in the presence of dissolved oxygen. Ion Chromatography verified near complete defluorination of PFOS. Hydrated electron was detected in the V$_2$C-H$_2$O$_2$ solution, which is supposed to be the key reason leading to the reduction of PFOS. The findings from this work of high reactivity and efficiency of PFAS degradation employing V$_2$C nanosheets coupled with the addition of a mild oxidant under environmentally relevant conditions can translate to other applications in contaminant removal, such as degradation of halogenated disinfection byproducts.

Z

Zahra Fakhraai—Invited Speaker
Professor, Department of Chemistry and Chemical and Biomolecular Engineering
University of Pennsylvania
USA

Day 1, August 5, 2024, 12:30 PM, Mitchell Auditorium

Title: Stabilizing Ti3C2Tx MXene Films by Removal of Highly Confined Water
Co-Authors: Hui Fang, Anupma Thakur, Amirhossein Zahmatkeshsaredorahi, Vahid Rad, Ahmad Arabi Shamsabadi, Masoud Soroush, Xiaoji G. Xu, Babak Anasori

MXenes thin films are prone to oxidation in ambient conditions, which highly depends on their synthesis conditions and surface terminations. Strategies to improve their stability include producing MXene-polymer composites, modifying surface terminations, or annealing MXenes in a vacuum at moderate temperatures. Here, we investigate the details of Ti3C2Tx MXene oxidation and stability under various conditions using high resolution atomic force microscopy (AFM) imaging and measure their conductivity using spectroscopic ellipsometry. The results show that MXene monoflakes are stable and resist oxidation even at elevated temperatures up to 600 oC in air. However, stacked MXene layers, oxidize readily when heated to above 300 oC. We demonstrate that this is due to confined water trapped between stacked MXene layers, which can be removed only when MXene films are annealed under vacuum at temperatures as high as 600 oC—while annealing at lower temperatures only removes surface-absorbed water. We demonstrate that removing the
confined water by annealing multilake Ti3C2Tx MXene films under vacuum at 600 oC dramatically improves their stability. We also demonstrate that the removal of highly adsorbed water affects the termination state of MXene and its conductivity. These findings provide fundamental insights into the kinetics of confined water and its role in the oxidation and charge transport in Ti3C2Tx MXenes.

Zdenek Sofer – Invited Speaker
Professor
University of Chemistry and Technology Prague
Czech Republic

Day 2, August 6, 2024, 4:20 PM, Mitchell Auditorium

Title: MXene chemistry and topochemical conversion for energy storage applications
Co-Authors: Lukáš Děkanovský, Jalal Azadmanjiri, Martin Havlík, Bing Wu, Jiří Šturala, Vlastimil Mazánek, Jan Luxa

The field of MXene chemistry is rapidly advancing, characterized by the emergence of novel terminations and surface functionalization strategies. MXenes can be transformed into a diverse array of related compounds through controlled reactions with chalcogens and various other reagents. By converting titanium-based MXenes and other variants to chalcogenides, composite materials can be generated while preserving the original morphology. These materials demonstrate enhanced properties suitable for a wide range of applications such as energy storage and photocatalysis. Through specific chemical processes, MXenes based on vanadium, niobium, and molybdenum can be converted into chalcogenides or vanadates/niobates, offering opportunities for the development of high-performance materials for applications in photocatalysis, supercapacitors, and batteries. Additionally, covalent functionalization strategies can be employed to stabilize the surface of MXenes and tailor their properties, thereby enhancing charge storage capacity for high-energydensity supercapacitors. The presentation will also showcase the use of various zwitterionic molecules for functionalization to achieve increased capacitance.

Poster Presentation Abstracts

A

Adam Walter
Drexel University
USA
As a novel family of nanomaterials discovered in 2022 at Drexel University, one-dimensional lepidocrocite titanium oxide nanofilaments (1DLS), offer promise in a variety of applications. With a base-unit cross-section of just $2 \times 3 \text{TiO}_6$ octahedra, they have a theoretical surface area of $\sim 1,000 \text{m}^2/\text{g}$ - a single gram could extend to the sun and back 1.7 times. However, the most important aspect of these materials is the ease at which they can be fabricated. Mixing abundant, commercially available Ti-containing precursors with a simple quaternary ammonium organic base (tetramethylammonium hydroxide) at temperature.

Titanium carbide MXene free-standing membranes (MFMs) have garnered significant attention for their efficiency in ion separation from water, owing to their aligned nanochannels and unique surface chemistry. However, their application in the selective separation of precious ions is seldom and remains to be experimentally explored. In this study, we focused on adjusting the interlayer spacing of MFMs and, consequently, the size of their nanochannels to either match or exceed the diameter of the desired ions. This adjustment facilitates the permeation of precious ions, including $\text{Y}^{2+}$, $\text{Cr}^{2+}$, and $\text{Ce}^{2+}$, through the membrane while rejecting other ions, allowing for their selective separation. We investigated the correlation between membrane surface chemistry and ion selectivity, showcasing the potential of controlling MXene surface chemistry to enhance the efficiency of selective ion separation. Additionally, we extended the lifetime and stability of MFMs through in situ cross-linking via thermal treatment. Our findings pave the way for the practical implementation of these membranes in the selective separation of precious ions, a crucial process for technologies essential to fostering a circular economy and achieving a clean energy future.

Two-dimensional (2D) materials, often referred to as atomically layered materials, boast extraordinary properties that are compelling for both foundational research and practical
applications. These properties arise from their atomic-scale planar structure and constituent elements, which can be adjusted during the synthesis process. This study focuses on MXenes, a recent addition to the expanding family of 2D materials, acclaimed for their versatility in various applications. MXenes can be represented by the chemical formula Mn+1XnTx, where M denotes a transition metal, X signifies nitrogen or carbon, and T stands for surface terminations like F, O, or OH. This research specifically centers on Ti-based MXenes. We introduce a novel method of transfer of MXenes prepared by Liquid Phase Exfoliation (LPE) method into UHV. This is achieved by drop-casting on a pre-prepared conductive substrate surface, followed by immediate vacuum drying to retain the surface condition. The objective of this study is to comprehend the oxidation processes occurring under ambient conditions and to delve into the long-term stability of the material. In-situ analysis conducted using a combination of X-ray Photoelectron Spectroscopy (XPS) and Atomic Force Microscopy (AFM). Samples then exposed to air for durations of 1h, 24h, 5 days, 10 days, 1 month, and 2 months. Their compositional changes tracked after each exposure to comprehensively understand the stability of the material. Thus, this fundamental study will reveal many important aspects of MXenes stability, will help establish a roadmap to engineer their properties, and so control the performance of devices based on these new materials.

Ajay Pratap
Boise State University
USA

Title: Enhancing triboelectric nanogenerators with MXene-fortified PVBVA: A novel additive manufacturing approach for advanced energy harvesting
Co-authors: Isaac Little2, Fereshteh Rajabi Kouchi, Hailey Burgoyne, Tony Varghese, Zhangxian Deng, David Estrada

While the adoption of soft contact structure designs in Triboelectric Nanogenerators (TENGs) has been a favored approach to enhance their durability, this method often presents a significant challenge in simultaneously achieving high output performance. Traditional TENGs are often limited by their reliance on specific tribo-materials, which can restrict their practicality and performance. To address these limitations, we present a novel fabrication method for a 3D-printed TENG, that is adaptable to a variety of tribomaterials, including human skin. Our innovation lies in the integration of a high-performance polymer, Poly (vinyl butyral-co-vinyl alcohol-covinyl acetate) (PVBVA), with MXene, a two-dimensional material, onto an aluminum foil substrate. This combination significantly enhances the triboelectric properties of the device. Our findings show that the PVBVA layer alone yields a triboelectric output of approximately 110 V. However, with the introduction of MXene at a concentration of 2.75 mg/ml, the output escalates to 150 V, and further increases to 250 V at a concentration of 5.5 mg/ml, demonstrating a substantial enhancement in performance. Beyond energy harvesting, we leveraged this TENG technology in a water energy harvesting system, effectively extracting energy from sources such as raindrops. Additionally, we developed a 2 x 2 touch sensor array utilizing this technology. This sensor array is capable of generating charge through the triboelectric effect and dynamically mapping the output voltage values in response to skin touch, showcasing its potential for human-machine interaction and touch-sensitive interfaces.
Title: **MXene Enabled Wearable Energy Storage Solutions**
Co-Authors: Alex Inman, Magdalena Zywolko, Tetiana Hryhorchuk, Lingyi Bi, Kyle Matthews, Yury Gogotsi

E-textiles can create new user experiences and provide comfortable monitoring of patient vitals. To realize the potential of E-textiles there is a need for textile-based energy storage. Current research into textile-based energy storage often leads to devices with insufficient energy to power the electronics necessary to realize this future. MXenes are a conductive 2D material with high energy capacity that can be integrated into textiles making them an ideal candidate for textile-based energy storage. We demonstrate the use of MXenes in two different textile-based devices to power fully programmable microcontrollers capable of motion tracking and environmental sensing for extended times.

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Title: **Sustainable Lignin-MXene Composite Adsorbent for Hg(II) Removal from Water**
Co-authors: Armanbek Nursharip, Chingis Daulbayev, Jakpar Jandosov, Joseph C. Bear, Rosa Busquets, Vassilis J. Inglezakis, Alzhan Baimenov

Heavy metal pollution in water poses a severe health threat. This study investigates a novel and sustainable approach for mercury removal using macroporous aerogel composites derived from rice husk lignin and modified with MXene. These composites exhibited high specific surface area (320 m²/g) and remarkable potential for Hg(II) removal. Notably, 20 wt.% MXene modification increased the maximum adsorption capacity to 135.8 mg Hg²/g, exceeding bare lignin aerogel (82.4 mg Hg²/g) and surpassing commercial adsorbents. The composite effectively removed Hg(II) even from tap water spiked with high metal concentrations (10 mg/L). These findings highlight the potential of lignin-MXene aerogels for real-world application in water purification and environmental remediation.
Ankita Rawat
Jawaharlal Nehru University
India

Title: **Highly Sensitive Ti3C2Tx/MoSe2 (2D/Quasi-2D) Heterojunction based Photodetector**
Co-authors: Abhishek Kumar Singh, Surendra Kumar, Gaurav, Rajput, Ritesh Kumar Chourasia, Nitesh K. Chourasia*, Pawan Kumar Kulriya*

Two-dimensional (2D) materials, which can be synthesized using low-temperature methods like liquid exfoliation, are now being considered for electronics and optoelectronics applications due to their unique optoelectronic properties and ability to be processed into various structures. In this article, a 2D material i.e., Ti3C2Tx/MoSe2 with a nanometer-thick Ti3C2Tx MXene (Tx stands for surface terminating species, including -F, -OH and -O) and MoSe2 film has been fabricated by a successive interfacial assembly of liquid exfoliated 2D MXene and MoSe2. Photodetectors (PDs) made of Ti3C2Tx/MoSe2 over SiO2 on Si substrate exhibit significantly improved photodetection ability. The photo responsivity of Ti3C2Tx/MoSe2 PD is ~159 mA/W when illuminated by a 372 nm light intensity of 4.4 μW at a reverse bias of -1.5 V. The interface between the 2D and quasi-2D effect on the formation of the heterostructure played a major role in the enhancement of its photodetection performance. Observation of high responsivity (~159 mA/W), as well as external quantum efficiency (53 %) for Ti3C2Tx/MoSe2 PD, make it a promising material for a UV light photo switch and image sensors. This work sheds light on the utilization of a combination of 2D MXene and quasi-2D MoSe2 materials in high-performance optoelectronic devices.

Annabelle Bedford
Purdue University
USA

Title: **High-throughput Synthesis of Double Transition Metal MAX for Future Machine Learning**
Co-authors: Bethany G. Wright, Brian C. Wyatt, Babak Anasori

As the available compositions of MXene have grown, both novel synthesis and optimization of MXenes are critically linked to the development of their precursor MAX phases. Based on the wide number of possible compositions and synthesis routes, machine learning is a promising technique to predict potential new compositions and synthesis techniques to yield higher quality MAX and MXenes. By leveraging machine learning models, discovery of novel MAX and MXene compositions can be expedited reducing the cost and time investment associated with synthesis. However, very limited data is available to train the machine learning models. This study uses high-throughput processing of three double-transition metal solid solution MAX phases (Ti,Nb)2AlC, (Ti,Ta)2AlC, and (Ti,V)2AlC to optimize sintering temperature and molar ratios effect on phase stability and atomic occupancy as measured via x-ray diffraction, scanning electron microscopy, and energy dispersive spectroscopy analysis. These phases have a tunable compositional space of their M elements allowing for study of the effects of composition on temperature, in addition to the ability to measure their M’ and M’’ occupancies. By systematically investigating these synthesis conditions on both successful and unsuccessful MAX synthesis and the resultant purity and composition of the MAX phases, these datasets can serve to improve machine learning algorithms to study other MAX systems for scalable and efficient synthesis of MAX phases and the resulting MXenes.
Ashley Koluda  
University of Pennsylvania  
USA  

Title: **Development of human-scale dry EEG based on 2D MXene for dynamic brain monitoring**  
Co-authors: Sneha Shankar, Eugenia Angelopoulos, Mariam Josyula, Nina Petillo, Kathryn Davis, Flavia Vitale  

Electroencephalography (EEG) is crucial for non-invasive recording of electrical brain activity for diagnosis and treatment of neurological disorders. Traditionally, EEG requires gel-based electrodes, which are time-consuming to apply and require skin-irritating abrasives and pastes. Recently, we have introduced dry EEG electrodes, using Ti3C2 MXene, which enhance comfort and usability with minimal skin preparation. Here, we advance this technology towards clinical use by fabricating a flexible EEG headset. We developed a reduced montage headband consisting of 8 channels positioned equidistantly on the head circumference. These electrodes, made from Ti3C2 MXene-infused hydroxylated PVA pillar templates (diameter: 8 mm, height: 8 mm), penetrate through hair contacting the scalp without needing gels. Individual electrodes are connected to the recording amplifiers via off-the-shelf EEG connectors attached to leads. Owing to the high electrical conductivity and surface area of Ti3C2 electrodes, the average 10 Hz impedance with the scalp is 2.1 ± 1.8 kΩ (n=5 subjects). To further validate this dry Ti3C2 MXene EEG technology in a realistic scenario, we recruited healthy participants and recorded EEG in the sitting position and during walking at regular speed. A preliminary analysis of the EEG recordings shows that signal quality of the MXene electrodes is comparable with clinical gelled electrodes, while reducing skin prep and electrode placement time by ~2X. Furthermore, we demonstrated successful recording in a realistic dynamic application. Our novel dry EEG technology can improve comfortability, reduce placement and skin preparation time, and reliably transmit relevant brain signals, supporting its potential as a comfortable, easy-to-use EEG monitoring technology.

Austin Vorhees  
Purdue University  
USA  

Title: **Thermally stable high-temperature additive-free Ti3C2Tx MXene fibers**  
Co-authors: Ken Usman, Nithin Chandran, Anupma Thakur, Kartik Nemani, Joselito M. Razal, Babak Anasori  

The advancement of aerospace, automotive, energy, and electronics industries necessitates materials capable of withstanding higher temperatures and extreme environments. Integration of thermally stable fiber reinforcements becomes crucial for achieving reduced weight, increased tensile strength, enhanced thermal shock resistance, prolonged service life, and high-temperature stability (>1000 °C) in composites. Particularly, ceramic fibers with high strength, high thermal stability, and high thermal shock resistance are crucial for next-generation engineering materials. MXenes as 2D nanoceramics are gaining interest as high-temperature carbide additives in metal and ceramic composites. Similar to their bulk transition metal carbide and nitride counterparts (such as TiC, NbC, TaC), MXenes’ interior transition metal carbide/nitride core lends the potential of their use...
in extreme conditions, such as high-temperatures (> 1500 °C). In this study, we present the systematic approach for additive-free wet spinning of Ti3C2Tx MXene fibers and their high temperature phase behavior up to 1000 °C. We will present the structure and phase stability and evolution of these fibers at different temperatures as the first steps in the development of additive-free ultra-high temperature fibers. This finding underscores the potential of MXene fibers for ultra-high-temperature applications.

