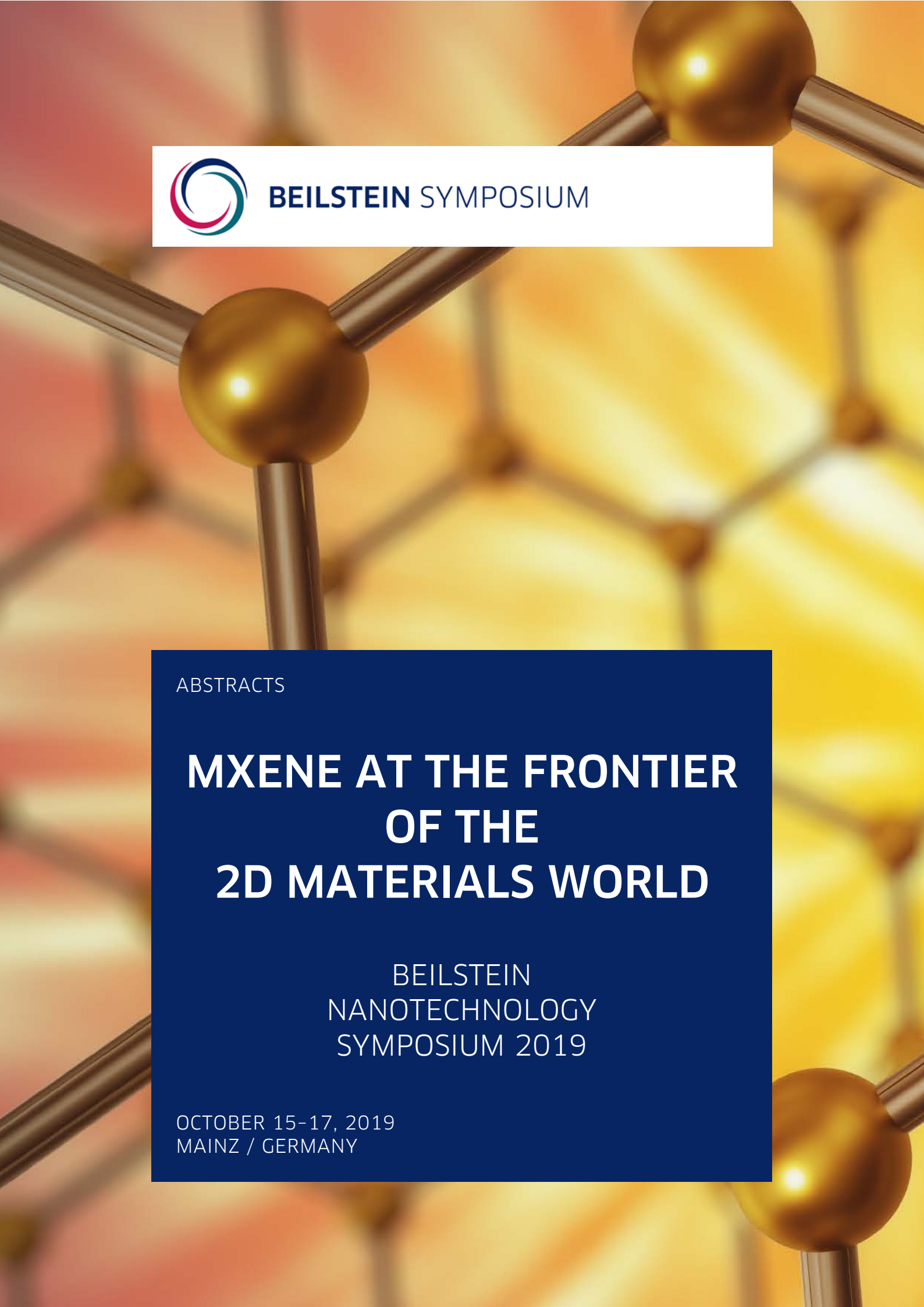

BEILSTEIN SYMPOSIUM

ABSTRACTS

MXENE AT THE FRONTIER OF THE 2D MATERIALS WORLD

BEILSTEIN
NANOTECHNOLOGY
SYMPOSIUM 2019

OCTOBER 15–17, 2019
MAINZ / GERMANY

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GENERAL INFORMATION

INTRODUCTION

The goal of this symposium is to provide a forum for discussion of hot topics and fundamental questions in the rapidly growing field of MXenes. With about 30 MXenes reported, an infinite number of solid solutions possible, more than 1000 papers published, and the first industrial products on the horizon, it is important to exchange information and build a community of researchers working in the field.

The symposium will bring together leading international experts and those researchers who are just entering the exciting world of 2D carbides and nitrides to explore new synthesis methods, better understand properties and find new applications of MXenes.

The conference hotel is located in Mainz near Frankfurt, directly on the banks of the river Rhine. The number of participants is limited to about 60 including 20 invited speakers and the program is designed specifically to allow sufficient time for discussions and exchanges of thoughts and ideas.

SCIENTIFIC ORGANIZERS

Yury Gogotsi / Drexel University, USA

Xinliang Feng / TU Dresden, Germany

Johanna Rosén / Linköping University, Sweden

DATES

- **Scientific program** October 15–17
- **Travelling days** October 14 and October 18
- **Welcome reception** October 14 at 7 pm

WEBSITE

You will find the website of this symposium at

www.MXene.beilstein-symposia.org

TWITTER

Please use the hashtag **#BeilsteinMXene** for this symposium.

Follow the Beilstein-Institut: **@BeilsteinInst**

CONFERENCE HOTEL

The conference, lunches and dinners will take place at:

Favorite Parkhotel Mainz Karl-Weiser-Str. 1 55131 Mainz Germany	T +49 6131 8015 0 F +49 6131 8015 420 empfang@favorite-mainz.de www.favorite-mainz.de

ORGANIZATION AND CONTACT

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SCIENTIFIC PROGRAM

Tuesday, October 15

9:00	**Welcome and introduction** Martin G. Hicks, Wendy Patterson
	Chair: Tawfique Hasan
9:20	**The rise of MXenes** Yury Gogotsi
10:00	**Graphene and MXene from electrochemical approaches: prospects for functional applications** Xinliang Feng
10:40	**Coffee break**
11:10	**Expanding the structural and elemental space of MAX phases and MXenes** Johanna Rosén
11:50	**MXene-enabled electronic applications** Husam N. Alshareef
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	Chair: Xinliang Feng
14:00	**Properties and applications of MXenes from first-principles perspective** Mohammad Khazaei
14:40	**Two-dimensional titanium carbonitride, a novel member of the MXene family** Michael Naguib
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16:00	**Poster Session**
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9:40	**Tailoring the surface chemistry of 2-dimensional MXenes** Per O.Å. Persson
10:20	**Coffee break**
10:50	**When molecular science meets 2D materials: Orchestrating multiple functions** Paolo Samorì
11:30	**Observing MXenes with soft X-ray light** Tristan Petit
12:10	**Lunch**
	Chair: Susan Sandeman
14:00	**Triple hybridization of MXene/Chevrel and carbon electrodes in saturated LiCl solution for fast energy storage: Fundamental aspects of hybrid devices** Mikhael D. Levi
14:40	**2D $Ti_3C_2T_x$ MXene materials for electrochemical energy storage** Hui Shao
15:20	**Coffee break**
15:50	**Water treatment and environmental remediation applications of two-dimensional metal carbides (MXenes): Opportunities and challenges** Khaled Mahmoud
16:30	**Electrochemical water desalination with transition metal carbides and dichalcogenides** Volker Presser
17:10	**End of talks**
19:00	**Dinner**

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	Chair: Yury Gogotsi
9:00	**2D crystals for inkjet-printed (opto)electronics and sensors: Towards manufacturability** Tawfique Hasan
9:40	**MXene conductive inks for energy storage and electronics** Chuanfang Zhang
10:20	**Coffee break**
10:50	**MXene chemistry for applications** Vadym Mochalin
11:30	**MXenes for biomedical applications** Susan Sandeman
12:10	**Lunch**
	Chair: Yury Gogotsi
13:40	**2D transition metal carbide (MXene) thin film for EMI shielding** Chong Min Koo
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15:00	**Farewell and final remarks**
15:20	**End of program**
19:00	**Dinner**

ABSTRACTS

Tuesday	The rise of MXenes
9:20	**Yury Gogotsi**
	A.J. Drexel Nanomaterials Institute and Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, United States of America

Numerous compounds, ranging from clays to boron nitride (BN) and transition metal dichalcogenides, have been produced as 2D sheets. Although many of these materials remain subjects of purely academic interest, others have jumped into the limelight due to their attractive properties, which have led to practical applications. Among the latter are carbides and nitrides of transition metals known as MXenes (pronounced “maxenes”), a fast-growing family of 2D materials. The family of 2D transition metal carbides and nitrides (MXenes) has been expanding rapidly since the discovery of Ti_3C_2 at Drexel University in 2011 [1]. More than 30 different MXenes have been reported, and the structure and properties of numerous other MXenes have been predicted using density functional theory (DFT) calculations [2,3]. Moreover, the availability of solid solutions on M and X sites, control of surface terminations, and the discovery of ordered double-M MXenes (e.g., Mo_2TiC_2), i-MAX phases and their MXenes offer the potential for producing dozens of new distinct structures.

This presentation will describe the state of the art in the field. The manufacturing of MXenes, their delamination into single-layer 2D flakes and assembly into films, fibers and 3D structures will be briefly covered. Synthesis-structure-properties relations of MXenes will be addressed on the example of Ti_3C_2. The use of MXenes in ceramic- metal- and polymer-matrix composites, smart fibers and textiles will also be discussed. The versatile chemistry of the MXene family renders their properties tunable for a large variety of applications [3-5]. Oxygen or hydroxyl-terminated MXenes, such as $Ti_3C_2O_2$, have been shown to have redox capable transition metals layers on the surface and offer a combination of high electronic conductivity with hydrophilicity, as well as fast ionic transport [4]. This, among many other advantageous properties, makes the material family promising candidates for energy storage and related electrochemical applications [4], but applications in plasmonics, electrocatalysis, biosensors, water purification/ desalination and other fields are equally exciting.