Ayesha Zaheer
University of Naples Federico-II
Italy

Title: MXene Flakes Decoration with AuNPs for Enhanced Bio-sensing
Co-authors: Z.U.D Babar, F. Pisani, R. Velotta, B. Della Ventura, V. Iannotti

Biosensors offer a rapid, efficient, affordable, and real-time monitoring solution for detecting Escherichia coli in drinking water, a pathogen responsible for many infectious diseases. Here, we introduce a cost-effective biosensor using 2D-Ti3C2 MXene and gold nanoparticle composites (MX@AuNPs). The MAX phase was etched via an HF + HCl etching approach and delaminated using LiCl to obtain a stable colloidal suspension containing single/few-layer MXene flakes. The MX@AuNPs were prepared by an in-situ self-reduction method, followed by an innovative photochemical immobilization technique (PIT) to covalently immobilize antibodies over MX@AuNPs. The etching and subsequent delamination processes were investigated using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDXS). XRD confirms the removal of interleaved aluminum, and the increase in c-spacing indicates successful exfoliation and subsequent delamination. Confirmation of successful MX@AuNPs synthesis was achieved through SEM, DLS, and UV-vis spectroscopy. Dynamic light scattering (DLS) analysis reveals an increase in the hydrodynamic radius of the flakes after decorating MXenes with AuNPs, confirming composite formation. SEM analysis shows the in-situ formation of AuNP clusters throughout the MXene sheets, confirming successful incorporation and providing numerous sites for antibody immobilization. UV-vis spectra exhibit a prominent peak of AuNP alongside the typical MXene peak, further indicating MX@AuNPs formation. The fabricated biosensor demonstrates the combined synergistic properties of both MXene and AuNPs, capable of reaching a low detection limit and rapid response time. Our groundbreaking approach, which streamlines water quality monitoring, holds promise for detecting various other pathogens and environmental pollutants.

Banani Talapatra
Central University of Punjab
India

Title: MXenes as a supporting component of electrocatalysts for Oxygen Evolution Reaction
Co-authors:
Electrochemical water splitting presents a promising aspect for both mitigating fossil fuel use and storing energy from renewable sources in the form of hydrogen fuel. However, the four electron transfer process, OER, remains a bottleneck, as, even with catalysts, the overpotential is quite high (around 300 mV). Iridium and Rubidium oxide are proved to be good electrocatalysts but are very costly. Now the aim is to synthesize an electrocatalyst to achieve a low overpotential at a feasible cost. MXenes are known to have a high surface area, high electroconductivity and are extremely hydrophilic, which makes them quite a promising component of electrocatalysts for OER. Electrochemical measurements can provide insight into the electronic interaction, stability and structural change in different MXene based catalysts.

Ben Davis
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Drexel University
USA

Title: **Gas-Phase MXene Synthesis via Dry Halogen-Based Etching**
Co-authors: Hyunho Kim, Yury Gogotsi

Developing cost-effective methods of MXene synthesis is of the utmost importance for the industrial implementation of this rapidly growing family of 2D materials. The aqueous etching process typically used is time- and labor-intensive due to the many washing cycles needed to remove etchants from the MXene dispersion and later separate and collect delaminated MXene flakes. Aqueous etching with HF and HCl also results in an uncontrolled mixture of O, OH, F, and Cl surface terminations, which have a significant impact on the material properties. Recently, gas phase synthesis has been increasingly investigated as a potential alternative to traditional solution processing of MXenes. Gas-phase etching of MAX phases has the potential to save time, eliminate water waste, and produce MXenes with a single surface termination depending on the gas used. The present work investigates the ability of halogen-containing vapor to etch MAX phases and form MXenes.

Ben Reigle
Undergraduate Student
Purdue University
USA

Title: **Optimal Techniques for Nonlinear Optical Measurements of MXenes**
Co-authors: Jeffrey Simon, Colton Fruhling, Sasha Boltasseva, Vlad Shalaev

Nonlinear optical properties in MXenes have been measured with both the z-scan and I-scan techniques. In both techniques, the optical transmission through the sample is monitored as the fluence (intensity per area) is modulated. In the z-scan technique, the optical beam is focused to a point and the sample is translated through the focus, resulting in a changing beam area. In the I-scan technique, the intensity of the laser is modulated while the beam area is held constant. The I-scan technique has several advantages when working with emerging materials such as MXenes. Specifically, we can collect low-power reference transmission measurements to easily determine sample modification and consistently measure non-uniform samples. Using the I-scan technique,
we can also easily monitor the intensity-dependent reflection of the sample. This becomes important in MXenes such as Ti3C2Tx, which have a transition from dielectric to metallic optical properties in the near-infrared spectrum. When pumping the MXene, generated charge carriers could dramatically shift the crossover point, resulting in significant modulation in sample reflection. With the altered I-scan technique, we investigate the nonlinear absorption (NLA) and nonlinear reflection (NLR) of a variety of thin films of carbide MXenes containing transition metals Ti, Nb, and V in structures M4X3, M3X2, and M2X on fused silica and analyze the effects of sample thickness.

Benjamin Chacon
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Title: Zero-G Immune Impact of M4X3 MXenes
Co-authors: Laura Fusco, Linda Giro, Marco Orecchioni, Carlo Iorio, Lucia Gemma Delogu, Yury Gogotsi

MXenes are emerging as promising new candidates for a plethora of advancements in biomedical applications. Although their usefulness is proven, their biological properties, implications, and behaviors in extreme environments remain vastly unknown. The immune system of astronauts is significantly compromised by the microgravity environment encountered in spaceflight, rendering them susceptible to various diseases that pose a serious threat to their well-being. Immune cells exhibit remarkable sensitivity to gravitational changes, and the microgravity environment can impact diverse aspects of immune cell function through various mechanisms. In this work, we selected three different MXene compositions, Ta4C3, Nb4C3, and Mo2Ti2C3, with the aim to investigate their immune cell interactions in microgravity at a single-cell level. To achieve this, we utilize the high-dimensional technique of single cell mass cytometry by time-of-flight (CyTOF), in which it has previously been reported to detect these three MXenes without the need of additional material functionalization. We demonstrated that peripheral blood mononuclear cells (PBMCs) readily internalize these MXenes and identified no toxic effects to any of the immune cell subpopulations. We investigated the role of microgravity on the uptake of MXenes and viability of PBMCs both with simulated microgravity and as part of the European Space Agency's (ESA) 83rd parabolic flight campaign. Our findings show that microgravity reduces MXene uptake by immune cells while still maintaining full biocompatibility. These results illuminate the biological and immunological impact of MXenes under microgravity and open the door for further investigations on immune modulation and space medicine.

Bita Soltan Mohammadlou
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Title: MXenes Characterization using X-Ray Computed Tomography
Co-authors: Stefano Ippolito, Lingyi Bi, Alex Inman, James Fitzpatrick
MXenes represent a class of two-dimensional materials consisting of transition metal carbides, nitrides, and/or carbonitrides. They show unique physicochemical properties which make them promising candidates for applications in energy storage, catalysis, and electronics, due to their high conductivity and mechanical strength. Characterizing MXenes is essential for unravelling their functional properties and expanding their range of applicability in many technological areas. To explore the structural and functional characteristics of MXenes, researchers have utilized various characterization methods, such as XRD, Raman Spectroscopy, XPS, FTIR, TEM and others. However, the use of x-ray computed tomography for this purpose has not been explored yet. Nano-CT is a non-destructive imaging technique that uses X-rays to offer high-resolution three-dimensional imaging, enabling detailed analysis at both nano and micro scales. In this study, we exploit nano-CT to examine various MXene samples, including MXene-coated textiles, aerogels, and composites. They demonstrated how nano-CT images clarify the distribution of MXenes within textile fibers using various coating techniques. Additionally, this technique identifies structural defects such as pores and flake aggregations. This information is crucial for quality control and for informing strategies to enhance the properties of MXene composites, as well as supporting our understanding of the mechanical behavior of these materials under various loading conditions. Furthermore, the 3D porosity of MXene-based aerogels was examined, providing insights essential for applications in filtration and gas storage. Overall, nano-CT has proven to be an invaluable tool for advancing our understanding and development of MXene materials.

Bright Ngozichukwu  
Texas A&M University  
USA

Title: Long-Term Stability of Ti4N3Tx Measured Through Spectroscopic and Electrochemical Measurements  
Co-authors: Eugenie Pranada, Denis Johnson, Abdoulaye Djire

MXenes are gaining increasing attention in electrocatalysis due to their unique attributes like high conductivity, large surface area, and adjustable electronic structures. Despite this interest, most research focuses on the performance of newly synthesized MXenes, even though many are stored in solvents for extended periods. Currently, there is lack of understanding on how the electrocatalytic activity of MXenes is affected after prolonged solvent immersion. In this study, we examine the electrocatalytic behavior of a Ti4N3Tx nitride MXene over 230 days in various solvents, including water, ethanol, N-N dimethylformamide (DMF), dimethyl sulfoxide (DMSO), and acetonitrile (ACN). We assess its electrocatalytic performance through the hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR), tracking overpotential, Tafel slope, and limiting current density over this extended period. Our results show that the HER activity of Ti4N3Tx MXene remains stable after 230 days, with consistent overpotential and Tafel slope values across all solvents. Raman spectroscopy indicates only slight formation of TiO2, suggesting minimal degradation. However, the ORR behavior changes over the same period, with altered overpotential and Tafel slope. Notably, the number of electrons transferred per product molecule shifts from 4 to 2 in all solvents, indicating a change in the reaction mechanism. These findings suggest that the impact of solvents on MXene electrocatalysis varies depending on the type of reaction, likely influenced by the type and density of the terminal groups. These findings can be used to establish MXene-solvent relationships to broaden the utilization of MXenes and facilitate their integration in solvent-based applications.
C

Chandra Adhikari  
Fayetteville State University  
USA

Title: **First-principles Study on Two-Dimensional (Ti, Ta) Double-Transition Metal Carbide MXenes**  
Co-authors: Bhoj R. Gautam

Two-dimensional layered structured transition metal carbide, nitride, or carbonitride, called MXenes, have recently received great attention in the materials science community because of their excellent electrical conductivity, mechanical strength, volumetric capacitance, larger surface-to-volume ratio, high thermal conductivity, and chemical stability, which make them a promising candidate for electronic devices applications, sensors, energy storage devices, oxygen evolution reaction and hydrogen evolution reaction catalysts and so on. We theoretically study the stability of double transition metal carbides made up of titanium and tantalum, their electronic structures, magnetism, optical properties, and their applicability for electrode materials for energy storage applications. Study shows that the (Ti, Ta) double transition metal carbides are comparatively stable with a 1:1 atomic ratio. The magnetic properties of (Ti, Ta) double-transition metal carbides are different than those of single-transition metal carbides of Ti and Ta. This work is supported by the Department of Energy BES-RENEW award number DE-SC0024611.

D

Daryl Hurwitz  
University of Pennsylvania  
USA

Title: **Rapid Fabrication of Customizable MXene/Polydopamine (MXPDA) Electrodes**  
Co-authors: Spencer R. Averbeck, Raghav Garg, Flavia Vitale

In the evolving field of neuroelectronic implants, traditional rigid devices frequently cause tissue damage and immune reactions, while also lacking customization and having limited electrodes, restricting spatial resolution. Recent advances with MXenes specifically $\text{Ti}_3\text{C}_2\text{T}_x$, have shown excellent biocompatibility, electrical conductivity, surface hydrophilicity, mechanical properties and processability in aqueous dispersions, making them distinct among carbon-based nanomaterials. However, MXene structures suffer from mechanical fragility and vulnerability to oxidation. Herein, utilizing MXene (MXPDA) functionalized with polydopamine (PDA), enhances mechanical flexibility and environmental stability, fabricating flexible, customizable microelectrode arrays (MEA) using direct ink writing. The method allows rapid fabrication of MEAs tailored for patient-specific surgical settings, facilitating precise electrode placement for optimal neural
recording and stimulation. MXPDA inks exhibit superior rheological properties—~2.5 times higher zero-shear viscosity compared to MXene at the same concentration—and long-term stability compared to unmodified MXene inks. While displaying better electrochemical characteristics, with significantly higher charge storage capacity and more stable decay. These findings demonstrate that incorporating PDA not only enhances the viscosity and structural integrity of the inks but also improves their performance and longevity in vivo applications. By overcoming the challenges of existing neuroelectronic interfaces, such as stable and safe integration with soft tissues, this approach combines the unique properties of nanomaterials to produce scalable, high-resolution, and biocompatible devices. To eventually enable neuroelectronic implants to be fabricated within the operating room, significantly enhancing the accessibility and effectiveness of these devices.

David Kumar Yesudoss  
Texas A&M University  
USA  

Title: Electrochemical Synthesis of Formamide from CO2 and NH3 using Titanium Nitride (Ti2N) MXene  
Co-authors: Abdoulaye Djire

Formamide can be electrochemically synthesized using CO2 and NH3 as reactants. Amides play a crucial role in various industrial applications, including pharmaceuticals, agrochemicals, and polymers. The conventional method of amide production involves high energy consumption and leads to environmentally harmful outcomes. Recently, there has been a growing interest in electrochemically synthesizing organonitrogen chemicals from atmospheric pollutants. While copper (Cu) has been extensively studied as a catalyst for these processes, its limited tunability restricts the formation of a diverse range of C-N products. In contrast, MXenes, a novel class of 2D-layered materials, exhibit properties such as high surface area, hydrophilicity, and surface tunability, making them promising candidates for C-N coupling electrocatalysis. In this study, we employed a novel 2D Ti2N MXene as an electrocatalyst for the reduction of CO2 in the presence of NH3 in an alkaline environment, resulting in the production of formamide. The presence of NH3 facilitated nucleophilic attack on the carbocation intermediate, leading to the reduction of CO2 to formamide. The results were confirmed using 1H-NMR spectroscopy and were comparable to those obtained with the well-known Cu catalyst. Our current findings highlight the C-N coupling ability of Ti2N MXene, and lay foundation for the broader objective of coreducing CO2 and earth-abundant nitrogenous waste molecules, ultimately forming a diverse array of organonitrogen chemicals.

Deniz Cakir  
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USA  

Title: Synthesis and Characterization of Mo-Based MXenes via Atmospheric Pressure Chemical Vapor Deposition (APCVD)  
Co-authors: Yury Gogotsi
MXenes are two-dimensional transition metal carbides, nitrides, and carbonitrides with unique properties, including high conductivity and mechanical flexibility, making them promising materials for energy storage, catalysis, and electronics. Mo-based MXenes (Mo2CTx, Mo1.33Tx, etc.) stand out due to their distinctive electronic structure and superior electrochemical properties, making them suitable for lithium-ion batteries, supercapacitors, and electrocatalysis applications. This study investigates the direct synthesis of Mo-based MXene using precursors such as MoCl4 and CH4 in atmospheric pressure chemical vapor deposition (APCVD), offering insights into tailoring properties. Compared to the time-consuming selective etching method, APCVD significantly shortens synthesis times from over a week to just a few hours, enhancing the efficiency and scalability of MXene production. The synthesis and characterization of Mo-based MXenes via APCVD offer valuable insights into tailoring their properties for specific applications, contributing to the advancement of MXene-based technologies. APCVD enables shorter synthesis times compared to conventional methods, enhancing the efficiency and scalability of MXene production processes. It allows the synthesis of high-purity and highly crystalline MXene layers by adjusting various parameters for process optimization and evaluating outcomes through comprehensive techniques. X-ray diffraction (XRD) and scanning electron microscopy (SEM) provide detailed insights into the crystal structure, morphology, and composition of the synthesized Mo-based MXene. In conclusion, this study demonstrates that APCVD is an effective method for the synthesis of Mo-based MXene, and the obtained MXene could be a significant step in potential applications.

Dheeban Govindan
New Jersey Institute of Technology
USA

Title: Efficient Antiviral Air Filtration Based on MXene and MXene/Laser Induced Graphene Surface Coatings
Co-authors: Fangzhou Liu, Wen Zhang, Mengqiang Zhao

Removal of airborne viruses can lead to an improvement in public health, especially in hospitals, train stations, and airports. Removal of these infectious particles from contaminated air can be achieved with air filters, which usually trap the particles based on size. However, these filters are costly and accumulation and proliferation of microbes in the filter are associated problems. Here, we designed MXene-based surface coatings that can lead to enhanced biological effects. Uniform MXene-based surfaces were fabricated through spray coating on commercial air filters, with a limited increase in the pressure drop during air filtration. Compared to pristine air filters, the MXene-coated ones improved virus removal efficiency from 50~% to ~80%. Close to 100% removal of the viruses was achieved by applying a low voltage (< 5 V) or microwave to the MXene-based surfaces. This is ascribed to the excellent electronic conductivity and electromagnetic wave absorption properties of MXenes. The airborne virus removal performance can be further improved by the hybridization of MXenes with laser-induced graphene, which also achieved a negligible pressure drop during air filtration.
Two-dimensional (2D) transition metal carbo-chalcogenides (TMCCs) consist of a core early transition metal carbide with a chalcogen surface (e.g., S, Se, Te). These materials have a combination of high electrical conductivity, attributed to the presence of the core carbon layer, and high electrocatalytic activity, owing to their chalcogenide surface. These properties render them suitable for various applications, including use as active materials in batteries, supercapacitors, and electrocatalysis. Here, we describe the synthesis of 2D TMCCs via simple and scalable process. Initially, we obtained FexM2X2C (M: transition metal, X: chalcogen, C: carbon) using a solid-state synthesis method. Subsequently, we produced multilayer TMCCs (m-TMCC) using a room-temperature chemical purification procedure. We then introduced lithium between the layers of m-TMCCs either electro- or mechano-chemically. Finally, delamination of the layers was achieved by adding deionized water and sonication, allowing the use of the materials in forms such as colloidal dispersion, free-standing paper, or aerogel. Electrocatalytic measurements revealed the excellent electrocatalytic performance of 2D Ta2Se2C for hydrogen evolution reaction (HER), suppressing both mTa2Se2C and 2D TaSe2. 2D Ta2Se2C required an overpotential of about 264 mV for 10 mA cm-2 current density. It also demonstrated a Tafel slope of 91 mV.dec-1 and a large electrochemically active surface area (ECSA) of 780 m2.g-1 as a synergistic effect of the extensive surface area provided by few-layered or single nanosheets and the point defects in the structure like vacancies which increase the number of exposed active sites within 2D Ta2Se2C. Thus, TMCCs emerge as promising electrocatalyst candidates for HER.

MXenes are a family of two-dimensional transition-metal carbides and nitrides discovered at Drexel University in 2011 with a general formula of Mn+1XnTx, where M stands for an early transition metal (Ti, V, Nb, Mo), X stands in for either carbon or nitrogen, n = 1−3, with Tx representing surface terminations acquired through MXene’s top-down etching process such as −OH, −O−, and −F. They are biocompatible, conductive and possess a host of qualities ideal for medical applications. Kidney failure affects tens of thousands of people yearly and current dialysis technology is expensive, cumbersome and requires many liters of medically clean water. Sorption cartridge dialysis supplies portable and accessible dialysis without requiring liters of medical grade water or a dedicated facility. Herein we demonstrate how a lithium-free NaF MILD method etched Ti3C2Tx MXene could serve as the ideal adsorbent for the removal of urea and creatinine from a testing solution both in a dynamic adsorption column setup and a kinetic adsorption on small scale samples. With a
maximum reported removal of Urea at ~35 mg/g, the sorbent cartridges can be miniaturized to the size of a consumer smartphone. The effectiveness of Ti3C2Tx MXenes has been demonstrated for a panel of different toxins and cytokines this work expands on previous papers and shows improvements to the material and the ability to reuse any potential sorbent cartridge. This could lead to the development of reusable, eminently portable, effective at-home and on-the-go dialysis systems for people suffering from kidney damage, sepsis or acute poisoning.

Eric Vertina
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USA

Title: MXene Property Prediction via Deep Learning
Co-authors: Oren Mangoubi

MXene synthesis is too slow to explore the vast MXene property space - there are likely an infinite number of possible MXenes - necessitating the need for fast methods, such as machine learning methods, that can quickly predict properties and provide guidance to experimentalists. However, existing machine learning methods fail to account for atomic structure information that can be encoded by representing MXenes as graphs - constituent atoms as nodes and bonds between atoms as edges - potentially leading to lower property prediction accuracy. We introduce a novel method for predicting MXene properties which uses graph neural networks to predict target features from MXene graph structures and chemical formulas. Specifically, our model uses graph contrastive learning, a type of graph neural network method, to transform input features from a graph dataset to a lower-dimensional representation space that enables high-accuracy predictions for downstream machine learning models. We obtain the following RMSEs for downstream models predicting properties from an unpublished MXenes dataset: 0.418 J for Work Function, 0.518 eV$^{-1}$ for Density of States at Fermi Level, 21.65 N/m for Bulk Modulus, 0.067 for Poisson’s Ratio, 14.56 N/m for Shear Modulus, 35.66 N/m for Young’s Modulus, and an accuracy of 0.82% for Magnetic (T/F). We apply our method to predict important MXene properties which, to the best of our knowledge, have not been successfully predicted by existing deep learning methods that include atomic structure information as model input.

Fereshteh Rajabi Kouchi
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Title: High-Resolution Aerosol Jet Printed MXene Supercapacitor for Energy Storage Applications
Co-authors: Fereshteh Rajabi Kouchi, Tony Valayil Varghese, Naqsh E Mansoor, Shruti Nirantar, Myeong-Lok Seol, Nicholas McKibben, Josh Eixenberger, Hailey Burgoyne, Karthik Chinnathambi, Christopher E Shuck, Yury Gogotsi, Jessica E. Koehne, David Estrada
Wearable electronics demand the accelerated development of flexible energy storage devices to enable portability and avoid complex wiring. Additive electronics manufacturing can create lightweight, flexible, lowcost sensors and energy storage devices with complex geometries. However, the lack of multifunctional nanomaterial inks and the availability of diverse materials limit on-demand printing, and material selection is crucial because the printed device’s performance depends on the design, material, printing method, and postprinting process. MXenes, transition metal carbides, nitrides, and carbonitrides have gained considerable interest in energy conversion and storage applications due to their excellent electrical conductivity, rich surface chemistry, thermal conductivity, hydrophilicity, and superior dispersibility in various solvents. Aerosol Jet printing (AJP) is a promising technique for additive electronics manufacturing. AJP ink development requires tuning the ink rheology including viscosity, surface tension, and solid loading to obtain suitable fluid dynamic parameters for jetting the ink. In this study, we demonstrate the synthesis, characterization, and formulation of Ti3C2Tx nanomaterial ink using the high-resolution AJP technique, with a specific focus on supercapacitors for energy storage. We show that aerosol jet-printed MXene supercapacitors exhibit an areal capacitance of 67 mF cm-2, which is within the highest performance range for printed supercapacitors reported so far. These results highlight the potential of aerosol jet printing of MXene inks as a path towards on-demand manufacturing and rapid prototyping of low-cost, efficient, and flexible printed electronic and electrochemical devices.

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Title: Enhancing Na-S Battery Performance by Controlling the MXene Composition
Co-authors: Pawel Michalowski, Ruocun (John) Wang, Tetiana Hryhorchuk, Moses Abraham, Kate Harrison, Vibha Kalra and Yury Gogotsi

Room-temperature sodium sulfur (Na-S) batteries emerge as promising candidates for long-term, reliable, large-scale energy storage, leveraging the abundance and widespread availability of sulfur and sodium resources. However, challenges such as sluggish Na ion transport kinetics, severe polysulfide shuttling, and slower polysulfide conversion kinetics compared to lithium counterparts underscore the need for tailored material development for Na-S batteries. The utilization of conductive MXenes as cathode hosts and additives has shown potential in enhancing Na-S battery performance by chemically restraining polysulfides and expediting their conversion kinetics. Nevertheless, the efficacy of this enhancement hinges upon the MXene composition, an area that requires further investigation. Our study, involving a combination of spectroscopic analyses (UV-Vis, inductive coupled plasma optical emission spectroscopy, secondary ion mass spectroscopy, and X-ray photoelectron spectroscopy), electrochemical characterizations, and theoretical computations, elucidates the influence of M3X2Tx MXenes' transition metal (M) outer layer (Ti and Mo) and carbon (X) layer (oxygen and nitrogen doping) on polysulfide adsorption and electrocatalytic conversion to mitigate the polysulfides shuttling effect for advancing high-performance sodium-sulfur batteries.
**Mo2Ti2C3 MXenes as combinatorial nanoplatforms for cancer therapy**

Co-authors: Berfin Illyada Ozturk, Benjamin Chacon, Ahmet Ceylan, Yury Gogotsi, Acelya Yilmazer

Emerging strategies for cancer treatment encompass immunotherapy, gene therapy, photodynamic therapy (PDT), and photothermal therapy (PTT), all of which have demonstrated or hold the promise of enhancing therapeutic efficacy. MXenes, thanks to their intrinsic physiochemical properties, have been recognized as extremely promising candidates for cancer treatment. In this work, we analyzed the photothermal (PTT) or photodynamic (PDT) therapeutic characteristics of Mo2Ti2C3, a two-dimensional nanomaterial belonging to the MXene family. Furthermore, detailed in vitro analysis was conducted to determine if MXenes was able to trigger any immunotherapeutic response through inducing immunogenic cell death. In vitro and in vivo results showed that Mo2Ti2C3 MXenes were able to induce effective PTT and PDT in a breast cancer model. Based on the transmission electron microscopy imaging, MXenes-induced PTT resulted in immunogenic cells death of breast cancer cells and phagocytosis in a dendritic cell line. To summarize, it is suggested that Mo2Ti2C3 MXenes can be potential nanoplatforms to offer a combinatorial therapeutic approach for breast cancer.

**Spatial Transcriptomic Evaluation of MXene Quantum Dot-Treated Tumors**

Co-authors: Recep Uyar, Dogantan Celik, Ahmet Ceylan, Yury Gogotsi, Lucia Gemma Delogu, Sanjiv Dhingra, Acelya Yilmazer

Nanomedicine holds promise in revolutionizing tumor treatment strategies. However, the intricate tumor microenvironment (TME) poses challenges, housing diverse immune cell populations alongside tumor cells. Despite advancements in nanoparticle-based therapies, understanding the nuanced interactions within the TME remains elusive. In this study, we employed spatial transcriptomics to unravel the gene expression landscape and discern the impact of nanoparticle exposure on immune cell dynamics within the TME. Utilizing Ti3C2Tx MXene quantum dots (MQDs), we tracked their distribution in orthotopic breast cancer models. Our findings revealed distinct responses in tumor and immune cells contingent upon MQD accumulation, unveiling a tumor-suppressive phenotype in regions with variable MQD accumulation. Furthermore, pathway analysis and cell deconvolution unveiled alterations in B cells and neutrophils induced by MQDs, including recruitment, activation, and neutrophil degranulation. Through spatial transcriptomics, we delineated the molecular and cellular changes instigated by MQDs within the TME. Future studies leveraging spatial omics approaches with diverse nanoparticles hold promise in refining nanotherapeutic design for enhanced efficacy.
MXenes are a family of 2D transition metal carbides, nitrides, and carbonitrides with unique properties. MXenes have manifested promise for a wide range of biomedical applications, including regenerative medicine, infection treatment, cancer treatment, immune modulation and labeling. Mesenchymal stem cells (MSCs) are multipotent stem cells that can migrate to the site of injury, help regulate immune homeostasis by immunomodulation and repair or regenerate the tissues. MSCs are widely used in regenerative medicine and medical applications. Since they have a migration capability, labeling MSCs is essential to track the effect of the MSCs for both in vivo and biomedical applications. Previously, Nb4C3Tx, Mo2Ti2C3Tx, and Ta4C3Tx MXenes were reported for label-free detection with single-cell mass cytometry by time-of-flight (CyTOF) and immune profiling. Herein, we tested Nb4C3Tx, Mo2Ti2C3Tx, and Ta4C3Tx MXenes cytotoxicity, proteomics, and labeling of primary mouse MSCs. Cytotoxicity assay showed that Nb4C3Tx, Mo2Ti2C3Tx, and Ta4C3Tx MXenes are non-toxic to the MSCs. Proteomic analysis of MXene-treated MSCs revealed that developmental pathways are activated during Ta4C3Tx administration, indicating differentiation of the MSCs, while Nb4C3Tx administration did not activate the developmental pathways and showed similar results with control. MSCs treated with Nb4C3Tx, Mo2Ti2C3Tx, and Ta4C3Tx MXenes can be detected with CyTOF without performing further nanomaterial modification. We proved that MXenes could be used as a facile, non-toxic labeling agent for MSCs.

Stretchable electrodes possessing strain-insensitive properties of electrical conductivity, mechanical durability, electrochemical activity are central to various advanced technologies based on stretchable electronics. However, conductive electrode materials (e.g., metals and metal oxides) are usually intrinsically brittle, and cracks on the electrode will be generated under small stretching. Additionally, the conventional one-factor-at-a-time (OFAT) method for stretchable conductor fabrication is time-consuming due to the complex relationships between materials and structural
design. Here, we show a robotic/machine learning (ML) integrated workflow including feasible area definition, artificial neural network (ANN)-based active learning loops, SHapley Additive exPlanations (SHAP) and finite element simulation to accelerate the discovery of MXene/single wall carbon nanotube (SWCNT)-based ultrastretchable conducting layer. Under the guidance of suggested parameters from well-trained ANN model, a MXene/SWCNT-based conducting layer with excellent electromechanical performance was built, where MXene provides the high electric conductivity and SWCNT provides the high stretchability. After coating a thin-layer gold, we fabricated a stretchable gold electrode with metal-like conductivity (2.2 × 10^7 S·m), exceptional stretchability with tiny resistance response (<10% resistance increases under 900% strains), and enduring electromechanical stability (600% strains over 50,000 cycles). Furthermore, we made a stretchable Zinc-MnO2 battery with strain-resilient specific capacities and columbic efficiencies under 300% strain. Our methodology consisting of robot-assisted experiments, data science, and simulation tools, offers an unconventional design platform to accelerate the invention of strain-insensitive stretchable electrodes with customizable opportunities.

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Title: Scalable Synthesis of High-Quality Ti2CCl2 MXene by Chemical Vapor Deposition (CVD)  
Co-authors: Ben Davis, Teng Zhang, Yasunori Hioki, Yury Gogotsi

The synthesis methods for the MXene materials family have been developed from selective chemical etching using acid to Lewis-acid molten salt (LAMS) method, and chemical vapor deposition (CVD) as well as direct synthesis over the last 13 years. The newest CVD approach can provide the highest quality crystal thanks to the bottom-up assembly from their molecular precursor. However, the yield of CVD MXene using Ti foil is rather limited compared to top-down approaches starting from the MAX phase precursor. Here, we report a scalable CVD method using Ti powder instead of Ti foil. The powder allows a larger amount of MXene product in one batch using a 1-inch tube furnace without complicated parts. The formation of Ti2CCl2 MXene is formed on the surface of Ti powder particles, with a superior crystal quality based on Raman spectroscopy. The produced MXene-covered-Ti powder can be further processed with solvent and salt to obtain delaminated CVD-Ti2CCl2 which will be compared with acid-Ti2CTx and LAMS-Ti2CCl2. Our finding offers a cost-effective and scalable synthesis of high-quality Ti2CCl2 that can accelerate further advance and development of MXene applications.

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City University of Hongkong  
China

Title: Electrochemical Properties of Mo4V6C4T10, MXene in Aqueous Electrolytes  
Co-authors: Faisal Rehman, Mohit Saraf, Teng Zhang, Ruocun Wang, Tridip Das, Zhengtang Luo, Yury Gogotsi, Kaili Zhang
MXenes represent the most recently discovered and least studied sub-family of out-of-plane ordered double transition metal carbides with 11 atomic layers, probably the thickest of all 2D materials. Molybdenum (Mo) and vanadium (V) in Mo\textsubscript{4}VC\textsubscript{4}T\textsubscript{x} offer multiple oxidation states, making this MXene potentially attractive for electrochemical energy storage applications. Herein, we evaluated the electrochemical properties of Mo\textsubscript{4}VC\textsubscript{4}T\textsubscript{x} free-standing thin films in acidic, basic, and neutral aqueous electrolytes and observed the highest gravimetric capacitance of 219 F g\textsuperscript{-1} at 2 mV s\textsuperscript{-1}) in a 3 M H\textsubscript{2}SO\textsubscript{4}. Further, we investigated the intercalation states of four different cations (H\textsuperscript{+}, Li\textsuperscript{+}, Na\textsuperscript{+}, and K\textsuperscript{+}) in MXenes through \textit{ab initio} molecular dynamics (AIMD) simulation and used density functional theory (DFT) calculations to assess the charge storage mechanisms in different electrolytes. These studies show hydrated Li\textsuperscript{+}, Na\textsuperscript{+}, and K\textsuperscript{+} ions forming electric-double layer (EDL) at the MXene surface, which is the primary charge storage mechanism. This work shows the promise of Mo\textsubscript{4}VC\textsubscript{4}T\textsubscript{x} MXene for energy storage in aqueous electrolytes.

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USA

Title: \textbf{The Analysis of Paramagnetic Defect Centers in Ti3C2Tx}  
Co-authors: Yuan Zhang, Ahmet Güngör, Emre Erdem, Yury Gogotsi

The need for having energy storage devices having higher energy and power density is increasing to store the intermittent energy acquired from clean energy sources such as wind, hydro, and solar power. Supercapacitors are advantageous as energy storage devices due to their high power density and long cycle life. The selected electrode materials carry great importance in the electrochemical performance of supercapacitors and there are a lot of ongoing research on using MXene as electrode material in supercapacitors. It is known that the defects can affect both electronic conductivity and chemical stability of the synthesized Ti3C2Tx, however, there is limited information on the paramagnetic defect centers that exist in the Ti3C2Tx. This work aimed to focus on the analysis of paramagnetic defect centers in Ti3C2Tx, Ti3C2Tx were synthesized at different HF concentrations and the paramagnetic defect centers were analyzed using X-Band EPR Spectroscopy. This work is anticipated will pave the way for further analysis on different types of MXenes as well.