References

[1] M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J.-J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum, Two-Dimensional Nanocrystals Produced by Exfoliation of Ti_3AlC_2, *Advanced Materials*, **23** (37), 4248-4253 (2011).
[2] M. Naguib, O. Mashtalir, J. Carle, V. Presser, J. Lu, L. Hultman, Y. Gogotsi, M.W. Barsoum, Two-Dimensional Transition Metal Carbides, *ACS Nano* **6** (2) 1322–1331 (2012).
[3] B. Anasori, Y. Gogotsi (Ed.) *2D Metal Carbides and Nitrides (MXenes): Structure, Properties and Applications* (Springer), 2019.
[4] B. Anasori, M. Lukatskaya, Y. Gogotsi, 2D Metal Carbides and Nitrides (MXenes) for Energy Storage, *Nature Reviews Materials*, **2**, 16098 (2017).
[5] K. Hantanasirisakul, Y. Gogotsi, Electronic and Optical Properties of 2D Transition Metal Carbides and Nitrides (MXenes), *Advanced Materials*, **30** (52) 1804779 (2018).

Tuesday	**Graphene and MXene from electrochemical approaches: prospects for functional applications**
10:00	**Xinliang Feng**
	Faculty of Chemistry and Food Chemistry & Center for Advancing Electronics Dresden, Technical University Dresden, Germany

The discovery of graphene one decade ago has inspired the development of functional graphene for practical applications. Enormous research suggests a bright future of the graphene industrialization. However, for a long time there has been a huge gap between laboratory-scale research and commercial application due to the challenging task of reproducible bulk production of high-quality graphene at low cost. The future research and application of graphene materials urgently calls for the efficient, reliable and smart chemical synthesis and processing, which need to play a key enabling role. Electrochemical exfoliation of graphite has emerged as a promising wet-chemical method with advantages such as up-scalability, solution processability and eco-friendliness.

In this lecture, we will discuss the recent progress in electrochemical exfoliation of graphite and 2D materials including black phosphorous and MXenes. The solution exfoliation of graphite is relying on the smart processing of graphitic precursors at the thin-thickness level under electrochemical control. This strategy offers the reliable means to produce high quality, solution-processable graphene on a large scale and at low cost. This approach is further extended to the exfoliation of black phosphorous and MXenes as new type of 2D materials. The prospects for the functional applications of exfoliated graphene, black phosphorus and MXenes will be provided, particularly in the fields of flexible electronics, energy technologies, functional foams & coatings.

Tuesday	**Expanding the structural and elemental space of MAX phases and MXenes**
11:10	**Johanna Rosén**
	Materials Design, Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

The exploration of new MAX phases and MXenes is an active area of materials discoveries. A more recent addition to the field is a new type of atomic laminated phases, coined i-MAX, in which the M-atoms in (M12/3M21/3)2AlC are in-plane chemically ordered. The first phase discovered was (Mo2/3Sc1/3)2AlC, and it has been shown that this was a first example of a large, more than 30 reported to date, set of thermodynamically stable phases, typically realized from an interplay between theoretical predictions and experimental verification.

Using the i-MAX phases for MXene synthesis allows a new route for tailoring the MXene structure and composition: By employing different etching protocols, it is possible to I) remove only the Al atoms, and obtain a MXene with in-plane elemental order, or II) remove Al and one of the M-elements, and obtain a MXene with ordered vacancies. The i-MAX phases realize 3D and 2D materials with elements beyond those traditionally associated with MAX phases and MXenes, and expand the range of attainable properties. This has implications for the tuning potential of these materials in applications for, e.g., energy storage and catalysis, as well as for new diverse magnetic MAX phase and MXene properties.

Tuesday	**MXene-enabled electronic applications**
11:50	**Husam N. Alshareef**, Jehad El-Demellawi, Shaobo Tu, Yongiju Lei
	Materials Science and Engineering, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia

MXenes are one the most fascinating families of 2D materials. They exhibit a unique set of properties including excellent electrical conductivity, surface redox activity, ability to intercalate many types of ions and molecules, tunable interlayer spacing, and large surface area. As a result, they have great potential in a large number of applications. In our group, we have been focusing on developing processes and devices that capitalize on the excellent properties of MXenes.

In this talk, I will review some of these recent developments showing that MXenes can be used as electrical contacts for devices and circuits. Specifically, we fabricated thin film electronics (including transparent CMOS) using all-MXene electrical contacts integrated with n-type and p-type oxide semiconductors, with excellent performance. Further, we have developed a synthesis process to produce highly textured ferroelectric crystals such as $KNbO_3$ and $LiNbO_3$ that inherit the 2D character from MXenes.

Capitalizing on the abundant surface charges of MXenes, we have developed MXene-polymer hydrogels with unique sensing capabilities that outperform existing hydrogel sensors. Recently, we have shown that MXenes can be used as fillers that enhance the dielectric constant of polymers more than any other carbon-based conductive filler due to their conductivity, large surface area, and abundant surface charges. Further, we have combined spectroscopy and microscopy to provide a fundamental understanding of MXene surface plasmons, and how functional groups on the surface of MXenes can change their plasmonic character. Further, we have demonstrated electrochemical microsupercapacitors with very high frequency response that outperform commercial Al electrolytic capacitors based on MXene interdigital electrode materials. These and other recent developments in our group will be discussed.

Tuesday	**Properties and applications of MXenes from first-principles perspective**
14:00	**Mohammad Khazaei**
	New Industry Creation Hatchery Center (NICHe), Tohoku University, Sendai, Japan

Reducing the dimensionality of a system is often associated with enhanced quantum effects and increased correlations, resulting in exceptional electronic, optical, and magnetic properties. Specifically, two-dimensional materials present opportunities for manifestation of concepts and phenomena that may not be prominent or have not been observed in bulk materials. Among various two-dimensional (2D) materials particularly the transition-metal-containing ones provide an excellent ground for exploring and exploiting the internal degrees of freedom of electrons — charge, orbital, and spin — and their interplay for fundamental research and device applications.

There are many transition metal-based 2D materials in the literature. Among them, nowadays MXenes are truly at the cutting edge of materials research and promote new scientific and technological horizons. I have performed systematic research on this very promising family of advanced materials to exploit their novel and unique properties.

In this presentaion, I would like to discuss the trivial and nontrivial electronic structures, magnetic, work function, and surface state properties of MXenes as well as their possible applications as thermoelectric or piezoelectric materials.

Tuesday	**Two-dimensional titanium carbonitride, a novel member of the MXenes family**
14:40	**Michael Naguib**
	Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, United States of America

The chemical space of two-dimensional (2D) materials has expanded significantly in the recent years by introducing MXenes, which is a large family of 2D transition metal carbides and carbonitrides of composition $M_{n+1}X_nT_z$; M is an early transition metal (e.g. Ti, V, Nb, Mo), X is carbon or nitrogen, *n* =1-3 and Tz stands for mixture of surface terminations (e.g. O, OH, F).

The chemical diversity of MXenes is combined with a wide range of potential applications ranging from electrochemical energy storage to catalysis. Most of studies on MXenes focused on the first reported MXene *viz.* $T_i3C_2T_z$, much smaller number of studies focused on other transition metals including ordered mixed and solid solutions at the M sites in MXenes. While nitrogen doping nanomaterials including transition metal carbides and oxides are known to be a very promising approach for altering materials properties and performance, very limited number of studies focused on carbonitride MXene.

Herein, the characteristic differences between $Ti_3C_2T_z$ and Ti_3CNT_z MXenes from both structure and surface chemistries points of views are discussed based on experimental results obtained using multiple techniques and theoretical calculations. Also, the performances of Ti_3CNT_z as electrode materials for electrochemical energy storage electrocatalysis in addition to their performance as catalysts are compared to that of $Ti_3C_2T_z$.

Wednesday	**On MXenes and clays: or what happens between the sheets**
9:00	**Michel W. Barsoum**
	Department of Materials Science and Engineering, Drexel University, Philadelphia, PA, United States of America

Discovered in 2011, the 2D early transition metal carbides known as MXenes - obtained by etching the A-layers from the MAX phases - have generated substantial interest in the scientific community because of their potential in an ever-expanding host of applications. Whether during etching or use, it is critical to understand what happens in the interlayer space. In most applications, the first step is to etch and wash MXene multilayers, MLs, until they disperse.

Using primarily XRD diffraction, the relationship between etchant used and washing protocols and the swelling of the interlayer space of Ti3C2Tx MLs is elucidated. How changing the intercalant cations can change the spacing, and even the nature of ML $Ti_3C_2T_x$ from hydrophilic to hydrophobic, is discussed. How to render MXenes oxidation resistant in aqueous solutions is described. Lastly, the similarities of MXenes and clays are overviewed.

Wednesday	**Tailoring the surface-chemistry of 2-dimensional MXenes**
9:40	**Per O.Å. Persson**
	Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

Transition metal carbides, carbonitrides and nitrides, MXenes, constitute the latest addition to the ever-growing family of two-dimensional (2D) materials.[1] Since their discovery in 2011, MXenes have outperformed existing materials for a range of applications such as energy storage [2], water filtering [3], electromagnetic shielding [4], as catalysts for H_2 evolution from water [5] and as astonishingly effective materials for capturing CO_2 [6] to name but a few examples. Their outstanding performance is accredited to a range of properties, e.g. hydrophilic and conductive, that can be attributed to a rich transition metal chemistry. Ultimately, the range of properties are dictated by the tailoring potential of the MXenes. In this respect, MXenes stand out in stark contrast to commonly employed 2-dimensional structures.