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Title: \textbf{Highly porous Ti3AlC2 MAX-phase synthesis for MXene with enhanced properties}  
Co-authors: Ivan Baginskiy, Serhii Dukhnovskyi, Veronika Kaurkovska, Margaryta Potashna, Veronika Zahorodna, Stefano Ippolito, Oleksiy Gogotsi, Yury Gogotsi
MXenes, large family of 2D carbides and nitrides, nowadays are among the most studied nanomaterials worldwide. MXenes are synthesized by selective wet-chemical etching of ternary carbides and nitrides of early-transition metals - layered ceramic materials MAX-phases that were initially developed for structural and high-temperature applications. The requirements for MAX-phases as a precursor for MXenes differ drastically from those of structural MAX materials. However, MAX phase synthesis has not been optimized yet for MXene manufacturing. Here we demonstrate developed highly porous Ti$_3$AlC$_2$ (porosity about 70%) from an inexpensive titanium sponge instead of expensive highly pure titanium powder and explain the mechanisms of reaction sintering and formation of porous MAX phase. MAX phase sintered in such way can be easily ground into individual grains without time-consuming crushing and milling steps. Synthesis yield of Ti$_3$C$_2$Tx MXene from porous Ti$_3$AlC$_2$ was 65%. MXene obtained from this MAX phase, Ti$_3$C$_2$Tx, shows larger flake size and higher electrical conductivity up to 16 500 S/cm in thin films, compared to the materials produced from the costly fine titanium powder. The proposed approach may apply to the synthesis of other Ti-based and beyond-Ti MAX phases.

Acknowledgement: Supported by European Commission under HORIZON-Europe projects #101131147 “ESCUAPE”, #101086184 “MX-MAP”, #872370 “SALSETH”.

James Fitzpatrick
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Title: Multifunctional MXene-Polymer Composites: Controlling Structure and Properties
Co-authors:

MXenes, a family of two-dimensional (2D) transition metal carbides and nitrides, have attracted significant attention in recent years for their unique optical, electronic, and chemical properties, to name a few. These nanomaterials have a general formula of Mn+1XnTx where M is a transition metal, X is carbon and/or nitrogen, and Tx represents a variety of surface terminations. MXenes can be tailored for an incredibly broad array of applications, but are still often hindered by manufacturing, stability, and mechanical challenges. Many of these challenges can be overcome by integrating the 2D material into polymer matrices, leading to composites with distinct properties that can serve specific or multiple functions. While many such materials have been fabricated, research into composite systems is still lacking in this field. Challenges such as dispersibility and interfacial compatibility persist with many MXene composites, hindering further progress in creating high performance materials. Herein, solution processing methods to fabricate MXene polymer composites for multifunctional applications are explored. The roles of MXene synthesis, delamination, and composite processing are investigated to determine effects on composite structure and resultant properties. By carefully selecting process parameters, various composites with broad ranging electrical, optical, and mechanical properties can be formed to serve a myriad of purposes. Dielectric properties of polymers can be modified or enhanced by MXene integration as well, leading to piezoelectric, pyroelectric, or highly capacitive functionalities. The work
documented here opens the doorway for a new generation of composites that can be produced effectively and efficiently.

Jesus Medina
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Ireland

Title: 3D printed Silicon/MXene electrode for enhanced Sodium-Ion batteries
Co-authors: Kavin Arunasalam, Dr. Apostolos Koutsioukis, Prof. Valeria Nicolosi.

Silicon stands out as a promising material for negative electrodes in sodium-ion batteries due to its high theoretical capacity, low working potential, and abundance. However, challenges such as volume expansion, unstable solid electrolyte interphase, low conductivity, and capacity retention hinder its performance. Attempts to mitigate these issues include strategies such as particle size reduction, creating porous structures, and incorporating conductive materials. MXene, a class of 2D transition-metal carbide and nitride, in particular, Ti3C2Tx, shows promise in enhancing the electrical conductivity and mechanical properties of silicon particles. Previous studies have demonstrated MXene’s effectiveness as a conductive additive for metal-ion battery electrodes, improving structural stability and enabling the fabrication of thick electrodes for high-energy applications [1]. We explored the synergy between MXenes and 3D printing technologies to further enhance the mechanical properties and ion diffusion pathways within the electrode structure. 3D printing has emerged as an alternative to conventional electrode fabrication techniques due to its versatility in designing electrodes at a macroscopic level. Through this approach, we aim to enhance the porosity and conductivity of electrodes, facilitating increased exposure of active materials for ion intercalation. Electrochemical and physical characterization techniques such as SEM, AFM, and XRD were employed to evaluate the performance of the resulting electrodes. This research presents a novel approach to optimizing sodium-ion battery electrodes, leveraging the high capacity of silicon with the unique properties of MXene and the versatility of 3D printing technology.


Juan Lopez Luna
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Title: Compulsions detection with MXene-based electromyography
Co-authors:

Obsessive-Compulsive disorder (OCD) is a mental and behavioral disorder characterized by the presence of persistent and intrusive thoughts (obsessions) and repetitive behaviors (compulsions). OCD affects 1.2% of U.S. adults, with reported impairment in half of the cases. Moreover, approximately 40% of OCD patients do not respond to treatment. Deep Brain Stimulation (DBS) has emerged as a potential therapeutic solution. Nevertheless, response rates outcomes are limited and are primarily done in an open-loop fashion. Studies have reported that close-loop stimulation yields promising outcomes for treating OCD and binge eating. However, the monitoring requirements
significantly impact the battery life of the implanted device. Here, we report using a wearable with MXene electrodes to continuously acquire high-quality neuromotor signals at the forearm to detect effective compulsions in patients with mild to severe OCD. We built a sleeve with detachable snap buttons fabricated using hydroxylated PVA aerogel templates dip-coated in Ti3C2Tx MXene arranged equidistant across the forearm. Using a custom-made device, we captured eight single-ended electromyography (EMG) channels and transmitted the data via Bluetooth. The single-patient data was acquired in a clinical setting; the protocol consisted of equally spaced blocks of symptom provocation, followed by effective or ineffective compulsions and a comparison movement. We developed a machine-learning algorithm that detected effective compulsions with 80% accuracy. Together, this work is a proof-of-concept for a MXene-based wearable capable of detecting effective compulsions, serving as a first-in-class objective symptom detection platform using EMG with the potential for closing the loop in DBS systems for treatment of OCD.

Karamullah Eisawi
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Title: MXenes Hybrids: Potential iodine gas sorbents in nuclear waste
Co-authors: Brian Riley and Michael Naguib

Nuclear energy is the primary source of low-carbon power supply worldwide. However, the environmental risk posed by the release of volatile, toxic radioactive iodine gases is critical. Research into novel porous sorbent materials for capturing radioactive iodine gas has expanded rapidly over the past decade. MXenes, a family of 2D transition metal carbides, nitrides, and carbonitrides, display fascinating physical and chemical attributes, including customizable surface terminations and interlayer spacing, a large surface area, and outstanding electronic conductivity. In this study, we propose MXene hybrids as promising sorbents for radioiodine capture. We synthesized Ag-Ti3C2Tx hybrids by growing Ag nanoparticles on the surface of Ti3C2Tx MXene sheets through the direct reduction of AgNO3 in colloidal dispersion of delaminated Ti3C2Tx in water. Our results revealed that Ag-Ti3C2Tx hybrids that exhibit an iodine uptake exceeding 0.62 (iodine)/g(sample), suppressing both silver mordenite zeolite (AgZ) and silver-functionalized silica aerogel (AgAero). These findings highlight the potential of MXene hybrid material as an efficient sorbent for capturing iodine gas.


Kateryna Shevchuk
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MXenes, a large family of two-dimensional materials, have attracted a lot of interest due to their large chemistry space and diverse chemical, electrical, mechanical, and optical properties. MXenes follow the general formula Mn+1XnTx (n = 1, 2, 3, or 4) with M representing an early transition metal, X—carbon and/or nitrogen, and T—surface terminations (=O, –OH, and –F). In particular, MXenes’ metallic conductivities and redox-active surfaces make them attractive for electrochemical energy storage. Recently, we demonstrated that partial oxidization of Ti3C2Tx MXene by cycling the material at 1.2 V vs. Ag wire led to enhanced pseudocapacitance in water-in-salt electrolytes. However, there is a fine line between partial oxidation of Ti3C2Tx MXene and complete oxidation that leads to the formation of titania and carbon. The extent of oxidation is difficult to measure with conventional X-ray and electron-based techniques. This work focuses on using in situ electrochemical Raman spectroscopy to analyze the oxidation processes in Ti3C2Tx MXenes at the high anodic potential. Raman spectroscopy has proven to be a powerful technique for detecting the natural oxidation of Ti3C2Tx MXenes. The ability to perform Raman spectroscopy in situ during electrochemical reactions will allow us to expand our knowledge of MXene electrochemistry and its partial oxidation. The findings will help achieve higher energy density in MXene-based energy storage devices.

Kuanysh Zhussupbekov
Trinity College Dublin
Ireland

Title: **Self-assembled moiré superstructure of Ti3C2Tx MXene**
Co-authors: Kuanysh Zhussupbekov, Andrea Cabero del Hierro, Samuel Berman, Dahnan Spurling, Ainur Zhussupbekova, Stefano Ippolito, David D. O'Regan, Igor V. Shvets, Yury Gogotsi and Valeria Nicolosi

Nanoscale periodic moiré superlattices within two-dimensional (2D) heterostructures offer an opportunity to exploit new electronic and atomic characteristics that are not present in their pristine 2D and bulk counterparts.1–6 However, a detailed understanding of the atomically reconstructed moiré superlattice and the resulting novel electronic structure on the microscopic level is currently lacking in many systems. This understanding is crucial for gaining fundamental knowledge and mastery over interconnected moiré phenomena. In this study, we thoroughly examine and compare the self-assembled moiré superlattices of Ti3C2Tx MXene through experimental scanning tunneling microscopy and spectroscopy, accompanied by first-principles simulations of MXene moiré superlattices. We examined three distinct self-assembled moiré patterns with wavelengths of approximately 2.32 nm, 2.17 nm, and 1.12 nm. Our experiments reveal that the moiré superstructure with wavelengths of 1.12 nm exhibits a non-monotonic behavior in the moiré periods within the conduction band. Our findings shed light on MXene moiré superstructures which may find use in quantum devices.
Investigation of Titanium Nitride MXene Charge Storage Mechanism in Nonaqueous Electrolytes

Co-authors: Abdoulaye Djire and Mark Barteau

The increasing demand of renewable energy requires innovation of energy storage devices. The ideal device must have high energy and power densities. Novel 2D materials, such as MXenes, show promise in meeting both requirements due to intercalation mechanisms. Here, we hypothesize that an intercalation reaction can occur in non-aqueous electrolytes on a titanium nitride MXene, with a large voltage window that enables high energy density. To this end, we have investigated non-aqueous electrolytes based on lithium and sodium salts using a Ti4N3Tx electrode. We used 1M lithium hexafluorophosphate (LiPF6) and sodium hexafluorophosphate (NaPF6) in 1:1 volume dimethyl carbonate and ethylene carbonate to further understand the intercalation chemistry of the Li and Na ions, respectively. In both media, cyclic voltammetry (CV) experiments performed on the electrode displayed a wider voltage window relative to aqueous systems, reaching 3V, while maintaining the intercalation chemistry. Galvanostatic charge discharge (GCD) and electrochemical impedance spectroscopy (EIS) experiments were performed to gain further information on the capacity, energy density, and reaction characteristics. Unexpectedly, irreversible side reactions that led to the formation of Li3N species in the solid electrolyte interface (SEI) were observed in the Li-based electrolyte. This prevented the long-term cycling of the electrode. On the other hand, stable cycling was achieved in the Na-based electrolyte exhibiting more promising charge storage capability. In summary, MXenes, especially nitrides, could play a significant role in electrochemical charge storage, but further studies have to be performed to understand the choice of the intercalation ion and its mechanism.

How does sodium polyphosphate used to prevent Ti3C2Tx degradation in water impact electronic properties of thin films?

Co-authors: Andrew M. Fitzgerald, Dawei Liu, Tom Kohen, Mary Qin Hassig, Kateryna Kushnir Friedman, Jeannine M. Coburn, Joshua R. Uzarski, Michel W. Barsoum, Ronald L. Grimm, Lyubov V. Titova.

Titanium carbide, Ti3C2Tx, where Tx stands for surface terminations -OH, -F, and -O, is the first discovered member of 2D MXene family [1]. Its hydrophilic nature enables fabrication of high-quality thin films from Ti3C2Tx aqueous suspensions. High conductivity of resulting films makes them attractive for flexible electronics, electromagnetic shielding, and THz devices [1-3]. However, degradation of Ti3C2Tx in aqueous environments due to oxidation and hydrolysis presents a challenge. Capping MXene flake edges and defects with sodium polyphosphate improves chemical
stability in solution [4,5]. Here, we investigate the effect of sodium polyphosphate on the electronic properties of thin films using a four-point probe measurement of DC conductivity and time-domain THz spectroscopy measurement of complex frequency-resolved conductivity [2,6]. We find that polyphosphates improve MXene conductivity, possibly acting as bridges that facilitate interflake transport and passivating defects that act as carrier traps.

Approved for public release

Leopoldo Posada Escobar
University of Maryland
USA

Title: Impact of Surface Modifications on the Physiochemical Properties of Ti3C2Tx MXene
Co-authors:

MXenes, a recently discovered family of two-dimensional transition metal carbide/nitride nanomaterials, have garnered considerable attention from researchers due to them exhibiting various advantageous properties such as high electrical conductivity, mechanical sturdiness and flexibility, and high colloidal stability in aqueous solutions. As a result of this, MXenes have found applications in many fields, such as energy storage, smart textiles, flexible electronics, optoelectronics, catalysis, filtration devices, and sensors. Due to the success MXenes have had in these and many other fields, there has been a recent shift towards using these nanomaterials in biomedical and environmental applications. However, it has been recently discovered that when solutions of MXenes are made in more complex media (e.g., buffers), which are ubiquitously used in these fields, they tend to have adverse effects on the physiochemical properties of MXenes, such as reducing their electrical conductivity and increasing surface oxidation. Therefore, this project aims to develop a molecular level understanding of the complex interactions that occur at the MXene surface when these materials are suspended in complex media. Simultaneously, we intend to develop a strategy to modify the MXene surface with the effect of reducing the detrimental effects produced when suspended in complex media by using a combined computational and experimental approach.

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Missouri University of Science and Technology
USA

Title: MXene-based Stimuli-Responsive Transdermal Patches for Wound Healing
Co-authors: Lev Suliandziga, Fateme Fayyazbakhsh, Vadym Mochalin, Yue-Wern Huang, Ming Leu
In this presentation, we report our results on novel stimuli-responsive hydrogel-based transdermal patches (HTPs), for alleviation of inflammation and localized drug delivery towards wound healing. For purposes of this study, a titanium carbide MXene was incorporated into a gelatin-alginate hydrogel mixture. Following addition of ibuprofen (IBU) into the mixture, the resulting bioink was fabricated into HTPs using a 3D printer and characterized. Drug release was induced through NIR irradiation of the transdermal patches and quantified using UV-VIS spectroscopy. The biocompatibility, anti-inflammatory properties, and the HTP’s effects on wound healing were assessed, using human dermal fibroblasts as an in-vitro model. Included in the presentation are the experimentally derived correlations between the degree of external stimuli and the rate of drug release, as well as the immunomodulatory activity of MXene-doped HTPs. Our findings position MXene-incorporated hydrogels as promising candidates for on-demand drug delivery, with simultaneous alleviation of inflammatory response, in field of smart wound care.

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Italy

Title: An Alternative Cell Labeling System Based on the New Two-Dimensional Nanomaterials MXenes
Co-authors: Laura Fusco, Arianna Gazzi, Chacon Benjamin, Christopher Eugene Shuck, Marco Orecchioni, Klaus Ley, Yury Gogotsi, Lucia Delogu

Transition metal carbides and nitrides (MXenes), are a novel family of 2D nanomaterials rapidly growing as multimodal nanoplatforms in biomedicine. Tracking and labeling of biological processes using biocompatible contrast agents over a certain period of time is vital for precise diagnosis and treatment. Over the past two decades, cell labeling strategies have remained the same, with the same critical technological limitation: a lack of chemical versatility. Moreover, none of the current cell labeling tools can be applied with single-cell mass cytometry by time-of-flight (CyTOF), a disruptive technology in research and the clinic that is already replacing flow cytometry worldwide. To date, novel methods are tremendously needed in translational medicine to enable cell labeling/tracking by single-cell mass cytometry. Using MXenes as a model, we propose a versatile multiplexed label-free single-cell detection strategy based on CyTOF and ion beam imaging by time-of-flight (MIBI-TOF). This strategy, Label-free sINgle-cell tracKing of 2D matErials by mass cytometry and MIBI-TOF Design (LINKED), enables nanomaterial detection and simultaneous measurement of multiple cell and tissue features.