The first MXene to be discovered was $Ti_3C_2T_x$, and this material has remained the archetype MXene ever since. Currently, in excess of 20 complementary structures have been synthesized with many more predicted from theoretical investigations.[7] The general formula to describe MXenes, $M_{n+1}XT_x$, identifies that the tailoring potential in the MXene family is vast. In addition to choice of thickness (n) and X element, for instance, M can be a range of single transition metal elements, or an extensive set of combinations between multiple M elements in an ordered or disordered condition. Similarly, the range and corresponding potential mix of terminating elements or molecules is an apparent key in determining the final MXene properties.

The present contribution discusses recent advances in structural ordering and tuning of surface terminations, as revealed by high resolution electron microscopy and spectroscopy in combination with X-ray photoelectron spectroscopy methods.

References

[1] M. Naguib, et al. *Adv. Mater*. 2011, 23: 4248-4253
[2] B. Anasori, M. R. Lukatskaya, Y. Gogotsi, *Nature Reviews Materials* 2017 2: 16098
[3] C. E. Ren et al., *J. Phys. Chem. Lett.*, 2015, 6: 4026-4031
[4] F. Shahzad et al *Science* 2016, 353: 1137-1140
[5] C. H. Wang, et al., *Energy Environ. Sci.*, 2013, 6: 943-951
[6] I. Persson et al. *Adv. Mater.* 2019, 31: 1805472
[7] M. Khazaei, et al. *Adv. Funct. Mater.* 2013, 23: 2185-2190

Wednesday	When molecular science meets 2D materials: Orchestrating multiple functions
10:50	**Paolo Samorì**
	Institut de Sceinces et d'Ingénierie Supramolécule, Université de Strasbourg, France

During the last decade the scientific community has witnessed a tremendous progress on the production and properties optimization of 2D materials for numerous technological applications in opto-electronics, energy (generation and storage), photonics, etc. Next major steps forward from both fundamental and more technological viewpoint require the fine tuning of the properties of such extraordinary materials, in view of the specific applications. Such a modulation can be achieved by combining the unique characteristics of the single layers with the virtually-infinite variety of molecular systems each holding specific properties, thereby developing advanced hybrid materials exhibiting enhanced or novel functions for the chosen applications.

In my lecture, I will review our recent activity on the covalent and non-covalent functionalization of layered materials with ad hoc (macro)molecules in order to create artificial responsive hetero-structures as well as functional foams and coatings which can operate as selective chemical sensors. I will describe how the same approaches can be exploited to fabricate highly sensitive pressure sensors which can monitor heartbeats, thus holding great potential for their integration in medical diagnostic devices or sport apparatus.

Overall my lecture will shows the disruptive potential of chemical approaches to generate smart 2D materials-based hybrid systems with tailored made properties to address societal needs in electronics, sensing and energy applications

References

[1] For review articles on leveraging the production of graphene in liquid media via supramolecular approaches: (a) A. Ciesielski, P. Samorì, *Chem. Soc. Rev.* 2014, 43, 381-398. (b) A. Ciesielski, P. Samorì, *Adv. Mater.* 2016, 28, 6030–6051.
[2] For liquid-phase exfoliation of 2D materials to generate multiresponsive inks: (a) A. Ciesielski, S. Haar, M. El Gemayel, H. Yang, J. Clough, G. Melinte, M. Gobbi, E. Orgiu, M.V. Nardi, G. Ligorio, V. Palermo, N. Koch, O. Ersen, C. Casiraghi, P. Samorì, *Angew. Chem. Int. Ed.* 2014, 53, 10355–10361. (b) M. Döbbelin, A. Ciesielski, S. Haar, S. Osella, M. Bruna, A. Minoia, L. Grisanti, T. Mosciatti, F. Richard, E.A. Prasetyanto, L. De Cola, V. Palermo, R. Mazzaro, V. Morandi, R. Lazzaroni, A.C. Ferrari, D. Beljonne, P. Samorì, *Nat. Commun.* 2016, 7, 11090.
[3] For reviews on tuning the properties of 2D materials via molecular approaches: (a) S. Bertolazzi, M. Gobbi, Y. Zhao, C. Backes, P. Samorì, *Chem. Soc. Rev.* 2018, 47, 6845-6888. (b) M. Gobbi, E. Orgiu, P. Samorì, *Adv. Mater.* 2018, 30, 1706103.

[4] For responsive hybrid van der Waals heterostructures: (a) M. Gobbi, S. Bonacchi, J. Lian, Y. Liu, X.-Y. Wang, M.-A. Stoeckel, M.A. Squillaci, G. D'Avino, A. Narita, K. Müllen, X. Feng, Y. Olivier, D. Beljonne, P. Samorì, E. Orgiu, *Nat. Commun.* 2017, 8, 14767. (b) M. Gobbi, S. Bonacchi, J.X. Lian, A. Vercouter, S. Bertolazzi, B. Zyska, M. Timpel, R. Tatti, Y. Olivier, S. Hecht, M.V. Nardi, D. Beljonne, E. Orgiu, P. Samorì, *Nat. Commun.* 2018, 9, 2661.
[5] For pressure sensors based on molecule-graphene hybrids: C.-B. Huang, S. Witomska, A. Aliprandi, M.-A. Stoeckel, M. Bonini, A. Ciesielski, P. Samorì, *Adv. Mater.* 2018 in press (DOI: 10.1002/adma.201804600)

Wednesday 11:30	**Observing MXenes with soft X-ray light**
	Tristan Petit
	Institute for Nanospectroscopy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany

MXenes are an exciting 2D materials family with a fast-growing number of members due to the high versatility of their chemical and physical structure and surface terminations. MXenes have led to significant developments in widely diverse fields such as electrochemical energy storage, biomedical or sensing applications, which often rely on strong interactions with their environment. These interactions are however generally poorly understood so far and would strongly benefit from the development of *in situ/operando* methods that can be applied to probe changes in the chemical and electronic structure of MXenes exposed to different environments.

Synchrotron-based soft X-ray spectroscopies, composed in particular of X-ray absorption (XA), emission (XE) and photoemission (PE) spectroscopies, are particularly adapted to the characterization of MXenes. Especially, the use of synchrotron light allows energy-sensitive measurements, high spatial resolution and environment flexibility. The soft X-ray energy range (200-2000 eV) is well-adapted for MXenes because transition metal L-edges and light elements (C, N, O, F) K-edges lie in this range and can be excited separately. The complementarities of these different methods will be discussed in this presentation and opportunities for their application to MXenes will be highlighted, especially in terms of *in situ/operando* characterization in liquid environment.

First examples of characterization of $Ti_3C_2T_x$ (T_x being the surface termination) MXenes using XAS in vacuum and in aqueous medium will be presented. In particular, strong changes of the MXene chemical structure after intercalation with organic molecules and ions will be highlighted. Using X-ray Photoelectron Emission Microscopy (X-PEEM), chemical mapping of individual micrometer-sized MXene flakes in vacuum with a spatial resolution <30 nm will also be presented. These results will illustrate the high relevance of soft X-ray spectro/microscopy for the characterization of electronic and chemical structure of MXene materials and further perspectives will be discussed.

Wednesday

14:00

Triple-hybridization of MXene/Chevrel and carbon electrodes in saturated LiCl solution for fast energy storage: Fundamental aspects of hybrid devices

Mikhael D. Levi

Department of Chemistry and BINA-BIU Center for Nanotechnology and Advanced Materials, Bar-Ilan University, Ramat-Gan, Israel

Electrochemical capacitors are vital systems for fast energy delivery. Their surface-based adsorption/redox mechanisms enable high-power densities and long cycling life at the expense of the relatively low documented energy densities. A general approach frequently used in different fields of modern material science consists of designing new materials or devices via integration (or hybridization) of contrastingly different material properties linked to these devices. Recently new concepts of hybridization of battery and supercapacitor electrodes have been intensively developing and discussed in the energy storage field [1,2]. The hybridization implies matching intrinsic electrochemical windows for battery and supercapacitor components of the integrated electrode. Next, when such a hybrid electrode is coupled with another supercapacitive electrode in an asymmetric cell, their further hybridization is required in order to significantly increase the cell voltage.

With the goal of achieving simultaneously high-energy and high-power density of hybrid negative electrode, we have recently proposed the use of pseudocapacitive 2D MXene (Ti_3C_2) as a convenient matrix to incorporate intercalation particles of one of ultrafast battery material, namely, the Chevrel phase electrode (Mo_6S_8) for fabrication of free-standing, flexible, binder-free hybrid electrodes [3]. Further hybridization was extended to its integration with a positive nanoporous carbon electrode revealing the maximum pseudo-equilibrium cell voltage of 2.05 V, the highest ever reported for MXene-based materials in cells of asymmetrical geometry using aqueous electrolytes. Important innovation is the use of saturated (14 M) aqueous LiCl solution of high electric conductivity, low density and viscosity revealing much better performance than the conventional aqueous solution of LiTFSI [4]. We believe that rapid progress in the field of hybrid energy storage systems operating in aqueous-based electrolytes will soon be intensively explored resulting in a wide spectrum of high energy and power density applications.

References

[1] H. S. Choi and C. R. Park, *J. Power Sources*, **2014**, 259, 1–14.
[2] X. Guo, X. Xie, S. Choi, et al. *J. Mater. Chem. A*, **2017**, 5, 12445–12452.
[3] F. Malchik, N. Shpigel, M.D. Levi, T. S. Mathis, A. Mor, Yury Gogotsi, and Doron Aurbach, *J. Mater. Chem. A*, **2019**, 7, 19761-19773.
[4] L. Suo, O. Borodin, T. Gao, et al. *Science*, **2015**, 350, 938–43.

Wednesday

14:40

2D $Ti_3C_2T_x$ MXene materials for electrochemical energy storage

Hui Shao[1,2], Pierre-Louis Taberna[1,2], Patrice Simon[1,2]

[1] CIRIMAT, UMR 5058, Université Paul Sabatier, CNRS, Toulouse, France

[2] Réseau sur le Stockage Electrochiimique de l'Energie (RS2E), FR CNRS 3459, Amiens, France

2D transition metal carbides, carbonitrides and nitrides, also known as MXenes, are synthesized by selectively remove the A atom layer from parent MAX phase using etchant such as aqueous fluoride-containing acidic solutions [1]. MXenes have shown great potential in electrochemical energy storage devices due to its electronic, mechanical and optical properties. Herein, we will present our strategies to optimizing the electrochemical performance of $Ti_3C_2T_x$ MXene in both aqueous and non-aqueous systems. In sulfuric acid electrolytes, a $Ti_3C_2T_x$ MXene hydrogel electrodes demonstrated a high volumetric capacitance of 1500 F cm^{-3} and 350F g^{-1} for the gravimetric capacitance, exceeding those conventional carbon materials [2].

Differently, MXene electrodes performances were limited in non-aqueous systems [3,4]. It is crucial to increase MXenes capacitance in non-aqueous electrolytes since non-aqueous systems can offer a larger voltage window (> 2.5 V), thus lead to high energy density. Interestingly, our recent results demonstrated that tailored $Ti_3C_2T_x$ MXene electrodes could deliver capacitance up to 200 F g^{-1} with a 2.4 V voltage range in non-aqueous Li^+-containing electrolyte, by controlling the architecture [5]. Moreover, we proposed a new Lewis acidic etching synthesis route for preparing MXenes with enhanced electrochemical performance in non-aqueous electrolyte. The obtained $Ti_3C_2T_x$ MXene delivers a Li-ion storage capacity up to 738 C g^{-1} (at a potential range of 2.8 V) as well as high rate performance in a carbonate $LiPF_6$-based electrolyte. This offers new opportunities for MXene materials for future energy storage applications.

References

[1] Anasori, B., Lukatskaya, M. R., & Gogotsi, Y. (2017). *Nature Reviews Materials*, 2(2), 16098.

[2] Lukatskaya, M. R., Kota, S., Lin, Z., Zhao, M. Q., Shpigel, N., Levi, M. D., Halim, J, Taberna, P. L, Barsoum, M, Simon, P, Gogotsi, Y. (2017). *Nature Energy*, 2(8), 17105.

[3] Lin, Z., Rozier, P., Duployer, B., Taberna, P. L., Anasori, B., Gogotsi, Y., Simon, P. (2016). *Electrochemistry Communications*, 72, 50-53.

[4] Lin, Z., Barbara, D., Taberna, P. L., Van Aken, K. L., Anasori, B., Gogotsi, Y., Simon, P. (2016). *Journal of Power Sources*, 326, 575-579.

[5] Wang, X., Mathis, T. S., Li, K., Lin, Z., Vlcek, L., Torita, T., Osti, N, Hatter, C, Urbankowski, P, Sarycheva, A, Tyagi, M, Mamontov, E, Simon, P, Gogosti, Y. (2019). *Nature Energy*, 1.

Wednesday	**Water treatment and environmental remediation applications of two-dimensional metal carbides (MXenes): Opportunities and challenges**
15:50	**Khaled Mahmoud**
	Qatar Environment and Energy Research Institute, Hamad Bin Khalifa University, Doha, Qatar

Characteristic properties of two-dimensional (2D) transition metal carbides and nitrides (MXenes), such as high conductivity, hydrophilicity, and catalytic activity have led to a growing research interest for their use in environmental remediation and water treatment applications. The ability to process MXenes into flexible films with negative surface charge and hydrophilicity adds a possibility to control ion flux and biofouling by applying a small potential to the membrane. MXene shows a much higher antibacterial efficiency toward both Gram-negative and Gram-positive bacteria as compared with other 2D nanomaterials.

Consequently, MXene membranes demonstrated outstanding water flux, selective rejection to salts and organic molecules, which makes it ideal UF/NF membrane materials. Moreover, MXene has been successfully used for the efficient adsorption and removal of heavy metals such as Hg, and Cu. This talk summarizes the recent advances in the applications of MXenes as adsorbents, desalination membranes, electrodes for electrochemical deionization, and catalytic or antibacterial agents for water purification and other environmental remediation processes.

The overview also features discussions on the computational attempts, biocompatibility, and environmental impact in the exploration of MXenes for water applications, highlighting the challenges and opportunities of these advanced 2D materials. The biocompatibility and cytotoxicity assessment of MXene and their impact on the environment will be highlighted.

Wednesday	**Electrochemical water desalination with transition metal carbides and dichalcogenides**
16:30	**Volker Presser**
	Department of Chemistry, University of Southampton, United Kingdom

Capacitive deionization (CDI) accomplishes energy-efficient water desalination by electrosorption of ions at the interface between saline solutions and nanoporous carbon electrodes.[1] The strictly physical process of ion electrosorption yields salt adsorption capacities of typically 15-20 mg/g (mg salt per g of the electrode) have been reported. The use of carbon limits the maximum achievable charge storage capacity and restricts the applicability of CDI to very low salt concentrations (typically below 20-50 mM). This issue originates from unfavorable co-ion expulsion from carbon nanopores concurrently occurring during counter-ion adsorption. Only once all co-ions have become depleted in the pores, permselective ion removal is accomplished. To transfer CDI from a niche technology to a more largescale use, new electrode materials and cell concepts need to be explored.

The use of Faradaic electrode materials has had a transformative impact on the research field for electrochemical water desalination. The presentation will summarize key aspects of the implementation of ion intercalation materials for the deionization of aqueous media with ion concentration levels typical brackish water and seawater. We demonstrate the facile use of pseudocapacitive materials to effectively remove cations and anions from saline media. Transition metal carbides (MXene) are ideal candidates for this task per their ability to afford permselective ion intercalation even at high molar strength.[2]

With enhanced ion mobility and lowered energetic barriers, there is even an improved desalination performance when increasing the salt concentration from low (10 mM) to high levels (1 M). Careful design of the MXene electrodes and operation within the electrochemical window enables performance stability. The presentation will compare the electrochemical desalination of Ti_3C_2- and $Mo_{1.33}C$-MXene with the results obtained from transition metal dichalcogenides, such as MoS_2 and TiS_2.[3] While MoS_2 is a nearly perfect pseudocapacitor and yields a desalination performance comparable to MXene, TiS_2 features distinct cation intercalation peaks which allow the design of desalination batteries. The dependence of ion intercalation potentials on the type of cation further allows selective ion removal for advanced sustainable technologies.[4]

References

[1] M. E. Suss, S. Porada, X. Sun, P. M. Biesheuvel, J. Yoon and V. Presser, *Energy & Environmental Science* 2015, 8, 2296-2319.

[2] a) P. Srimuk, J. Halim, J. Lee, Q. Tao, J. Rosen and V. Presser, *ACS Sustainable Chemistry & Engineering* 2018, 6, 3739-3747; b) P. Srimuk, F. Kaasik, B. Krüner, A. Tolosa, S. Fleischmann, N. Jäckel, M. C. Tekeli, M. Aslan, M. E. Suss and V. Presser, *Journal of Materials Chemistry A* 2016, 4, 18265-18271.
[3] a) P. Srimuk, J. Lee, S. Fleischmann, S. Choudhury, N. Jäckel, M. Zeiger, C. Kim, M. Aslan and V. Presser, *Journal of Materials Chemistry A* 2017, 5, 15640-15649; b) P. Srimuk, J. Lee, A. Tolosa, C. Kim, M. Aslan and V. Presser, *Chemistry of Materials* 2017, 29, 9964-9973.
[4] P. Srimuk, J. Lee, S. Fleischmann, M. Aslan, C. Kim and V. Presser, *ChemSusChem* 2018, 11, 2091-2100.

Thursday	**2D crystals for inkjet-printed (opto)electronics and sensors: Towards manufacturability**
9:00	**Tawfique Hasan**
	Cambridge Graphene Centre, Engineering Department, Cambridge University, United Kingdom

Two-dimensional (2D) crystals have shown huge promises in a wide variety of applications with large form factors. The ability to formulate their functional inks is of paramount importance for additive manufacturing of these devices [1,2].

In the first part of my talk, I will discuss fundamental aspects of droplet drying and how solvent composition engineering enables uniform deposition. I will discuss our observation on a new phenomenon [3,4] that allows us to deform the shape of a drying droplet, sharply deviating from the natural spherical cap geometry. I will show that our ink formulation enables high device-to-device uniformity for a wide range of 2D crystals, their hybrids and heterostructures for applications in photonics, (opto)electronics and sensing [5,6]. I will then present our recent results on pure solvent based MXene inks suitable for additive patterning for transparent electronics [7].

In the final part of my talk, I will briefly discuss other traditional printing technologies that we use in our laboratory to print functional materials on to conformable substrates [8] as well as scalable, large format print technologies.

References

[1] G. Hu et al. Functional inks and printing of two-dimensional materials, *Chemical Society Reviews*, 47, 3265-3300 (2018).
[2] L. Ng et al. Functional Inks and Printing of Graphene and Related 2D Materials: Technology, *Formulation and Applications*, (Springer, 2019).
[3] G. Hu et al. Black phosphorus ink formulation for inkjet printing of optoelectronics and photonics, *Nature Communications*, 8, 278 (2017).
[4] G. Hu et al. Wafer-scale inkjet-printed 2d crystal devices enabled by solutal Marangoni effect, Under review (2019).
[5] X. Wang et al. Realization of vertical metal semiconductor heterostructures via solution phase epitaxy, *Nature Communications*, 9, 3611 (2018).
[6] T.-C. Wu, Inkjet-printed CMOS-Integrated Graphene-Metal Oxide Sensors for Breath Analysis, Under review (2019).
[7] S. Liu et al. Inkjet printed transparent electronics, Under preparation.
[8] L. W. T. Ng et al. Conformal printing of graphene for single and multi-layered devices on to arbitrarily shaped 3D surfaces, *Advanced Functional Materials*, 1807933 (2019).