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Title: Colorful MXene inks for multifunctional textiles
Co-authors: Tetiana Hryhorchuk, Danzhen Zhang, Kseniiia Vorotilo, Bita Soltan Mohammadlou, Genevieve Dion, Yury Gogotsi

Textiles are the ultimate wearables, providing 24/7 next-to-skin coverage of large areas of our body. They present large surface areas to host sensing devices. Great effort has been made to impart
electronic properties - movement tracking, biological signal monitoring, and actuation functions for haptic interactions—by incorporating conductive materials into traditional textiles. However, these metal and carbon-based conductive materials not only limit the hues to silver, black, and grey but also require a large amount to be deposited for sufficient electrical conductivity—an approach that makes these textiles dull and harsh, deviate from the vibrant and comfortable textiles we love and experience every day. MXenes could pose a solution. MXenes are a family of two-dimensional transition metal carbides and nitrides with the highest electrical conductivity among solution-processible nanomaterials. MXenes exhibit distinct colors from green, blue to purple, gold of different shades depending on the transitional metal(s) present (e.g., Ti, V, Nb, Mo, and Cr) and their structuring. Moreover, the functional groups on the surfaces of MXenes allow them to establish strong interactions with the substrates, making them ideal conductive additives for durability and scale. Here, screen printing—a widely adopted technique in the textile industry—was demonstrated as an economical method for faithfully replicating MXene colors and achieving high conductivities on fabrics. Moreover, with the patterning capability of screen printing, different MXenes can be carefully placed and combined for various smart textile applications, such as multispectrum camouflage.

Liya Gebemedhin
Addis Ababa University
Ethiopia

Title: First-Principle Study of Graphene/MB2 (M = Fe, Mo) Vander Waals Heterostructures as Anode Materials in Rechargeable Lithium-Ion Batteries
Co-authors: Dr. Yedifana Setarge

The design of novel high-performance electrode materials are crucial to the advancement of next-generation energy storage systems. We present a variety of two-dimensional transition metal borides (MBenes)-based hetero-structures based on first-principles density functional theory, particularly B2Fe/graphene, graphene/B2Mo, graphene/B2Fe, and B2Mo/graphene, for application in lithium-ion battery anodes. Thermodynamic stability, structural, and electrical characteristics, as well as performance, are explored in lithium ion batteries (LIBs) with all heterostructures. The study went on to determine formation and adsorption energies using van der Waals forces in the DFT+D3 framework, as well as intermediate interlayer interactions. We investigated the electrochemical characteristics, including open circuit voltage (OCV) ranging from 0.1 to 2 V and theoretical capacities of up to 1040.1 mAh/g of B2Fe/graphene and 693.4 mAh/g of B2Mo/graphene, to illustrate the promise of these hetero-structures as anode materials. The MBene-based hetero-structure of B2Fe/graphene (-3.154 eV) exhibits more negative Li adsorption energies than the remaining heterostructures and better electronic conductivities. The metals with excellent electronic and ionic conductivities, DFT analysis, and CI-NEB technique estimates of lithium-ion mobility and diffusion rates demonstrate the efficiency of these materials. In particular, graphene/B2Mo has reduced energy barriers, indicating greater performance along the (001) plane. These findings are critical for the development of effective lithium intercalation batteries, emphasizing the importance of material composition and diffusion paths.

Lorena Manzanares
Ludwig Maximilians Universität
Title: **MXene interfaces for single-molecule biosensing**  
Co-authors: Lorena Manzanares, Dahan Spurling, Alan Szalai, Ece Büber, Tim Schröder, Valeria Nicolosi, Philip Tinnefeld

MXenes have primarily demonstrated their potential in biomedical fields as biomaterials, notably in dialysis and cardiac tissue engineering. Our work shifts the focus of MXenes within the biological context to a more molecular perspective, as we explore these materials for single-molecule biosensing, addressing fundamental aspects of fluorescence and biomolecular assemblies at MXene interfaces. Using single-molecule fluorescence confocal microscopy and DNA origami nanopositioners, we first explored the distance-dependent fluorescence intensity and lifetime of an emitter2 (ATTO 542) placed on transparent thin films made of spincoated Ti3C2Tx MXene 2D flakes.3 Each DNA origami structure carried a single dye molecule at predetermined heights. We developed a specific immobilization chemistry for DNA origami nanostructures based on the interaction between glycine and MXene, allowing precise orientation control on the surface. MXenes were found to quench the fluorescence of a dye located between 1 nm and 8 nm following a distance dependence of d-3, consistent with other transparent conductors.4,5 In contrast to other surfaces, these materials display ultrahigh axial sensitivity at short distances. We recently probed MXenes' utility in sensing single dye-labeled lipids in supported bilayers, serving as model cell membranes. By detecting sub-nanometer changes within the 5-nm-thick membranes, MXenes might reveal molecular aspects of certain diseases, drug-membrane interactions, and more. At a more basic level, we can gain a deeper understanding of lipid bilayers, providing experimental validation for computational findings.


Magdalena Zywolko  
PhD Student, Mercedes Benz  
Germany

Title: **MXene-enabled electrodes for wearable aqueous batteries**  
Co-authors: Alex Inman, Kyle Matthews, Ruocun (John) Wang, Lingyi Bi, Yury Gogotsi

The growing demand for connectivity and access to real-time information requires innovative solutions to improve the quality of life through wearable technologies. By embedding functionalities into fabrics and garments, everyday clothing can be transformed into textile-based devices (so-called electronic textiles or “etextiles”). While research efforts exist in textile-based energy storage for powering on-garment devices, the demonstrated applications have been confined to simple devices like LCD displays and LEDs, drawing negligible current and having limited applicability. The research on Lithium-ion batteries (LIBs) focuses on established form factors (e.g., jelly roll, pouch cell) encased in bulky and rigid metal housings, rendering them impractical for real-world wearable applications where batteries should be flexible and conformal to the human figure. This research
introduces MXenes, two-dimensional (2D) nanomaterials conductive and compatible with natural fibers, as a promising material for textile-based LIBs. MXene nanoflakes dip-coated onto textile substrates provided mechanically stable structural support for the active material and formed an electron pathway. The resulting flexible textile-based electrodes eliminated the need for current collectors, reducing the overall mass and thickness while maintaining the same capacity. Utilizing these electrodes, we assembled battery pouch cells encapsulated within a soft, self-adhesive linen patch that adheres comfortably to textiles on the human body. A proof-of-concept battery was integrated with commercially available microelectronics capable of collecting accelerometer data and wirelessly transmitting information in real-time. The proposed technology demonstrates significant potential, particularly in the wireless monitoring of patient’s vital signs, paving the way for lightweight and human-friendly textile-based electronics.

Marina Smirnova
Adam Mickiewicz University
Poland

Title: From Synthesis to Application: Developing High-Performance MXene Photocatalysts for Hydrogen Production
Co-authors: B. Scheibe, A. Lewandowska-Andralojc

Discovered just over a decade ago, MXenes have rapidly become the spotlight for leading scientists of our time. Their diversity has expanded quickly, leading to continuously growing ways of application due to their outstanding properties, such as the combination of electronic conductivity and hydrophilic surface. The Ti3C2Tx MXene shows promising properties to be applied as a photocatalytic substrate for hydrogen production via the photoinduced water-splitting process, potentially replacing noble metals like Pt in photocatalysis. However, numerous factors can affect the photocatalytic activity of MXenes. Firstly, the synthesis method and subsequent purification processes have predominant importance. Secondly, the specific protocol for preparing the photocatalytic system before its testing also plays a significant role. Depending on the concentration of the bulk MXene solution as well as the presence of intercalants, the preparation procedure for the MXene solution used in the photocatalytic system may require additional steps. In our investigation, we isolated various fractions of Ti3C2TX MXenes through differential centrifugation with decreasing RPMs. Each fraction differed in terms of lateral sizes of MXene flakes and the number of intercalant layers, factors that can strongly influence the photocatalytic activity for hydrogen generation. Upon comparing the co-catalytic activity of each MXene fraction in the photocatalytic system, we observed that the fraction of MXenes characterized by larger lateral sizes of flakes exhibited higher hydrogen evolution rate (mmol h⁻¹ g⁻¹) for Eosin Y/Ti3C2Tx/CoSO4 system compared to other MXene fractions.

Acknowledgments: This work was supported by the National Science Center (Grant Number: UMO2021/43/O/ST5/00137).

Matin Nejatbakhsh
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Iran
Title: Hydrogel-based blood filtration integrated with disposable electrochemical sensor based on copper ferrite nanozymes and MXene for detection of glucose
Co-authors: Fatemeh Zahra Sarshar

The development of simple and effective diagnostic systems is a major goal in the field of medicine. Biosensors, such as blood glucose strips, are among the first examples of such systems that have been commercially available. However, research is being conducted to enhance and improve their performance. One of these approaches is the substitution of enzymes with Nano enzymes or the construction of non-enzyme sensors. The use of Nano enzymes increases the stability of the sensor and reduces the cost of raw materials and fabrication. Essentially, nanozymes are the nanomaterials that can mimic the behavior of enzymes and accelerate the progress of a reaction through catalytic reactions, oxidation, etc. Considering that different sources report glucose ranges between 1-25 mM for blood and 1 μM to 1 mM for saliva, there is a need to develop a sensor with suitable selectivity, high sensitivity, and stability in neutral environments. With these considerations, it appears that the combination of copper ferrite and MXene could lead to the development of a sensor with appropriate sensitivity and selectivity for glucose, able to use in natural or near natural environments. Therefore, in this study, copper ferrite nanozymes, along with MXene, was employed as nanozymes to enhance the sensitivity and stability of disposable carbon-based electrode platforms, and the performance of the final sensor for glucose detection was investigated.

Md Abu Zahed
Postdoctoral Researcher
University of Pennsylvania
USA

Title Microfabricated Ti3C2Tx thin film-coated flexible microelectrode arrays for electrochemical sensing
Co-authors: Spencer Averbeck, Royce Dong, Raghav Garg, Flavia Vitale

MXenes are promising materials for bioelectronics due to their excellent electrical conductivity, high surface area, processibility, and ability to be produced in large quantities.[1] While MXene-based electrochemical sensors have demonstrated high sensitivity for diverse analytes like neurotransmitters, and pollutants, existing methods rely on drop-casting MXene composites onto bulky and rigid current collectors like screen-printed electrodes or glassy carbon.[2][3] This approach hinders the development of microelectrodes and limits their application in flexible sensors. Recently, Noriega et al. investigated the feasibility of pristine Ti3C2Tx electrodes (mm in diameter) for flexible and transparent electrochemical sensors.[4] Although Ti3C2Tx microelectrode arrays (≤ 200 µm in diameter) have demonstrated excellent performance for in vivo neural electrophysiology recording compared to traditional metal electrodes,[5] however, they have not yet been explored for electrochemical sensing of biomarkers like neurochemicals, pathogens, and drugs. This work introduces a highly flexible Au-based microelectrode (200 µm in diameter) array (MEA) fabricated on an SU-8 substrate. A microfabrication method is then applied to deposit a Ti3C2Tx thin film onto the MEA, serving as a transducing layer to enhance the specific and electrochemical surface area for highly sensitive electrochemical sensing. To further increase the catalytic activity of the microelectrodes, platinum nanoparticles are electrochemically deposited on
the Ti3C2Tx. As an initial proof of concept, these microelectrodes are used to detect H2O2, a byproduct of various biological processes and a key indicator of oxidative stress, which is linked to inflammation and wound healing. The electrode exhibits excellent sensitivity (906.2 µAmM⁻¹cm⁻²) and a low detection limit (0.1 µM).

Mohammad Arham Khan
University of Nebraska-Lincoln
USA

Title Engineering MXene-based Electrodes for Green Ammonia Production
Co-authors: Syed Ibrahim Gnani Peer Mohamed, Ahmed El-Harairy, Sahand Serajian, Mona Bavarian, Siamak Nejati

The traditional method of ammonia production utilizes steam methane reforming to supply hydrogen, a known process for its energy-intensive nature and CO2 footprint. To overcome these challenges, we demonstrate the growth of metal-containing macrocyclic polymers on MXene electrodes to engineer the selectivity and reactivity of the electrodes in preparing green fuel and fertilizers. We study the effect of the MXene functional group on the mass activity of various samples prepared via adding conductive microporous polymers as a thin film to a MXene-based electrode. Here, we used the Ti3C2Tx, and studied the role of coatings on MXene stability and performance in converting Nitrate to Ammonia. Additionally, the role of the MXene terminal group on the rate of reaction and growth of the polymers was assessed. The data shows that multifunctional electrocatalysts, through engineering the microporous domain and post-synthetic annealing can be prepared and fine-tuned to enhance the reaction yield. We highlight the role of the MXene terminal group on reaction yield and electrode stability. Similar studies on hydrogen evolution reaction (HER) are being conducted to identify the path for further suppression of the HER and enhance the yield and activity simultaneously.

Mohammad Mozafari
Research Assistant
Drexel University
USA

Title Tailoring Interlayer Spacing in MXene/GO Composite Membranes for Enhanced Gas Separation Efficiency
Co-authors: Ali Pournaghshband Isfahani, Saeed Khoshhal Salestan, Masoud Soroush

Two-dimensional (2D) nanomaterial-based membranes have shown great potential for molecular separation owing to their attractive properties, including remarkable molecular sieving capabilities that offer an opportunity to overcome the inherent trade-off between permeability and selectivity. Due to their high aspect ratios, adjustable surface chemistry, and unique 2D lamellar structure, MXene membranes, characterized by regular and aligned nanochannels resulting from surface terminations, hold promise for achieving significant improvements in gas separation performance. In this work, we introduce a novel highly permeable Ti3C2Tx MXene/graphene oxide (GO) composite membrane tailored for selective H2 separation. The results indicate that gas molecules with smaller
kinetic diameters pass through the membranes more rapidly than those with larger kinetic diameters, indicating that molecular sieving dominates gas transport. Integrating larger GO flakes will not only effectively mask defects formed by Ti3C2Tx nanosheets but also enhance the molecular sieving capabilities of the membrane pathways, thereby improving selectivity. Additionally, we use various characterization techniques to evaluate the physicochemical properties of composite membranes that influence gas transport behavior. We conduct molecular dynamics simulations to study the gas transport through the membranes. Through this simulation, we determine potential mechanisms underlying the reduction of interlayer spacing, which may improve gas selectivity, thereby achieving a more favorable balance between permeability and selectivity. These combined experimental and theoretical studies are expected to shed light on the feasibility of finely adjusting interlayer spacing in the nanocomposite membranes to enhance molecular sieving for efficient gas separation.

Mohsen Pilevar Khomami
The University of Alabama
USA

Title: Antimicrobial Mode-of-Action of Colloidal Mo2TiC2Tx and Mo2Ti2C3Tx MXene Nanosheets
Co-authors: Anupma Thakur, Hesam Jafarian, Khaled Mahmoud, Mark Elliott, Babak Anasori, and Mostafa Dadashi Firouzjaei

MXenes have gained significant attention due to their unique properties and potential applications in various fields. The chemical structure of MXenes, particularly the type of transition metal used, has a crucial influence on their properties, including their antibacterial performance. This study explores the antibacterial capabilities of double-transition metal (DTM) MXenes, namely Mo2TiC2Tx and Mo2Ti2C3Tx, compared to a conventional single-transition metal MXene (Ti3C2Tx). Through a series of experiments, including time- and concentration-dependent growth-inhibition assays and analyses of the changes in nanosheet size after ultrasonication, the study investigated the antibacterial effects against E. Coli, a model gram-negative bacterium. The role of atomic structure and morphology in antibacterial efficacy was investigated using advanced electron microscopy (TEM and SEM), while disk diffusion assays and metal ion release evaluations (for Ti and/or Mo) helped clarify the mechanisms underlying MXenes' antibacterial performance. No meaningful correlation was observed between the antibacterial performance and released metal ions of MXenes. Our results have also indicated that physical damage by sharp edges of MXene flakes (i.e., nanoknives) is one of the primary antibacterial mechanisms of Ti3C2Tx (mono-M), Mo2TiC2Tx, and Mo2Ti2C3Tx (DTM) MXenes. In this regard, after 2h of exposure to E. Coli, all ultrasonicated MXenes (1 h) achieved an inhibition ratio (IR) exceeding 98%, whereas the pristine Ti3C2Tx, Mo2TiC2Tx, and Mo2Ti2C3Tx samples only achieved an IR of 31.8, 16.9, and 13.9%, respectively. In addition, a clear visualization of nanoknives' effects was recorded in SEM images, where the edges of mono-M MXene nanosheet has penetrated the wall of an E.Coli cell.