Thursday	**MXene conductive inks for energy storage and electronics**
9:40	**Chuanfang (John) Zhang**
	Swiss Federal Laboratories for Materials Science and Technology (EMPA), Dübendorf, Switzerland

Two-dimensional transition metal carbides and nitrides, so-called MXenes, have shown outstanding performances in electrochemical energy storage, water purification, electromagnetic interfering shielding, single-atom catalysis and many other applications, and have quickly attracted intensive attention around the world. These cutting-edge applications require the production of high quality MXene nanosheets, high concentration MXene inks and scalable manufacturing of MXene-based devices. However, these have proven to be quite challenging and reports on these aspects are quite limited.

In this talk, I will begin with the introduction of MXenes by reviewing their synthesis, properties and applications. Then, I will illustrate the oxidation kinetics of MXene aqueous solutions, which is the prerequisite for the industrial application of MXenes.[1] Following up, high-quality MXene nanosheets synthesis, ink formulations for the efficient fabrication of high-performance transparent conductive films/coatings [2] and scalable production of micro-supercapacitors assisted by the additive-manufacturing techniques,[3] are demonstrated. The ink viscous nature also allows the MXene nanosheet network to perform as a conductive binder for Si nanoparticles, resulting in high mass-loading anodes with an ultrahigh areal capacity (5 times higher than that of commercial anode).[4]

In addition, formulation of organic MXene inks for scalable additive-free printing of energy storage devices, as well as formulation of composite ink for lithium-sulfur batteries, are also demonstrated.[5-7] The excellent charge storage and optoelectronic properties can be well attributed to the impressive electrical, mechanical and electrochemical nature of MXene nanosheet, holding great promises for the next generation applications including energy, environment and electronics.

References

[1] C. Zhang, et al., *Chemistry of Materials*, 2017. 29 (11), 4848-4856
[2] C. Zhang, et al., *Advanced Materials*, 2017, 29, 1702678
[3] C. Zhang, et al., *Advanced Functional Materials*, 2018, 28, 1705506
[4] C. Zhang, et al., *Nature Communications*, 2019, 10, 849
[5] C. Zhang, et al., *Advanced Science*, 2018, 5, 1800502
[6] C. Zhang, et al., *Nature Communications*, 2019, 10, 1795
[7] C. Zhang, et al., *Advanced Functional Materials*, 2019, DOI: 10.1002/adfm.201901907

Thursday

10:50

MXene chemistry for applications

Vadym N. Mochalin

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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 largely terra incognita. In this presentation we will discuss recent progress in understanding MXene chemistry and harnessing it for development of applications.

For example, during delamination and storage in ambient air environment, spontaneous oxidation of MXene flakes leads to formation of titanium oxide, a process that can be harnessed for simple, inexpensive, and environmentally benign manufacturing MXene–titania composites for optoelectronics, sensing, and other applications [5]. We show that partially oxidized MXene thin films containing the in situ formed phase of titanium oxide have a significant photoresponse in the UV region of the spectrum. The relaxation process of photoexcited charge carriers, which takes a long time (~24 h), can be accelerated in the presence of oxygen and water vapor in the atmosphere.

These properties of spontaneously formed MXene-titania thin films make them attractive materials for photoresistors with memory effect and sensitivity to the environment, as well as many other photo- and environment-sensing applications.

Other selected examples illustrating connections between understanding MXene chemistry and development of their applications will also be considered.

References

[1] Y. Li, S. Huang, C. Wei, C. Wu, V. N. Mochalin *Nature Communications*, 10, 3014 (2019)
[2] M. Naguib, V. N. Mochalin, M. W. Barsoum, Y. Gogotsi, *Advanced Materials*, 26(7), 992-1005 (2014)
[3] J. Yi, L. Du, J. Li, L. Yang, L. Hu, S. Huang, Y. Dong, L. Miao, S. Wen, V. N. Mochalin, et al., *2D Materials*, 6, 045038 (2019)
[4] Y. Dong, S. Chertopalov, K. Maleski, B. Anasori, L. Hu, S. Bhattacharya, A. M. Rao, Y. Gogotsi, V. N. Mochalin, R. Podila, *Advanced Materials*, 30(10), 1705714 (2018)
[5] S. Chertopalov, V. N. Mochalin, *ACS Nano*, 12(6), 6109-6116 (2018)

Thursday	**MXenes for biomedical applications**
11:30	**Susan Sandeman**
	School of Pharmacy and Biomolecular Sciences, University of Brighton, United Kingdom

The properties of MXenes make them highly suited to a range of biomedical applications. They are hydrophilic and so can more easily interact with biological media than their hydrophobic counterparts. They are conductive and so can be applied to neural signalling or as actuators for bio-sensing and triggered release of biomolecules. They have reversible intercalation properties which may lend themselves to adsorption of small biotoxins or targeted slow release systems. They have reactive surface chemistry which may be used to create hybrid systems and combinatorial medical devices related to adsorption. However, there are a limited number of studies related to the biocompatibility and biomedical efficacy of MXenes and findings are inconsistent.

In the following study a range of in vitro biocompatibility assays were used to characterise the interaction of Ti3C2Tx MXenes with human cells, bacteria and blood. Two medical device applications were then considered. The first was the use of MXene to address the challenge of urea removal in the wearable artificial kidney. The second was the use of MXene as an optoelectronic coating for accommodating intraocular lens design to treat cataracts. MXene effects on cell viability, necrosis, apoptosis, induction of inflammation, blood cell activation, bacterial growth and adsorption of biological toxins were investigated in addition to the development of methods to form transparent, conductive coatings for mechano-actuation.

No significant impact on cell growth dynamics was observed. MXenes did not alter viable cell growth, induce cell death by apoptotic or necrotic pathways or activate oxidative stress or other inflammatory pathways. MXenes were haemocompatible and did not induce activation of blood platelets, haemolysis or coagulation cascades. MXene did not exhibit antibacterial properties. No impact on the growth of gram positive and gram negative bacterial species occurred in contrast to known antimicrobial nanoparticles and silver modified graphene variants. MXenes were adsorptive for marker biological toxins and formed transparent electrically conductive thin films onto intraocular lenses with no negative impact on lens epithelial cell physiology.

Results support the development of MXenes for biomedical applications related to functional tissue replacement.

Thursday	**2D transition metal carbide (MXene) thin film for EMI shielding**
13:40	**Chong Min Koo**
	Materials Architecturing Research Center, Korea Institute of Science and Technology, Daedeok Innopolis, Daejeon, South Korea KU-KIST Graduate School of Converging Science and Technology, Korea University, Seoul, South Korea

MXenes are a family of 2D transition metal carbides, nitrides, and carbonitrides with the general formula $M_{n+1}X_nT_x$ (n = 1, 2, or 3; M = transition metal, e.g. Ti, Nb, Mo; X = C and/or N; T = surface termination, e.g. –OH, –F, –O).

Unlike other 2D materials, MXenes offer an attractive combination of high electronic conductivity (~5000 S/cm), low density, hydrophilicity, and processability. Transition metal carbide (MXene) have been considered as an effective EMI shielding material since outstanding EMI shielding effectiveness of MXene was reported in 2016. 10μm-thick Ti_3C_2 MXene film had the shielding effectiveness over 60 dB. However, still it is lack of understanding EMI shielding behavior of MXene materials, especially, at thin thickness. In this presentation, we present the EMI shielding behavior of MXene film in a wide range of thicknesses ranging from a few nanometers to forty micrometers.

It reveals that MXene is an ideal candidate material for light-weight thin film shielding applications.

Thursday

14:20

Scalable synthesis of $Ti_3C_2T_x$ MXene and a reactor design for MXene synthesis

Vitalii Balitskyi[2], Christopher E. Shuck[3], Yury Gogotsi[3], Oleksiy Gogotsi[1,2], **Veronika Zahordona[1,2]**

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Scaling the production of synthetic two-dimensional (2D) materials to industrial quantities has faced significant challenges due to synthesis bottlenecks whereby only a few (graphene, BN, MoS2) have been produced in large volumes for industrial use. These challenges typically stem from bottom-up approaches limiting the production to the substrate size or precursor availability for chemical synthesis and/or exfoliation. In contrast, MXenes, a large class of 2D transition metal carbides, nitrides, and carbonitrides, are produced via a top-down synthesis approach. The selective wet etching process does not have similar synthesis constraints as some other 2D materials. The reaction occurs in the whole volume. Therefore, the process can be readily scaled with reactor volume.

We designed and manufactured 1L and 2L computer-controlled reactors for synthesis of MXenes form MAX phase precursors. Details of the reactor design will be described and comparison of the data between large scale synthesis in the reactor and small-batch lab synthesis will be provided. The synthesis of 2D titanium carbide MXene ($Ti_3C_2T_x$) in two batch sizes, 1 and 50g, was studied to determine if large-volume synthesis affects the resultant structure or composition. Characterization of the morphology and properties of the produced materials using a variety of experimental techniques showed that the materials produced in both batch sizes are essentially identical.

This illustrates that MXene experiences no change in structure or properties when scaling synthesis, making them viable for further scale-up and commercialization.

POSTER OVERVIEW

No. 1:	**Influence of reducing environment on charge storage behavior of two-dimensional $Mo_{1.33}C$ MXene** Bilal Ahmed / Linköping University
No. 2:	**In situ X-ray absorption spectroscopy electrochemical study of intercalated $Ti_3C_2T_x$ MXene: Towards high capacitance performance** Ameer Al-Temimy / Helmholtz-Zentrum Berlin
No. 3:	**Multifunctional polymer composites doped with MXenes nanoparticles for advanced applications** Andrey Aniskevich / University of Latvia
No. 4:	**Wet chemical based synthesis and exfoliation of MAX phase Cr_2GaC** Christina S. Birkel / Arizona State University
No. 5:	**Multilayered 2D sheets of Ti_2NT_x MXene: anticancer, selective and stable after delamination** Magdalena Birowska / University of Warsaw
No. 6:	**Implication of the interstratification process at stake in MXene on physical properties** Stéphane Célérier / University of Poitiers
No. 7:	**Insights into the elastic properties of 3D RE-containing MAX phases and their potential exfoliation to 2D MXenes** Aurelie Champagne / University of Louvain
No. 8:	**Chemiresistors based on Ti_3C_2 MXene** Sergii Chertopalov / Czech Academy of Sciences
No. 9:	**Flexible MXene devices for plasmonic photodetection** Jehad K. El-Demellawi / KAUST
No. 10:	**Large-scale synthesis of titanium-based MAX and MXenes** Oleksiy Gogotsi / Materials Research Centre, Kiev
No. 11:	**pH-dependent distribution of functional groups on titanium-based MXene** Rina Ibragimova / Aalto University
No. 12:	**Human-like collagen protein coated 2D multilayered Ti_3C_2 and Ti_2C MXenes for improved biocompatibility** Agnieszka M. Jastrzębska / Warsaw University of Technology

No. 13:	**Quality of MXene dispersion in various polymeric systems** Kateřina Kopecká / SYNPO, Pardubice
No. 14:	**A MXene-based wearable biosensor system for high-performance in-vitro perspiration analysis** Yongjiu Lei / KAUST
No. 15:	**Surface structure of MXene nanosheets investigated by scanning tunneling microscopy** Zhongpeng Lyu / Aalto University
No. 16:	**Superfast high-energy storage hybrid device composed of MXene and Chevrel-phase electrodes operated in saturated LiCl electrolyte solution** Fyodor Malchik / Bar-Ilan University
No. 17:	**Polymeric composites with 2D nanoparticles MXenes** Mária Omastová / Polymer Institute SAS, Bratislava
No. 18:	**Study of MXene nanoparticles aging** Michal Procházka / Polymer Institute SAS, Bratislava
No. 19:	**Silanization as an efficient way of protecting MXenes against oxidation** Błażej Scheibe / Palacký University Olomouc
No. 20:	**Mo_4VC_4: a two-dimensional MXene with five atomic layers of transition metals** Christopher E. Shuck / Drexel University
No. 21:	**Stability of MXenes dispersions – oxidation and use for air purification** Nadia Todorova / NSCR Demokritos, Athens
No. 22:	**Synthesis of a thermoresponsive hybrid MXene with switchable conductivity** Minh Hai Tran / TU Darmstadt
No. 23:	**MXene-derived ferroelectric crystals** Shaobo Tu / KAUST
No. 24:	**Two-dimensional titanium carbide (MXene) in accommodating lens design** Emma Ward / University of Brighton
No. 25:	**3D printing of freestanding MXene architectures for current collector-free supercapacitors** Wenji Yang / University of Manchester
No. 26:	**Strategies for enhancing the electrochemical activities of MXenes *via* chemical doping with nonmetallic electron donors** Yeoheung Yoon / Korea Research Institute of Chemical Technology

No. 27:	**Simulation on mechanical behaviour of polymer/MXene nanocomposites** Daiva Zeleniakiene / Kaunas University of Technology

No. 28:	**Synthesis and characterization of scandium and lutetium containing two dimensional carbides** Jie Zhou / Linköping University

No. 29:	**Atomic defects in monolayer ordered double transition metals carbide ($Mo_2TiC_2T_x$) MXene** Rasoul Khaledialidusti / NTNU, Trondheim

Poster	**Influence of reducing environment on charge storage behavior of two-dimensional $Mo_{1.33}C$ MXene**
No. 1	**Bilal Ahmed** and Johanna Rosén
	Department of Physics, Linköping University, Sweden

The utilization of MXenes in a wide range of applications, including energy storage, electromagnetic interference shielding and gas sensing, has garnered the research attention of academic and industrial communities. Recently, divacancy-containing $Mo_{1.33}C$ MXene has shown outstanding charge storage performance with an excellent specific capacitance of 339 F/g. Herein, we present a simple and cost-effective approach to tailor the surface chemistry of $Mo_{1.33}C$ MXene by introducing a reducing environment at low-temperatures and demonstrate that the supercapacitive performance can be further improved due to the partial removal of surface functional groups. The utilization of inert and inert/reducing environments altered the surface chemistry of MXenes, enhanced the electrochemically active surface area and led to a superior specific capacitance of 465 F/g, corresponding to a volumetric capacitance of 1581 F/cm^3. The detailed transmission electron microscopy and X-ray photoelectron spectroscopy are carried out to investigate the relationship between processing parameters, MXene surface chemistry and charge storage behavior.

Poster

No. 2

In situ X-ray absorption spectroscopy electrochemical study of intercalated $Ti_3C_2T_x$ MXene: Towards high capacitance performance

Ameer Al-Temimy[1,2], Michael Naguib[3], Babak Anasori[4], Katherine A. Mazzio[1], Ronny Golnak[1], Mailis Lounasvuori[1], Florian Kronast[1], Kaitlyn Prenger[3], Narendra Kurra[4], Mykola Seredych[4], Mohamad-Assaad Mawass[1], Simone Raoux[1,5], Yury Gogotsi[4] and Tristan Petit[1]

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MXenes are a new class of 2D materials consisting of transition metals carbides and nitrides that demonstrate extraordinary properties for electrochemical energy storage applications. In particular, $Ti_3C_2T_x$ (T_x describes the surface termination) MXenes have shown very large capacitance in sulfuric acid due to the surface redox (pseudocapacitive) charging mechanism[1]. Intercalation of $Ti_3C_2T_x$ by cations or molecules induces a larger spacing between the MXene sheets[2] facilitating ion transportation but its possible impact on the MXene surface chemistry remains unknown. It could however eventually result in different surface redox mechanisms. Tracking the changes of MXene surface chemistry of $Ti_3C_2T_x$, especially the average oxidation of Ti atoms, in situ in various environments could provide more insights into their energy storage mechanism.

The change in the surface chemistry of $Ti_3C_2T_x$ MXene is extremely important for many MXene-based applications. X-ray Absorption Spectroscopy (XAS) using soft X-rays is an element-sensitive technique that is very sensitive to surface chemistry and transition metal oxidation states. Herein, we present an XAS study of pristine, urea, Li-, Na-, K-, and Mg-intercalated $Ti_3C_2T_x$ in different environments. Electrochemical reaction coupled with *in situ* XAS at the Ti L-edge was conducted to probe the changes in the Ti oxidation state of Na-, K-, and Mg-$Ti_3C_2T_x$ MXenes in sulfuric acid. The electrochemical performance has been dramatically enhanced after intercalation. This study provides a basis for electrochemical performance of MXenes by applying the Ti L-edge sensitivity to probe the differences in the oxidation state of Ti atoms.

1. M. R. Lukatskaya et al., *Adv. Energy Mater* 2015, 5, 1500589
2. Muckley, E. S. *et al.*, *ACS Nano* 2017, 11, 11118–11126

Poster

No. 3

Multifunctional polymer composites doped with MXenes nanoparticles for advanced applications

Andrey Aniskevich[1], Daiva Zeleniakiene[2], Maria Omastova[3], Leon Mishnaevsky Jr.[4] and Oleksiy Gogotsi[5]

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The aim of the research is development of advanced multifunctional composites with outstanding electronic and mechanical properties by incorporation of novel MXene nanosheets into polymer matrixes. The concept explored in the research accounts for finding and extending the application potential of advanced MXene-doped polymers and validation of their effectiveness compared to well- known carbon-based and particularly graphene-doped polymers.

Objectives of the research are considered as:

- Development of model-integrated technology methods for synthesis of various MXenes and manufacturing of MXene-polymer composites;
- Experimental characterization of morphology, electrical, thermo-physical, and mechanical properties of MXenes and MXene/polymer composites;
- Development of multi-scale modelling tools for assessment of operational properties of MXene-polymer composites;

Expected results of the research are based on up-scaling of novel technologies for “close-to-industrial” synthesis of MXenes and MXene-doped polymer masterbatches and implementation of MXenes into design of structural polymer composites, including FRPs.

Acknowledgements
This project has received funding from the European Union’s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 777810.

Poster	**Wet chemical based synthesis and exfoliation of MAX phase Cr_2GaC**
No. 4	Minh H. Tran[2], Jan P. Siebert[2], Lothar Bischoff[2] and **Christina S. Birkel**[1,2]
	[1] Arizona State University, Tempe, USA [2] TU Darmstadt, Germany

We have developed a wet chemistry based synthesis method to access selected MAX phases, such as Cr_2GaC. The advantage is the enhanced processibility that we demonstrate by depositing the precursor gel onto amorphous hollow carbon microspheres. The resulting particles are highly crystalline and exhibit an anisotropic morphology that is different from the typical MAX phase microstructure. We have elucidated the formation mechanism and have extended this approach to further MAX phases.

Targeting a Cr-based MXene, we attempted the chemical exfoliation of the Cr_2GaC particles. Using hydrofluoric acid, the X-ray powder diffraction data and electron micrographs suggest that the MAX phase dissolves leaving Cr–C structures as the product. We discuss alternative exfoliation conditions and the resulting products based on X-ray diffraction and electron microscopy studies.