Muhammad Sharif Uddin
Purdue University
USA
Title: Molten salt shielding approach for direct synthesis of MXenes
Co-authors: Anupma Thakur, Nithin Chandran B.S., Brian C. Wyatt, Babak Anasori

Two-dimensional (2D) MXenes are commonly synthesized by top-down method of selective etching of A layers from their parent layered ternary MAX phases. Recently, MXenes have been successfully synthesized by a direct bottom-up synthesis route in a sealed ampule, which bypasses the need for MAX phases. The advancements in direct synthesis methods would facilitate practical applications of the rapidly developing family of functional MXenes with one step synthesis of MXenes without the need of fabricating a precursor and subsequent etching. Here, we present our attempts at a molten salt shielding-assisted direct synthesis of MXenes by reacting transition metal, transition metal halides, carbon precursor, and molten salts in a tube furnace in a single step, thereby avoiding the need for a sealed environment. This approach could offer scalability while providing MXenes with a diverse range of surface functional groups, aiming to provide a better understanding of the effects of different precursors and synthesis conditions on the growth of directly synthesized MXenes.

Murali Guntakrinda
Korea National University of Transportation
South Korea

Title: Surface Modification of MXene for Better Dispersion in Organic Solvents and Environmental Stability
Co-authors: Young Ho Park, Insik In

Because of its easy solution processing, superior electrical conductivity, and two-dimensional morphology, titanium carbide MXene (Ti3C2Tx, Tx = –O, –OH, etc.) has demonstrated great promise in a wide range of applications. However, hydrophilicity of MXene remains a critical concern since it causes poor dispersion stability in organic solvents and spontaneous chemical degradation in ambient conditions. To overcome this, we created a novel ligand that modifies the surface of MXene nanosheets, giving them hydrophobic surface characteristics. Unlike the previous reports, the ligand functionalization did not result in the significant decrease of MXenes' electrical conductivity. Furthermore, the functionalized MXene demonstrated exceptional dispersion stability in a range of organic solvents, including ethanol, acetone, and others, as well as enhanced oxidation stability. Although both pristine and functionalized MXenes originally displayed comparable electromagnetic interference (EMI) shielding efficacy, the chemical degradation of pristine MXene in ambient conditions deteriorated its EMI shielding efficacy with the progression of time. However, functionalized MXene’s EMI shielding efficacy remains constant over time due to its improved oxidation stability.

Murphy Sarshar
Medical University of Isfahan
Iran

Title: Disposable sensor based on cobalt oxide nano-micro flowers/MXene nanozymes for detection of salivary uric acid
Co-authors: Mohammad Matin Nejatbakhsh
This research addresses the critical health implications of deviations in uric acid levels, which can lead to cardiovascular disease, acute kidney injury, kidney stones, gout, diabetes, and heart disease. In response to the need for non-toxic, low-cost, and simple materials for electrochemical sensor applications in real environments such as serum and saliva, this research presents a non-invasive, non-enzymatic, and disposable sensor for point-of-care detection of uric acid. The sensor, which leverages cobalt oxide nanostructured with MXene and is fabricated through an economical electrodeposition method, demonstrated an enhanced reaction interface with uric acid due to the significant alteration in the cobalt oxides' morphology by MXene. The sensor exhibited superior performance in saliva, a challenging medium, showing a wide linear response range, high sensitivity in saliva and serum, and up to 21 days storage stability. The sensor proved practical and selective in real applications, such as human serum. This research marks a significant advancement in non-enzymatic sensors, paving the way for further development and application in real-world scenarios.

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Nafiza Anjum
Florida State University
USA

Title: High-Yield, High-Quality MXene for Energy Storage Application
Co-authors: Egwu E Kalu, Okenwa I Okoli

Minimally Intensive Layer Delamination (MILD) synthesis has been demonstrated as the most effective route to synthesize good quality MXene for the energy storage application. However, in this method, synthesized MXene contains partially etched MAX phases and residual LiF crystals as impurity, which affect the stability, conductivity and electrochemical properties of MXene. Furthermore, the yield is very low compared to other methods. In this work, we demonstrate a modified, high-yield route using repeated ultrasonication and centrifugation to separate high quality MXenes from the impurities which displays improved conductivity and electrochemical performance, hence can be potential candidate for energy storage applications. The yield of the MXene prepared by this modified route was found to be double to the MXene prepared by traditional MILD method. It showed conductivity of 490 S/cm and electrochemical capacitance of 380 F/g (at.10 mV/s) whereas the traditional route yield MXene with conductivity 250 S/cm and capacitance of 270 F/g. The crystal structures and elemental analysis conducted using electron microscopes, X-ray diffractometers and Raman spectroscopy confirmed the high quality of the prepared MXene.

Navaneeth Madathil
National Institute of Technology
India

Title: MXene based Triboelectric Nanogenerators for energy harvesting
Co-authors: Suprja potu, Jitesh pani, B Lakshakoti, Anjaly babu, Hitesh borker, K Prakash, K Uday kuamr, R Rakesh kumar

Two-dimensional transition metal carbides and nitrides (MXenes) have multifunctional applications in energy storage, electromagnetic interference (EMI) shielding, sensors, and flexible electronics. However, utilization of MXenes for energy harvesting applications is limited and started recently with triboelectric nanogenerators (TENGs). This work introduces a simple and cost-effective approach for advancing the performance of TENGs by utilizing MXene-Silicone nanocomposite film and aluminium as a triboelectric pair. MXene is combined with Silicone, a flexible polymer matrix, to form a nanocomposite layer for TENG applications. The electronaccepting nature of Silicone film was enhanced by adding triboelectric negative MXenes. To reduce TENG’s device fabrication steps, nanocomposite films were prepared directly on the aluminium foil by the film casting technique. The fabricated MXene-Silicone nanocomposite based TENG exhibited an impressive power density of 14.9 W/m², which is 3-fold higher than a pristine Silicone-based TENG. Under consistent mechanical stimulation, the TENG was capable of producing sufficient power to illuminate two LED lamps and continuously operate a digital calculator. The stability and robustness of the TENG were evaluated through a series of tests spanning 10,000 cycles over a period of six months, demonstrating consistent performance. Finally, using Arduino boards and the Blink app, self-powered touch-sensing technology was developed for security applications. The developed technology can send wireless alerts or notifications to mobile devices in the event of unauthorized access. These results illustrate MXene’s potential as a preferred material for applications such as energy harvesting, wearable electronics, self-sustaining systems, and touch-sensitive technologies.

Ndye Maty Ndiaye
University Cheikh Anta Diop of Dakar
Senegal

Title: **Optimization of Lithium Titanate Anodes for High Energy and Fast Charging Li-ion Capacitors**
Co-authors: Ndye Maty Ndiaye, Prisca Viviani, Armin VahidMohammadi, and Yury Gogotsi

Lithium-ion capacitors (LIC) are hybrid energy storage devices which combine the advantages of both lithiumion batteries (LIB) and supercapacitors. Thanks to their high energy and power densities and good cycling stability, they have been considered as a promising energy storage device. In our work, we have been optimizing various electrode architectures based on lithium titanate Li₄Ti₅O₁₂ (LTO) anode to obtain high areal capacities comparable to those used in commercial cells. We investigated different thicknesses, as well as composition of the anode electrodes based on LTO to maximize the areal capacity while maintaining the highrate capability of the fabricated electrodes. LTO based anodes with active material loading of up to 70 wt.% were able to deliver areal capacity of 1.8 mA h cm⁻² at a current density of 50 mA g⁻¹. As our next steps and to further optimize the electrodes’ structure and performance, we are going to investigate the role of MXene additives in anode electrodes based on LTO active material.

Nisha Hiralal Makani
Postdoctoral researcher
Fayetteville State University
Title: Enhancing optical characteristics of Ti3C2 MXene quantum dots through hydrothermal and electrochemical synthesis methods
Co-authors: Angelina K. Locke, Joshua Abbott, Shubo Han, and Bhoj Gautam

The remarkable capabilities of Ti3C2 MXene quantum dots (QDs) have showcased their immense potential in various domains such as biological imaging, optical sensing, photoelectric conversion, etc. In this study, Ti3C2 QDs were synthesized via two distinct methodologies: hydrothermal and electrochemical routes. The hydrothermal approach involved the use of LiF and HCl to etch titanium aluminum carbide (Ti3AlC2), followed by controlled heating of the decanted solution to produce the QDs. Conversely, the electrochemical method employed a three-electrode configuration with Ti3AlC2 as the working electrode and an ionic liquid electrolyte to synthesize the QDs directly. Top of Form Structural characterization was performed using X-ray diffraction (XRD) and Scanning electron microscopy (SEM), confirming the successful etching of aluminum from the Ti3AlC2 phase. Atomic force microscopy (AFM) and transmission electron microscopy (TEM) were used to measure the size of the QDs, which fell within the nanometer range, confirming the formation of QDs. Optical properties were assessed through UV-Vis spectroscopy and fluorescence lifetime measurements, showing distinct absorption and emission profiles for both sets of QDs. The hydrothermally synthesized QDs exhibited UV absorption between 200-220 nm and visible emission from 300-450 nm. Conversely, electrochemically synthesized QDs absorbed violet to blue light 350-400 nm with broader emission 400-500 nm, indicating the potential for various fluorescence imaging applications. This study showcases an expandable strategy for creating high-grade QDs with tunable optical features, catering to the needs of advanced optoelectronic devices. Top of Form.

This work was supported by DOE BES-RENEW award number DE-SC0024611

Title: Novel PCL-MXene patches for effective cardiac tissue regeneration

Here we demonstrate development of novel patches for cardiac tissue regeneration. Integration of MXenes into electrospun polycaprolactone (PCL) membranes was studied in order to harness the unique properties of Ti3C2 MXenes for creation of conductive, biocompatible, and mechanically robust scaffolds that promote cell adhesion, proliferation, and functional maturation. We propose a new method for depositing Ti3C2T3 MXenes onto hydrophobic electrospun PCL membranes by oxygen plasma treatment. This innovative approach has a positive effect on fiber size and increasing porous structure, reducing the contact angle of the PCL membrane and provides deep impregnation
of MXene into the material. The resulted PCL-MXene composite membrane is non-toxic, possess biomedical structural properties and electrical conductivity required for cardiac tissue regeneration, with no significant differences observed between the various numbers of MXene depositions. Incorporation of MXenes into biodegradable PCL membranes is very promising in conferring electroconductivity and enhancing cellular response in tissue-engineered cardiac patches. These novel MXene-PCL cardiac patches have a big potential for real application providing mechanical support to damaged heart tissue and enabling electrical signal transmission, by mimicking the crucial electroconductivity required for normal cardiac function. After a detailed investigation of scaffold-to-cell interplay this technology has the potential for clinical application not only for cardiac regeneration, but also as neural and muscular tissue substitutes.

**Acknowledgement:** Supported by European Commission under HORIZON-Europe projects #101131147 “ESCUAPE”, #101086184 “MX-MAP”.

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Prachi Rajput  
CSIR-CSIO  
India  

**Title:** SERS-Enhanced Detection of Persistent Organic Compounds Using Au Nanoparticle-Modified Ti3C2 MXene  
**Co-authors:** Pooja Devi

Sustainable and scalable surface enhanced Raman scattering (SERS) substrates showing notable stability and sensitivity for the detection of probe analytes have been a quest for quite a few decades. In recent studies the 2D metal carbides i.e., MXenes have displayed promising potential as SERS substrate in sensitive detection of the analytes due to their excellent electronic properties and surface chemistry. Furthermore, MXene engineering with metallic nanostructures allows enhancement of their performance for real world application. In present work, we report a scalable approach to fabricate a Ti3C2/Au SERS substrate via in-situ Au NPs synthesis on the few layered Ti3C2 MXene nanosheets. The resulting substrate demonstrates exceptional sensitivity, with a detection limit (LOD) of 10-12 M for methylene blue (MB) dye, serving as the model analyte. An enhancement factor of 13.43×1011 was achieved, alongside signal repeatability (RSD ~ 16.2%) and signal retention (~83%) over a 5-month storage period. Additionally, the substrate's efficacy in detecting BDE-47, a common persistent organic pollutant (POP) in e-waste recycling sites, with a permissible limit of 10-6 M, was also assessed. The substrate reliably detects concentrations below this limit, underscoring its potential for environmental monitoring. The exceptional performance is attributed to the combined effects of electromagnetic enhancement from Au nanoparticles and chemical mechanisms inherent to MXene. These results underscore the MXene hybrids promise for pollutant detection and environmental surveillance.

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Prastuti Upadhyay  
Undergraduate Student, A. J. Nanomaterials Institute
Title: Regenerative MXene Air Filtration Systems for Ultrafine Particles
Co-authors: Dr. Yury Gogotsi, Dr. Michael Waring, Dr. Stefano Ippolito, Bita Soltan Mohammadlou

With the increase in harmful emissions from vehicle exhaust, smoke, road dust, industrial emissions, pollen, chemicals, or biological pathogens like viruses, the quality of the air we breathe is getting worse with time leading to an increased risk of respiratory tract diseases. This project will explore an innovative route to design, optimize, and produce regenerative air filtration systems based on a family of 2D materials, consisting of alternating transition metal and carbon or nitrogen layer called MXenes. MXene Air filtration systems are advanced systems designed to filter particles of specific size, shape, and density from the air. To date, these systems have been used to filter bioaerosols like viruses and particulate matter that are around 2.5 µm in diameter. Our systems show promising results with improved air filtration capacities compared to traditional commercial HEPA filters for particulate matter less than 100nm (which have a larger surface area, are more risk-averse, and are commonly referred to as Ultrafine particles). The commonly found HEPA filters in the market can only filter particulate matter that is less than 2.5 µm or 10 µm in diameter. Moreover, this project introduces a new concept of the “Regenerative MXene Air Filtration system” where the MXene-based air filtration system could be charged or recharged by supplying electrical energy. So, this project aims to target nanoparticles, metallic particles, or biological particle filtration in a regenerative MXene air filter system that could be used as a sustainable alternative.

Title: In-situ Synergistic Nickel Boride/Stacked-Vanadium Carbide MXene Composites: 0D/2D NixB/V2CTx as Electrode Material for High-Energy-Density Supercapacitors
Co-authors: Karthik Raj, Carmel Breslin

Vanadium carbide-MXene (V2CTx) 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. We have developed a composite material consisting of amorphous nickel boride (NixB NPs) and V2CTx. To prevent oxidation and restacking of the layers and to improve the performance of the SCs, NixB was decorated between the gaps and the surface. The V2CTx and its composites were prepared by simple etching and direct liquid-phase methods. Under the optimized conditions, the V2CTx/NixB-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 diffusion paths, swift electron transfer, and excellent cycling stability of the composites are due to the V2CTx layers surface entrapped/gaps
filled by the NixB NPs. For practical application, an asymmetric device with V2CTx/NixB-75 and rGO as positive and negative electrodes was fabricated. The V2CTx/NixB-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 of 89.98 % and a Columbic efficiency of 99.9% after 20,000 continuous cycles at 8 A g⁻¹. These results emphasized that the NixB/V2CTx with novel composite architecture are suitable for advanced energy storage applications.

Ray Yoo
Texas A&M University
USA

Title: Optimizing the Electrocatalytic Phenomena of Ti2N MXene Through Decoupling Surface and Bulk Structure and Phenomena
Co-authors: Denis Johnson and Abdoulaye Djire

The continued rise in global energy consumption, along with the associated environmental hazards, pose a significant risk to our society’s infrastructure unless the main source is changed. Electrocatalysis involving hydrogen evolution reaction (HER), nitrogen reduction reaction (NRR), and oxygen reduction reaction (ORR), provide a pathway for energy storage and conversion due to their enhanced environmental friendliness and efficient energy input compared to their thermocatalytic counterparts. Currently, the state-of-the-art electrocatalysts suffer from scarcity and high cost. MXenes, a novel family of two-dimensional (2D) transition metal carbide and nitride materials, show potential as cost-efficient and highly abundant electrocatalysts with limited knowledge on their electrocatalytic mechanisms. This is especially true when considering the oftenoverlooked nitride family of MXenes. Herein, we investigate the electrocatalytic performance of a Ti2N nitride MXene under different electrolytic mediums. The effect of surface phenomena is investigated through manipulation of the surface passivation layer, as evidenced by Raman and Fourier-transform infrared (FTIR) spectroscopies, scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). Successful decoupling of the bulk and surface phenomena is achieved through Raman laser power attenuation. Under acidic medium, the surface reactivity towards HER is poor but the bulk reactivity for NRR is favored, making it an optimal NRR catalyst. Under alkaline medium, the surface reactivity of the pristine Ti2N MXene for ORR is high, but also leads to surface passivation and thus hinders the electrocatalytic activity. Overall, these results provide fundamental insights into future optimization strategies of the Ti2N nitride MXene, along with other electrocatalysts, towards electrocatalytic applications.