Poster

No. 5

Multilayered 2D sheets of Ti_2NT_x MXene: anticancer, selective and stable after delamination

A. Szuplewska[1], A. Rozmyslowska-Wojciechowska[2], T. Wojciechowski[1], Sz. Pozniak[2], **Magdalena Birowska**[3], M. Popielski[3], M. Chudy[1], W. Ziemkowska[1], L. Chlubny[4], D. Moszczyńska[2], A. Olszyna[2], J. A. Majewski[3] and A. M. Jastrzebska[2]

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The 2D Ti_2NT_x MXene is expected to pave the way of MXenes into many effective applications. Unfortunately, the first experimental studies carried out on 2D Ti_2NT_x monolayers revealed large difficulties in its synthesis and confirmed its low stability realized through rapid oxidation and decomposition. At the same time, their biological properties were not explored hindering the progress in the development of these phases. Our theoretical calculations confirmed that the multilayered Ti_2NT_x structures possess higher stability in comparison to single layered structures. Therefore, Ti_2AlN MAX phase was successfully etched into Ti_2NT_x MXene and further delaminated to obtain multilayered 2D sheets of the appropriate stability for biological studies. The in vitro tests were carried out using two pairs of normal and cancerous cell lines. Additionally, the potential mode of action of 2D Ti_2NT_x was investigated using reactive oxygen test as well as SEM observations. Our results indicate that multilayered 2D sheets of Ti_2NT_x showed higher toxicity towards cancerous cell lines in comparison to normal ones. The decrease in cells viability was dose-dependent. Generation of the reactive oxygen species as well as 2D sheets internalization were identified mechanisms of toxicity. We have shown that the 2D Ti_2NT_x in its multilayered form exhibits fair stability and can be investigated using in vitro studies. This gives a promise for its future application in biotechnology and nanomedicine.

Acknowledgements
Support of NCN through the grant SONATA (UMO-2017/26/E/ST8/01073) is acknowledged. M.B. is funded by the National Science Centre grant no. UMO- 2016/23/D/ST3/03446.

Poster

No. 6

Implication of the interstratification process at stake in MXene on physical properties

Stéphane Célérier[1], Simon Hurand[2], Cyril Garnero[1,2], Sophie Morisset[1], Mohamed Benchakar[1], Aurélien Habrioux[1], Patrick Chartier[2], Vincent Mauchamp[2], Nathaniel Findling[3], Bruno Lanson[3] and Eric Ferrage[1]

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The MXenes, among which $Ti_3C_2T_x$ is the most studied, are a large family of 2D materials with proven potential in a variety of application fields (*e.g.*, energy storage and conversion, water purification, electromagnetic interference shielding, humidity sensor, etc). For most of these applications, MXenes properties depend, at least partly, on their water sorption ability and on the induced structural swelling, which is commonly considered a stepwise process, like in clay-like materials. In the present study, we rather evidence the systematic coexistence of different hydrates in MXene interstratified crystals. Hydration heterogeneity and related structure disorder are described from the quantitative analysis of X-ray diffraction data. This specific methodological approach allows disentangling the complex interstratification and rationalizing the prediction of MXene electrical properties.[1] The widespread use of this approach paves the way for a systematic and thorough determination of MXene structure, including order-disorder, and thus for grasping the influence of structural disorder (hydration heterogeneity) on a large number of MXene physical properties (*e. g.* optical transparency, capacitance). Deciphering this complex structural disorder is also essential in the design of new MXene-based materials for a variety of applications (supercapacitors, batteries, water treatment…).

In a second part of the poster, our recent project (MXENECAT) funded by ANR (Agence National de la Recherche) relating to "Synthesis and functionalization of advanced 2D transition metal carbides (MXene): application to oxygen electrocatalysis (MXENECAT)" and started in january 2019 will be briefly described.

1. *Chem. Mater*. 2019, 31, 454-461

Poster

No. 7

Insights into the elastic properties of 3D RE-containing MAX phases and their potential exfoliation to 2D MXenes

Aurelie Champagne, M. W. Barsoum and J.-C. Charlier

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MAX phases, with formula $M_{n+1}AX_n$, are layered ceramics composed of 2D $M_{n+1}X_n$ sheets separated by A layers [Fig.1 & 2(a)], where M represents an early transition metal, A an element from groups 13 to 16, X either a carbon or a nitrogen atom, and n varies from 1 to 3 [1]. The chemical exfoliation of 3D MAX phases into 2D MXenes (Fig.1), reported in 2011, constitutes a major breakthrough in the synthesis of novel 2D systems [2]. Most MXenes exhibit a unique combination of excellent physical and chemical properties [3]. Thanks to their versatile chemistry and the control of their surface terminations, MXene is now the largest 2D family competing in an impressive number of applications. Recently, a new route to increase the elemental combination and to optimize MXene performance was proposed, consisting in the addition of a fourth element to the parent MAX phase. Historically, most MAX phase alloys existed as random solid solutions.

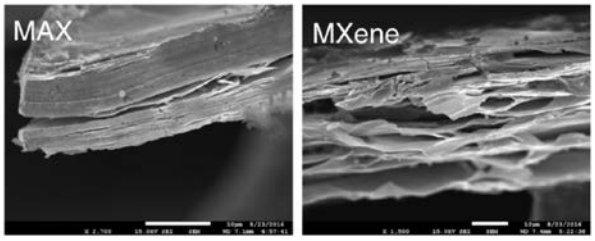

Figure 1: SEM images of a 3D MAX phase and the corresponding 2D MXene, after etching

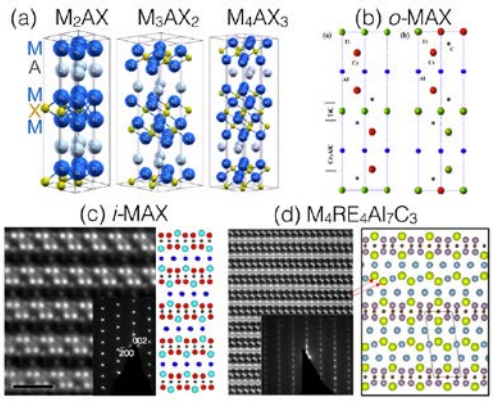

Figure 2: Atomic structures of different MAX systems, along with STEM images for (c) and (d).

In 2014, out-of-plane quaternary MAX phases (*o*-MAX) [Fig.2(b)] were discovered [4]. In 2017, in-plane ordered quaternary MAX phases (*i*-MAX) [Fig.2(c)] were theoretically predicted and successfully synthesized with the formula $(M^1_{2/3}M^2_{1/3})_2AlC$ where M^1 and M^2 are two metals ordered in-plane [5,6]. Recently, the existence of rare-earth (RE) containing *i*-MAX phases with the chemical formula $(M_{2/3}RE_{1/3})_2AlC$ was revealed [7], and similar layered family with stoichiometry $M_4RE_4Al_7C_3$ [Fig.2(d)] was simultaneously discovered and found to be ferromagnetic [8]. Since all these new MAX phases are Al-based, their conversion to 2D MXenes using chemical exfoliation should, in principle, be possible. To gain insight into the exfoliation possibility of RE-*i*-MAX phases, we perform ab initio calculations of electronic, vibrational, and elastic properties [9,10], from which both force constants and exfoliation energies are obtained. In addition, some materials properties, including bulk, shear, and Young's moduli, are computed and compared to experimental measurements.

[1] M.W. Barsoum, Progress in Solid State Chemistry 28 (2000), 201
[2] M. Naguib, Adv. Materials 26 (2014), 992
[3] M.R. Lukatskaya, Nature Comm. 7 (2016), 1
[4] Z. Liu, Acta Materialia 73 (2014), 186
[5] Q. Tao, Nature Communications 8 (2017), 1
[6] M. Dahlqvist, Science Advances 3 (2017)
[7] Q. Tao, Chem. Mater. 31 (2019), 2476
[8] Q. Tao, Phys. Rev. Materials 2 (2018) 114401
[9] A. Champagne, Phys. Rev. Materials 3 (2019) 053609 [10] A. Champagne, in preparation (2019).

Poster No. 8	**Chemiresistors based on Ti_3C_2 MXene**
	Sergii Chertopalov, Premysl Fitl, Martin Hruska and Jan Lancok
	Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic

The MXene family is a promising material for different applications as batteries, supercapacitors, semi-transparent electrodes, field-effect transistors, sensors, etc. The oxidation of $Ti_3C_2T_x$ MXene leads to metal-semiconductor heterostructure creation. We investigated spontaneously formed titania on MXene thin films for chemical gas sensors based on two different principles − chemiresistors and quartz crystal microbalance sensors. The thermal desorption and photo-stimulated desorption have been investigated and possible mechanism of the photo-stimulated desorption are proposed. Samples were exposed to different gases − argon, nitrogen dioxide, oxygen, and water vapor. A new method for fast and effective recovery by UV illumination at low temperature (~50°C) was utilized. It was shown that for active gases as oxygen, water vapor, and nitrogen dioxide the relaxation process of photoexcited charge carriers allows increasing the sensor sensitivity as well as decrease the time of sensor response.

Poster

No. 9

Flexible MXene devices for plasmonic photodetection

Jehad K. El-Demellawi, Dhinesh B. Velusamy and Husam N. Alshareef

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MXenes have recently exhibited impressive optical and plasmonic properties associated with their ultrathin atomic layer structure.[1] However, *their use in photonic and plasmonic devices is still marginally explored*. Herein, we have fabricated various flexible plasmonic photodetectors made of five different MXenes.[2] Amongst which, Mo_2CT_x have exhibited the best performance owing to its relative stability against oxidation, moderately high free carrier density and electrical conductivity.[3] The surface chemistry and the optoelectronic properties of the mechanically flexible photodetectors were thoroughly investigated.

The Mo_2CT_x flexible devices have exhibited broad photoresponse in the range of 400-800 nm with high responsivity (R, up to 9 A W^{-1}), detectivity (D^*, ~$5x10^{11}$ *Jones*) and reliable photoswitching characteristics. It is worth mentioning that despite being the first demonstration of MXene-based photodetection, the performance of Mo_2CT_x thin films considering their R and D^* is surpassing the majority of previously reported visible-band photodetectors based on solution-processed 2D materials. In particular, the responsivity of Mo_2CT_x devices were found to be ~18000 and ~1200 times higher than that of the *first reported* graphene [4] and MoS [5] photodetectors, respectively. We also show that in addition to their attractive performance and solution processability, our MXene-based devices possess a full visible spectrum coverage, highly stable operation and mechanical flexibility.