Royce Dong
PhD student
University of Pennsylvania
USA

Title: Microfabricating a multimodal neural interface integrating microLEDs and transparent Ti3C2Tx MXene electrodes for colocalized neural recording, imaging, and light-based stimulation.
Co-authors: Royce Dong, Raghav Garg, Sneha Shankar, Chris Wun, Spencer Averbeck, Placid Unegbu, Maggie Wagner, Yuzhang Chen, Dazhchen Zhang, Yuri Gogotsi, Brian Litt, Flavia Vitale
Light-based stimulation and control of neural activity is a powerful tool for neuroscience. However, studying complex brain activity with light-based stimulation in large animal models such as non-human primates is currently limited by the lack of scalable neurotechnologies integrating light sources and neural recording electrodes. For the few existing multimodal neural devices - mostly based on graphene - manufacturability, throughout, and material processing are still unaddressed issues. This work describes the microfabrication and characterization of a multimodal neural interface consisting of microLEDs and transparent Ti3C2Tx MXene microelectrode arrays, allowing for colocalized optical stimulation and electrical recording with high spatiotemporal resolution. We report scalable MXene microelectrode arrays with a transmittance of 60% at the reference wavelength of 550 nm and impedance of 587±152 kOhms at the reference frequency of 1 kHz. Importantly, we show that Ti3C2Tx MXene interacts minimally with microLED light output at 460 nm and 630 nm and does not give rise to photoelectric artifacts that are commonly observed in metal-based multimodal microelectrodes.

Sahand Serajian
University of Nebraska-Lincoln
USA

Title: Influence of Processing Methods on the Performance of Ti3C2Tx MXene-Integrated Polymer Electrolytes for Solid-State Batteries
Co-authors: Mona Bavarian

This research investigates the enhancement of ionic conductivity in solid electrolytes through the incorporation of Ti3C2Tx MXenes into polymer matrices. We explore two distinct MXene preparation methods: vacuum filtration and freeze-drying. The effects of each method on the ionic mobility and conductivity of the prepared electrolytes of same composition is studied through electrochemical impedance spectroscopy and differential scanning calorimetry. The electrolyte prepared using MXene obtained via freeze-drying method reduces the crystallinity of the prepared solid polymer electrolyte (SPE) by 4.9% leading to increase in the ionic conductivity of the SPE by one order of magnitude when compared to electrolytes prepared using MXene prepared through vacuum filtration method. Through the analysis of the frequency dependent impedance of the system and fitting the data to a representative equivalent circuit model and Voigt circuit representation, we highlight the potential of MXene composites in enhancing the performance of energy storage devices through reducing interfacial resistance and improving ion mobility. This investigation highlights the role of processing techniques in optimizing the functionality of two-dimensional materials in energy storage applications.

Sertan Kiziloz
University of Brighton
UK
Title: Optimising host response biology to advance wound dressing efficacy
Co-authors: Dan Hawthorne, Emma Ward, Avick Sinha, Grace Cooksley, Natalia Noriega, Dipak Sarker, Cyril Crua, Susan Sandeman

Chronic wounds are associated with multiple co-morbidities such as diabetes and pose a global burden. Chronic wounds remain in the inflammatory phase of the wound healing process where dysregulated inflammation and hyperosmotic stress are characteristics of chronic wounds. Wound dressings play a crucial role in the management of chronic wounds by providing an optimal wound healing environment, controlling exudate, and promoting tissue regeneration. Although advancements are being made in antimicrobial and moisture wound dressings, providing a wound dressing that can resolve the complex interplay of factors promoting failed wound resolution remains an open challenge. The wide range of biomedical properties of Ti3C2Tx MXene, adsorptive to inflammatory markers, biocompatibility and other biological properties are investigated in this study to show its effectiveness in wound healing. This study examined the effects of MXene and in combination with scavenger biomolecule in vitro to understand its effect on stress in HaCaT keratinocyte cell line. Stress was induced using mannitol. Comparisons were made between cells exposed to MXene and no MXene by carrying out scratch assay, enzyme linked immunosorbent assay (ELISA), real time polymerase chain reaction (rtPCR). Ti3C2Tx MXene was characterised by UV-vis spectrophotometry, dynamic light scattering (DLS), contact angle and scanning electron microscopy. The findings highlight that cells exposed to MXene significantly improved migratory response and repression of inflammatory upregulation and the expression were further primed in combination with scavenger biomolecule. Application of MXene can potentially provide new advances to wound dressing efficacy for chronic wounds.

Title: Machine Intelligence Accelerated Design of Conductive MXene Aerogels with Programmable Properties
Co-authors: Kieran James Barvenik, Tianle Chen, Haochen Yang, Yang Li, Meera Muthachi Kesavan, Joshua M. Little, Hayden C. Whitley, Zi Teng, Yaguang Luo, Eleonora Tubaldi, Po-Yen Chen

Designing ultralight conductive aerogels with tailored electrical and mechanical properties is critical for various applications. Conventional approaches rely on iterative, time-consuming experiments across a vast parameter space. Herein, an integrated workflow is developed to combine collaborative robotics with machine learning to accelerate the design of conductive aerogels with programmable properties. An automated pipetting robot is operated to prepare 264 mixtures of Ti3C2Tx MXene, cellulose, gelatin, and glutaraldehyde at different ratios/loadings. After freeze-drying, the aerogels’ structural integrity is evaluated to train a support vector machine classifier. Through 8 active learning cycles with data augmentation, 162 unique conductive aerogels are fabricated/characterized via robotics-automated platforms, enabling the construction of an artificial neural network prediction model. The prediction model conducts two-way design tasks: (1) predicting the aerogels’ physicochemical properties from fabrication parameters and (2) automating the inverse design of aerogels for specific property requirements. The combined use of model interpretation and finite element simulations validates a pronounced correlation between aerogel density and compressive strength. The model-suggested aerogels with high conductivity,
customized strength, and pressure insensitivity allow for compression-stable Joule heating for wearable thermal management.

Sokhna Dieng
PhD student, A. J. Nanomaterials Institute
Drexel University
USA

Title: Shrinking Lithium-Ion Batteries by Replacing Metal Current Collectors with MXene Films
Co-authors: Geetha Valurouthu, Kyle Matthews, John Wang, Yury Gogotsi

As the demand for renewable energy integration and portable electronic devices grows, high-performance energy storage devices are becoming increasingly important. Lithium-ion batteries are often the preferred choice due to their impressive energy density. Passive components, like current collectors, conductive additives, and binders, comprise around 25 wt% of a lithium-ion battery, with copper and aluminum foils commonly used as current collectors. In the past, these components often received less attention when developing high-power batteries, despite their significant contribution to the overall weight and volume. Since the active materials are reaching their theoretical performance limits, research interest in optimizing passive components has increased. To enhance the energy efficiency of Li-ion batteries, exploring the use of lightweight alternative materials and reducing the thickness of metal current collectors is critical. MXenes, a family of two-dimensional transition metal carbides, nitrides, and carbonitrides, have emerged as a promising solution. Among them, Ti3C2Tx MXene stands out for its excellent electrical conductivity (up to 20,000 S/cm), high surface area, good mechanical properties, and ease of solution processing, making it a suitable replacement for battery passive components. This study focused on replacing the conventional copper current collector with a thinner MXene film current collector for high-mass loading graphite anode electrodes. Our results showed improved capacities and rate performances of electrode materials using Ti3C2Tx MXene current collectors while reducing electrode weight and thickness. This study highlights the potential of MXene-based current collectors in improving the performance of lithium-ion batteries, paving the way for more efficient and lightweight energy storage solutions.

Spencer Averbeck
University of Pennsylvania
USA

Title: Scaling effects on the electrochemical performance of Ti3C2Tx MXene thin-film microelectrodes for neural recording and stimulation
Co-authors: Daryl Hurwitz; Raghav Garg; Michael S. Beauchamp; Flavia Vitale

In the last several decades there has been a growing interest in the development of technologies for neural recordings and therapeutic brain stimulation. Recently, 2D Ti3C2Tx MXene has emerged as a promising candidate for microscale recording and stimulation, due to its high electrical conductivity and volumetric capacitance. Here, we investigate the scaling effects on the electrochemical performance of thin-film Ti3C2Tx microelectrodes with diameters ranging from 25 µm to 500 µm. We
acquired electrochemical impedance spectroscopy (EIS), cyclic voltammetry (CV), and voltage transients (VT) measurements to characterize the recording and stimulation potentials of the microelectrodes. Through these experiments, we calculated impedance modulus at 1 kHz, cathodic charge storage (CSCc), and charge injection capacity (CIC) across the various electrode contact sizes. We found there was an increase in the magnitude of impedances at 1 kHz as the contact diameters decreased from 500 µm to 25 µm, increasing from 2.1 ± 1.3 kΩ in the 500 µm contacts to 315 ± 110 kΩ in the 25 µm contacts. Charge storage capacity increased steadily with decreasing contact size, increasing from 20 mC/cm2 to 90 mC/cm2 as the contact size decreased. For stimulation capabilities, we found a constant CIC value across all contact sizes, maintaining a cathodic charge injection capacity of ~600 µC/cm2 - a 3-fold increase compared to the ~200 µC/cm2 CIC for identically fabricated Platinum devices. Ultimately, our findings indicate that Ti3C2Tx microelectrodes are able to safely deliver electrical microstimulation, opening the door to further diagnostic research through electrophysiological recording and electrical stimulation.

Swapna Pahra
CSIR-Central Scientific Instrument Organization
India

Title: Engineered Ti3C2Tx MXene Based Multifunctional Electrocatalyst for Wastewater to Hydrogen Generation and Treatment
Co-authors: Pooja Devi

Abstract: Hydrogen generation via wastewater (WW) splitting is a sustainable approach to producing green hydrogen fuel. Over the last few years, enormous efforts have been made to develop oxide based efficient electrocatalysts for exploring WW H2 generation. Lately, MXenes have gained significant attention as an electrocatalyst due to their superior electrical conductivity and active basal planes. However, they are not fully studied in a WW environment as a multifunctional catalyst, which offers more challenge due to presence of contaminants. In the present work, a commonly used MXene i.e., Ti3C2Tx is engineered with transition metal alloys i.e., NiCo and NiMo via optimized electrodeposition. Followed by their characterized for optical, elemental compositions, morphological properties, etc., to confirm their synthesis. The polarization studies revealed that NiMo/Ti3C2 and Ti3C2/NiCo exhibited overpotentials of 45.8mV and 36.6mV, respectively, at 10mA/cm2, generating ~0.361 to 0.603mmolh⁻¹ of hydrogen from alkaline industrial WW. Additionally, NiMo/Ti3C2 and Ti3C2/NiCo degrade methylene blue ~82% and 86%, respectively. A scavenger study reveals the role of reactive oxygen species in pollutants degradation, while electrons for hydrogen generation. The promising catalytic activity of the engineered Ti3C2 could further be assigned to synergistic contributions from MXene and transition metals. Hence, this study contributes to the multifunctional activity of MXene for simultaneous wastewater treatment and hydrogen generation.

Sweta Sharma
AcSIR CSIR-CSIO
India

Title: Ti3C2/MoS2/SiNWs based dual functional electrode for photoelectrochemical wastewater to hydrogen generation and treatment
This study outlines the synthesis, optimization, and characterization of a Ti3C2 MXene-decorated MoS2/SiNWs photocathode, fabricated through hydrothermal and spray coating methods. The photocathode serves as a dual-functional system for photoelectrochemical (PEC) wastewater (WW) splitting, targeting hydrogen generation on the cathodic side and organic pollutant degradation on the anodic side, enabling simultaneous wastewater treatment and hydrogen production. Initially, SiNWs were synthesized via metal-assisted chemical etching (MACE), followed by a hydrothermal coating of MoS2 onto SiNWs, resulting in a type-II heterostructure formation. To enhance charge separation, Ti3C2 MXenes synthesized via LiF/HCl were spray-coated onto MoS2/SiNWs, yielding the Ti3C2/MoS2/SiNWs photocathode. PEC studies demonstrate the superior photocathodic activity of Ti3C2/MoS2/SiNWs over MoS2/SiNWs and SiNWs photocathodes. The fabricated heterostructure were characterized with XRD, UV, XPS, Mott-Schottky, and impedance analyses. Incident photon-to-current efficiency (IPCE) of Ti3C2/MoS2/SiNWs photocathode measures approximately 38.12%, surpassing MoS2/SiNWs (~15.26%), while long-term chronoamperometry study confirms its increased stability. In addition, the optimized electrodes exhibit efficient wastewater treatment, yielding a hydrogen production rate of 9.32µmol/h @ -0.78V vs RHE, with ~80.80% methylene blue degradation and total organic content (TOC) reduction to 1.520 mg/ml. Mechanistic studies via scavenger analysis elucidate hole-mediated MB degradation and electron-driven H2 generation. Overall, Ti3C2/MoS2/SiNWs photocathodes demonstrate outstanding performance, stability, and pollutant degradation efficacy, attributed to improved charge separation and utilization as outlined in the proposed mechanism.

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Title: Sodium aqueous supercapacitors based on Ti3C2 and activated carbon
Co-authors: Andrii Boichuk, Mahesh Eledath Changarath, Rafael Abargues, Juan P. Martinez-Pastor, Juan Francisco Sánchez Royo, Vitalii Vashchynskyi

In order to meet the needs of modern devices, power sources that are capable of delivering high power, good cycling and high capacity are becoming more important. The power of an electrochemical energy device is determined by the rate of electrochemical reactions that take place at each of its electrodes. In the case of hybrid supercapacitors, the reaction rate is limited by a Faraday electrode with an intercalation type of charge accumulation. Therefore, the development of novel 2D materials, such as MXenes with large surface area is very important now. In addition, MXenes single flakes remain stable for a long time in contact with water, which makes them effective in cheap and environmentally friendly aqueous supercapacitors. Our work is focused on investigating the electrochemical properties of hybrid supercapacitors formed on the basis of Ti3C2 and activated carbon obtained from apricot pits. Electrochemical studies were carried out in coin cells (CR 2032) in 1M aqueous solutions of Na2SO4, NaNO3 and Na2CO3. Based on the calculated values of the specific capacity, especially under high current conditions, we can conclude that this
combination of electronic materials could be used successfully for hybrid electrochemical systems with a high cycling rate and a high power density. Special attention should be paid to the transformation of the impedance spectra during the cycling, which indicates the stability of the charge accumulation processes on both electrodes during a thousand cycles.

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Title: Understanding the MXene-to-Oxide Transformation Process for Solid-Solution (V2-yNby)CTx MXenes and Electrochemical Properties of their Derived Oxides  
Co-authors: Marcelo A. Andrade, Ekaterina Pomerantseva

MXenes have been shown to be unique precursor materials for the synthesis of transition metal oxides for use as electrodes in intercalation energy storage as MXene-derived oxides exhibit morphologies not achievable with other precursors. The prospect of using solid-solution or multi-metal MXenes provides an exceptional avenue for creating composite-like materials with tightly bound heterointerfaces or create substitutional doping within a parent material, which can lead to further improvements in electrochemical performance. In this poster presentation, we will discuss details of the MXene-to-oxide transformation process using solid-solution (V2-yNby)CTx MXenes and the electrochemical properties of the derived oxides in Li-ion batteries. Oxidation of V2CTx and Nb2CTx resulted in bilayered vanadium oxide (BVO) with crumpled nanosheets and nanostructured amorphous Nb2O5 (nANO) nanospheres, respectively. SEM imaging showed nANO embedded in BVO nanosheets for oxides derived from solid-solution (V2-yNby)CTx MXenes. Electrochemical cycling in Li-ion cells revealed different behaviors: V2CTx-derived oxides showed redox processes, while nANO exhibited pseudocapacitive responses. Solid-solution MXene-derived oxides displayed composite behavior with notable exceptions. V1.75Nb0.25CTx-derived oxide electrodes achieved a high capacity of 296.8 mAh g⁻¹, possibly due to niobium doping into the BVO structure. V1.00Nb1.00CTx-derived oxide electrodes delivered 298 mAh g⁻¹, with contributions from both BVO and nANO phases. These electrodes showed improved electrochemical stability compared to those made by physically mixing Nb2CTx- and V2CTx-derived oxides. The study highlights that solid-solution MXenes are effective precursors for synthesizing oxides with unique compositions and morphologies leading to improved charge storage properties.

V

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Title: Understanding Water Transport through Ti3C2Tx MXene Membranes  
Co-authors: Ahamd A. Shamsabadi, Amir Aghaei, Anupma Thakur, Hui Fang, Zahra Fakhraai, Andrew P. Rappe, Mohtada Sadrzadeh, Babak Anasori, and Masoud Soroush
Water transport along nanochannels has become an area of significant interest due to its potential applications in water purification, desalination, and energy generation. MXenes are 2D transition metal carbides, nitrides, and carbonitrides, with high hydrophilicity, excellent electrical conductivity, and rich surface chemistry. Their hydrophilic nature, combined with high metallic conductivity, sets them apart from most other 2D nanomaterials. From a potential application point of view, experimental studies have mainly focused on how ionic transport occurs in MXene nanochannels. However, a comprehensive study on water transport in these nanochannels, particularly concerning the interaction of water molecules with cations of varied hydration diameters, remains elusive. Therefore, increasing the affinity of water molecules towards the nanochannel walls through the intercalation of cations with different hydration diameters could provide an effective approach to achieving fast water transport through MXene-based nanochannels. Here, we investigate the influence of cation intercalation on water transport through Ti3C2Tx MXene membranes. To this end, we intercalate different types of cations (using NaCl, KCl, LiCl, MgCl2, and CaCl2) with varied water affinities, allowing us to manipulate the number of hydrogen bonds interacted with the intercalated cation on the nanochannel walls of MXene membranes. Utilizing cations with different water affinities has allowed us to experimentally investigate their effect on water transport through these nanochannels. Furthermore, our findings provide important insights into the water transport mechanism in MXene-based nanochannels in general and support the application of the Hagen-Poiseuille equation to describe water transport in these nanochannels.

Vaihav Joshi
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USA

Title: Molten Salts Shielded synthesis of MXenes with in-situ Raman spectroscopy
Co-authors: Rose M. Snyder, John Jamboretz

Since their discovery in 2011, MXenes are on the rise due to their diverse applications ranging from energy storage, photonics, catalysis and biomedical sensing which are a result of their unique structure and properties. Although primary importance is given to the synthesis of pristine MXenes, during recent years, hetero MXenes have evolved and are being studied extensively. Hetero substitutions enhance the properties and characteristics while introducing flexibility and functionality to MXenes. One example is (VxNb1-x)2C, which is predicted to be an active and enhanced catalyst for oxygen evolution reactions (OER). Conventional methods of synthesizing MXene involves etching the A-element from parent MAX phase using hydrofluoric acid either produced in-situ or used ex-situ. Recent development in the field introduced various HF free methods to synthesize MXenes. Lewis Acid Molten Salts synthesis or LAMS is one of the promising synthesis methods involving the use of lewis acid to remove A-element. The process eliminates toxic hydrofluoric acid, improves reaction time and yields. However, the mechanistic studies of LAMS to synthesize MXenes is still largely unexplored. Existing in-situ methods rely on access to beamlines in huge facilities, which can either be inconvenient or at times inaccessible. In-situ Raman spectroscopy has proven to be an unorthodox technique to study such phase transformations. It’s easy, convenient and can be facilitated in common chemical laboratories. In this project, Molten Salts Shielded Synthesis along with in-situ raman is being used to shine light on the mechanistic pathways by characterizing phase transitions throughout the exfoliation process.
Valentina Nesterova  
Auburn University  
Australia  

Title: **Ti3AlC2 under Electrochemical Conditions: insights from ab initio simulations**  
Co-authors: Konstantin Klyukin

Improving the synthesis of MXenes requires a deep understanding of the atomistic mechanism of MAX phase etching reaction. The selectivity of the etching reaction depends on many factors, including surface terminations of MAX phases, their defect chemistry, choice of etching agent, and applied potential. Nevertheless, the behavior of MAX phases under electrochemical conditions remains unknown at the atomistic scale. In this work, we first used ab initio computational simulations to uncover the possible surface terminations of zigzag and armchair planes for Ti3AlC2 MAX phase. Using the computational hydrogen electrode approach [1] and considering all possible symmetric sites with adsorbed O, OH or H termination groups, we revealed the most stable configurations across different values of applied potential (Figure 1). Figure 1. Surface energies as a function of applied potential for armchair (a) and zigzag (c) planes of Ti3AlC2, stable surface terminations of armchair (b) and zigzag (d) planes. As a next step, we simulated the initial stages of etching reaching in the presence of F- and calculated energy barriers for Al and Ti extraction by employing DFT-based molecular dynamics using the approach discussed in our previous work. [2] Our research aims to improve the electrochemical etching conditions and shed light on various factors affecting etching selectivity.

We acknowledge funding support from the National Science Foundation (DMREF-2324156).

References:  

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Title: **Biomimetic Design and Dispersed Organization of Ti3C2Tx MXene flakes in Cellulose Nanofibers (CNF) Composite Membranes**  
Co-authors: Valeriia Poliukhova, James Fitzpatrick, Yuri Gogotsi, Vladimir V. Tsukruk

Controlled organization of Ti3C2Tx MXene within polymer networks is crucial for harnessing its full potential as a versatile 2D material in a broad spectrum of applications. Cellulose nanofibers (CNFs) extracted from natural plant sources are biodegradable and characterized by high aspect ratio, which provides a large interface area for interaction with MXene flakes. In this work, we develop Ti3C2Tx/CNFs composite membranes that ensure a controlled arrangement and distribution of single-to-few Ti3C2Tx MXene flakes within a cellulose matrix with bright light reflection. Leveraging
the unique properties of nanofibers with enhanced mechanical strength ultrathin membranes maintain high optical transparency up to 85 % with a volume fraction of MXene flakes < 1%. Our results not only expand the understanding of Ti3C2Tx/CNFs composites but also illustrate the potential of high-performance composite materials for advanced material science.

Vikash Khokhar
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USA

Title: From monodentate to polydentate organic ligands for hybrid-MXenes
Co-authors: De-en Jiang

The first successful controlled attempt to functionalize inorganic 2D transition metal carbide/nitride (MXenes) with amines was reported as organic-inorganic h-MXenes. However, the amido/imido groups at the interface were found to be monodentate, even for diamines used. Here, we explore the structure and stability of polydentate ligands on Ti3C2 using density functional theory and ab initio molecular dynamics simulations. We show the stability of polydentate imido groups even at high temperatures (~800 K), which can be instrumental in the design and synthesis of new stable h-MXenes.

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Title: Amplifying the differences in aluminium-based eutectic electrolytes through electrodeposition on MXenes
Co-authors:

Traditionally, rechargeable lithium metal battery systems relied on simple metal cationic species to conduct metal nucleation. However, this mechanism is less applicable to room-temperature rechargeable aluminium batteries (RABs), which utilise complex ionic species. In this work, we take advantage of two different MXenes, Mo2Ti2C3Tx and Ti3C2Tx, which have different metal-termination group bond strengths, interlayer spacings, and surface termination compositions, to amplify and visualise the differences between two promising RAB eutectic electrolytes (i.e., urea/AlCl3 and EMImCl/AlCl3). Better aluminium electrodeposition was observed on the Mo2Ti2C3Tx film in the urea/AlCl3 electrolyte but the same is true on the Ti3C2Tx film in the EMImCl/AlCl3 electrolyte, evidencing distinctive differences between the two electrolytes. Overall, due to the characteristics of aluminium, a good room temperature non-aqueous RAB will require different mechanisms as compared to conventional metal batteries, resulting in the need for audacious attempts towards system understanding and manipulation.
Xinle Zhang  
PhD Student  
Drexel University

Title: **Resolving the Structure of MXene-Derived Potassium Preintercalated Bilayered Vanadium Oxide using Atomic Pair Distribution Function Analysis**  
Co-authors: Timofey Averianov and Ekaterina Pomerantseva

Chemically preintercalated bilayered vanadium oxides derived from V2CTx MXene (MD-BVOs) have shown enhanced electrochemical performance as cathode materials in Li-ion batteries. While correlations have been made between the nature of chemically preintercalated ion and the (001) d-spacing calculated from X-ray diffraction (XRD) patterns, structures of MD-BVOs are poorly understood due to the lack of long-range order limiting the use of conventional structure refinement methods. Herein, we demonstrate the use of atomic pair distribution function (PDF) refinement to resolve the nanocrystalline structure of potassium preintercalated MD-BVO (MD-KVO). We employed a Na0.56V2O5 model, where the interlayer sodium atoms were replaced by experimentally established amounts of potassium and structural water oxygen atoms determined by energy dispersive X-ray spectroscopy and thermogravimetric analysis, respectively. The refinement of a modified model against the atomic PDF of MD-KVO led the interlayer distance increase from 8.90 Å to 9.57 Å, in agreement with the interlayer distance calculated from its XRD pattern. By applying spherical diameter in PDF refinements, the optimal fit suggests that the refined model best describes the structure within a 55.5 Å spherical spacing, indicating the local average crystallographic order dimension. In this poster presentation, we will demonstrate the correlation between the MD-KVO structure and its charge storage properties observed in non-aqueous K-ion batteries. By presenting the relationship between electrochemical performance and PDF refinement of MD-KVO, we propose that a similar methodology can be applied to other MD-BVO phases to establish structure-property relationships, charge storage mechanisms, and design strategies leading to improved performance.

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Title: **Critical Analysis of Hydrogen Storage in MXenes**  
Co-authors: Robert W. Lord, Pawel P. Michałowski, Sylwia Kozdra, Yury Gogotsi, Aleksandra Vojvodic
There is a large need to develop new hydrogen storage materials for the growing hydrogen economy. Recent studies have suggested that Ti-based two-dimensional MXenes (Ti2CTx and Ti3C2Tx, specifically; with Tx being the surface terminating functional group) can store large quantities, over 8 wt. %, of hydrogen. However, the atomic scale understanding of how and where these Ti-based MXenes store hydrogen is still lacking. Herein, we critically analyze the potential of MXenes as hydrogen storage materials and establish a framework of how to evaluate the hydrogen storage in these materials. A systematic evaluation of molecular and atomic hydrogen uptake and storage by stoichiometric and non-stoichiometric functionalized Ti2CTx MXenes (Tx being either bare, O, or F) is performed. We utilized a combination of density functional theory (DFT) calculations, experimental hydrogen uptake measurements by Ti2CTx, and layer-by-layer depth profiling using secondary ion mass spectroscopy (SIMS). By leveraging the capabilities of both the theoretical and experimental approaches, the intra- and inter-layer hydrogen storage location and capacities for the Ti2CTx are disentangled and the storage mechanisms are discussed. We identified that the intra-layer storage is critical and proceeds through interactions with a non-stoichiometric MXene consisting of either defects and/or vacancies with a range of hydrogen storage capacity of up to 1.5 wt.% for an oxygen-filled Ti defect, while the inter-layer hydrogen storage has a clear upper limit of 0.4 wt.%. which is only possible at high hydrogen pressures and temperatures.

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Title: Effect of CTAB Intercalation on the Electrochemical Performance of Ti3C2Tx MXene  
Co-authors: Yuan Zhang, Teng Zhang, Kyle Mathews, Yury Gogotsi

The intercalation of cationic surfactants, such as cetyltrimethylammonium bromide (CTAB), into twodimensional (2D) materials, such as MXenes, has emerged as a pivotal strategy to modify their intrinsic properties, including electronic characteristics, and surface charge. This method significantly broadens the application potential of MXenes in cutting-edge fields, such as electronics, energy storage, and catalysis. The process of CTAB intercalation facilitates the expansion of interlayer spacing within MXenes, thereby offering a route to tailor their electrical conductivity and band structure through the selective insertion of ions or molecules. Such modifications allow for the tunability of the hydrophilicity or hydrophobicity of the materials by varying surfactant concentrations. Despite the benefits of CTAB pre-intercalation in enhancing the electrochemical performance of MXene-based electrodes, the underlying mechanisms, particularly the distinction between steric and kinetic effects on ion storage, remain insufficiently explored. Moreover, the impact of varying intercalants and their concentrations on MXene characteristics across diverse applications necessitates further investigation. Additionally, the long-term stability and reusability of CTAB-intercalated MXenes under various environmental and operational conditions are crucial aspects that are yet to be fully understood. Addressing these knowledge gaps is essential for advancing MXene applications in fields, such as energy storage, adsorption, ion separation, and electrochemical actuation, where the precise tuning of material properties can lead to significant performance enhancements.
Yeonjin Baek
Auburn University
Australia

Title: **Cation-Intercalated Niobium Carbide (Nb2CTx) MXenes as a Cathode for Rechargeable Aluminum Batteries**
Co-authors: Bart Prorok, Majid Beidaghi

Rechargeable aluminum batteries (RABs) are considered an alternative to Li-ion batteries for some applications due to the high abundance and excellent theoretical specific capacity (2980 mA g⁻¹) of aluminum. Despite their potential, RABs encounter numerous challenges, such as poor cyclic life and low coulombic efficiency, primarily due to the strong interaction of intercalating ions and the cathode materials. While MXenes have demonstrated excellent potential as cathode materials for RABs, their charge storage mechanism in this system is still unclear. Also, the MXene-based cathodes usually show poor cyclic performance. In this study, we have developed a cation-intercalated Nb2CTx MXene cathode with significantly improved capacity and electrochemical stability. Intercalated cations change the interlayer environment as they interact with the inner surface functional groups. Also, those cations can decrease the electrostatic repulsion force between MXene layers and pillar the interlayer. Pre-intercalation of cations effectively alleviates stacking and expansion problems of cathode materials, making it easier for [AlCl4]⁻ to de-intercalate/intercalate in the Nb2CTxinterlayers. Pristine Nb2CTx and cation intercalated Nb2CTx MXene were evaluated as cathode materials for Al-batteries, and their performance was compared to investigate the effect of different cations on interlayer spacing and the change of the primary charge storage mechanism.

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USA

Title: **Electron Microscopy Characterization of 2D Titanium Carbide and Carbonitrile MXenes**
Co-authors: Teng Zhang, Danzhen Zhang, Yury Gogotsi, Eric Stach

MXenes, a family of two-dimensional transition metal carbides, nitrides, and carbonitrides, have garnered significant research interest globally due to their unique properties and tailoring capabilities. Despite the substantial collective efforts, fundamental aspects related to their structure and surface terminations remain unexplored. Understanding these fundamental properties, such as structure, chemistry, and defects, is crucial, and advanced scanning transmission electron microscopy (STEM) and spectroscopy methods with sub-atomic resolution play a pivotal role in this endeavor. While MXenes span diverse chemistries and structures, only a few studies have focused on the chemical components, atomic defects, and chemical bonding within these materials. This work represents the first systematic experimental study employing electron microscopy and electron energy loss spectroscopy (EELS) to investigate the chemical components, atomic defects, and chemical bonding in MXenes. The study explores the defect distribution and the surrounding chemical bonding in freestanding monolayers of Ti3C2, Ti3C1.5N0.5, Ti3CN and Ti3C0.5N1.5, terminated with –F, –OH, and =O, through atomic-scale characterization. The results demonstrate that the titanium vacancy concentration and surface functional groups can be controlled by tuning the nitrogen concentration in the
carbides/carbonitrides. This study highlights the potential for improving the stability and further applications of MXenes.

Yinan Yang
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Title: Understanding the Energetics and Reactivity of Ligands on MXene Surfaces
Co-authors:

The functionalization of MXene surfaces with ligands is of interest for tuning their optoelectronic and physicochemical properties. In particular, organic ligands offer a large degree of flexibility to modulate these properties, which may enable a wide range of applications. However, a comprehensive understanding of chemical interactions between organic ligands and MXene surfaces remains elusive. In this study, we employ density functional theory (DFT) calculations to quantify the binding strengths of various ligands to the Ti3C2 MXene surface. Additionally, we calculate the reactivity of a surface functionalized with alcohol ligands. Our results provide an energetic profile of Ti3C2 surface interactions that deepens the understanding of MXene surface chemistry for the future development of novel MXenes with tailored properties.

Young-Hwan Kim
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USA

Title: Covalent Surface Modifications of Two-Dimensional MXenoids

Surface modifications on two-dimensional (2D) inorganic materials serve as a unique platform for functionalizing and property tuning this extensive material family. The inorganic and organic surface modification strategies developed for halogen-terminated transition-metal carbides and nitrides (MXenes) show exceptional controllability and versatility, attributed to their robust in-plane and labile out-of-plane bonds. Here, we demonstrate the general applicability of this surface modification strategy to non-MXene halogenterminated 2D materials, termed MXenoids, encompassing at least 115 potential candidates. These surface modifications enable structural and band engineering, introduce organic chirality to hybrid structures, and achieve remarkable photophysical properties with a quantum yield reaching up to 22.0%. This study presents a universal approach to creating a library of surface-modified 2D materials, expanding their functional capabilities and property space.