The photodetection mechanism, as unveiled by spatially-resolved STEM-EELS and ultrafast femtosecond transient absorption spectroscopy, is shown to be dominated by the *intrinsic plasmon- assisted hot carrier generation*.

The demonstrated ability of coupling with light and dephasing of surface plasmons with a short lifetime, without the need of integration with other metallic plasmonic structures, as previously demonstrated with several 2D materials,[6] have led to a photoresponse outperforming that of many photoelectron-based devices. Moreover, the revealed specific ability to detect and excite individual surface plasmon modes, provide a viable platform for various MXene-based photonic and plasmonic applications.

[1] J. El-Demellawi, S. Lopatin, J. Yin, O. Mohammed, H. Alshareef, *ACS Nano* **2018**, *12*, 8485.
[2] D. Velusamy, J. El-Demellawi, A. El-Zohry, A. Giugni, S. Lopatin, M. Hedhili, A. Mansour, E. Fabrizio, O. Mohammed, H. Alshareef, *Adv. Mater.* **2019**, 1807658.
[3] H. Kim, B. Anasori, Y. Gogotsi, H. N. Alshareef, *Chem. Mater.* **2017**, *29*, 6472.
[4] F. Xia, T. Mueller, Y.-m. Lin, A. Valdes-Garcia, P. Avouris, *Nat. Nanotechnol.* **2009**, *4*, 839.
[5] Z. Yin, H. Li, H. Li, L. Jiang, Y. Shi, Y. Sun, G. Lu, Q. Zhang, X. Chen, H. Zhang, *ACS Nano* **2012**, *6*, 74.
[6] F. H. L. Koppens, T. Mueller, P. Avouris, A. C. Ferrari, M. S. Vitiello, M. Polini, *Nat. Nanotechnol.* **2014**, *9*, 780.

Poster

No. 10

Large-scale synthesis of titanium-based MAX and MXenes

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2D materials, like MXenes [1], provide very attractive building blocks for a very large variety of applications in electrical engineering, composites, energy and other fields [2-4]. However, availability and cost are the key factors limiting applications of advanced nanomaterials in industry.

There are currently many insulating and semiconducting 2D materials available and produced in large quantities, such as MoS_2, BN or clays. Graphenes, as mechanically exfoliated graphene platelets or reduced graphene oxide, are among the most conductive 2D materials available in industrial quantities. Transition metal carbides and nitrides (MXenes) are widely researched for their high metallic conductivity. MXenes have added metallically conductive 2D building blocks to the available list of 2D materials. More than 30 different MXenes have been reported, but most research is done of Ti_3C_2 and Ti_2C. And there is a good reason for this, as both are built of environmentally friendly and abundant elements, so their low-cost synthesis and safe use should be potentially possible. However, their production is still at a very early stage. One of the limiting factors for large-scale and low-cost manufacturing of MXenes is the cost and limited availability of MAX phases. However, making good-quality MXene in large quantities requires not just “a MAX”, but also a MAX phase with appropriate properties optimized for MXene synthesis. This presentation will address the synthesis of Ti_2AlC and Ti_3AlC_2 MAX phases in kilogram quantities and their use for manufacturing MXenes in 100-g quantities by selective etching in various acidic etchant [5, 6]. Effects of MAX phase quality on MXene properties will be discussed and our proprietary design of reactors for MXene synthesis from MAX phases will be described.

1. M. Naguib, et al., Two-Dimensional Nanocrystals Produced by Exfoliation of Ti3AlC2, Advanced Materials, 23, 4248 (2011)
2. F. Shahzad, et al. Electromagnetic Interference Shielding with 2D Transition Metal Carbides (MXenes), Science, 353 (6304) 1137-1140 (2016)
3. S. J. Kim, et al. Metallic Ti3C2Tx MXene gas sensors with ultrahigh signal-to-noise ratio, ACS Nano, 12 (2), 986−993 (2018)
4. B. Anasori, et al. 2D Metal Carbides and Nitrides (MXenes) for Energy Storage, Nature Reviews Materials, 2, 16098 (2017)
5. O. Gogtosi, V. Zahorodna, I. Hrysko, A. Serhienko, Y. Zozulya, V. Balitskiy, M. Seredych, B. Anasori, Y. Gogotsi. Scale-up of MXene Synthesis, 2018 IEEE 8th International Conference on Nanomaterials: Applications & Properties, Zatoka, September 9-14, 2018
6. O.O. Honcharuk, V. YU. Balitskiy, R. V. Voron, M.P. Brodnikovskiy, O.G. Gogotsi, V.V. Zahorodna, Y. I. Zozulya, M. Alhabeeb, B. Anasori, K. Malesky, Y. G. Gogotsi. Synthesis and Optical Properties of 2D Carbides MXenes, Book of Abstracts for 11th International Scientific-Technical Conference "Composite Materials", National Technical University of Ukraine "Igor Sikorsky Kyiv Polytechnic Institute", April 2018, pp.118-120. UDC 542;546;62.

Poster	**pH-dependent distribution of functional groups on titanium-based MXene**
No. 11	**Rina Ibragimova,** Martti Puska and Hannu-Pekka Komsa
	Aalto University, Finland

It has been shown that during the synthesis of MXenes their surfaces are usually functionalized by O, OH, and F, and further suggested that controlling the surface allows controlling their properties. However, understanding of the surface structure suffers from the significant discrepancy between computational and experimental studies. Experiments consistently show formation of surfaces with mixed terminations, while computational studies point towards pure terminated surfaces.

We study the formation of mixed functionalization on the surface of titanium based two-dimensional carbides Ti_2C and Ti_3C_2 using a multi-scale modelling scheme. Our scheme is based on calculating Gibbs free energy of formation by a combination of electronic structure calculations with cluster expansion and Monte Carlo simulations. Our calculations show formation of mixtures of O, OH, and F on the surface with the composition depending on pH, temperature, and the work function. On the other hand, our results also suggest a limited stable range of compositions, which subsequently also limits the tunability of MXene properties. [1]

1. R. Ibragimova, M. J. Puska, HP. Komsa, *ACS Nano*, **Just Accepted Manuscript**, DOI: 10.1021/acsnano.9b03511

Poster

No. 12

Human-like collagen protein coated 2D multilayered Ti_3C_2 and Ti_2C MXenes for improved biocompatibility

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Interactions that occur on material-biological matrix interface are of far importance for the development of new bioactive systems. Understanding and controlling these mechanisms may lead to new functionalities of the materials used in e.g. nanomedicine. It is expected that 2D materials (including MXenes) can face this challenge among other nanostructures. The MXenes phases are a member of the intriguing family of 2D materials beyond graphene [1]. They are a good candidates for many applications however, their potential toxicity is now of crucial importance for their further development [2]. Due to the increasing number of reports suggesting their toxic behavior [3], there is a high demand for in-depth studies on finding simple, low-cost and green approaches for controlling their interactions towards living organisms.

Herein, we present a simple, low-cost and fully green approach for controlling potential cytotoxicity of the 2D MXenes after delamination. We take advantage of interactions that occur between the surface of MXene phases and natural human-like collagen protein. We also demonstrate that the step-by-step adsorption and desorption of collagen from the surface of 2D MXenes can be easily controlled using in situ zeta potential measurements coupled with dynamic light scattering (DLS) method. The obtained results proved the electrostatically-driven unprecedented susceptibility of the MXenes' surfaces to collagen. Surface-modification reduced MXenes' toxicity in vitro i.e. lowered decease of cells' viability as well as reduced their oxidative stress. This indicates better biocompatibility of the 2D Ti_3C_2 and Ti2C MXenes surface-modified with collagen which is involved in many bio-interactions as an important building block of the human body. The presented study opens a new horizon for designing of the defined surface properties of the MXenes and paves the way for their future successful management for nano-medicinal applications.

[1] Naguib M, Kurtoglu M, Presser V, Lu J, Niu J, Heon M, Hultman L, Gogotsi Y, Barsoum M W, Adv. Mater. 23 (2011) 4248-4253.
[2] Lin H, Chen Y, Adv. Sci. 5 (2018) 1800518
[3] Jastrzębska A M, Szuplewska A, Wojciechowski T, Chudy M, Ziemkowska W, Chlubny L, Rozmysłowska A, Olszyna A, J. Hazard. Mater. 339 (2017) 1-8.

Acknowledgments
The study was accomplished thanks to the funds allotted by the Ministry of Science and Higher Education from the budget for science in the years 2016-2019 (project no. JP2015027774) as well as National Science Centre, within the framework of the research project 'SONATA BIS 7' no. UMO 2017/26/E/ST8/01073.

Poster

No. 13

Quality of MXene dispersion in various polymeric systems

Kateřina Kopecká[1], Vladimír Špaček[1], Mária Omastová[2] and Michal Procházka[2]

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Ever increasing demands on material properties, not only for hi-tech applications but also for materials intended for everyday use, motivates material engineers to develop new strategies and approaches for the design and production of more sophisticated materials. One of the most promising technique is replacement of traditional microfillers by nanoscaled fillers for the preparation of polymer composites. MXenes are among the newest candidates in the group of layered materials for enhancing properties of polymer composites. MXenes possess good electrical and thermal conductivities and, when used as fillers, they have a potential to improve mechanical properties such as stiffness and durability of polymers. The alpha and omega for profiting from incorporation of the fillers is their quality dispergation and homogenous distribution within the polymer matrix.

Incorporation of MXenes was tested for four different polymer matrices. A water-based epoxy system (CHS-EPOXY 200V 55), high-solid epoxy system (CHS EPOXY-520), acrylate system (Contasol 6492), and polyurethane acrylate lacquer (AQ CC 080). The stability of polymer/MXene dispersion was evaluated as well as the distribution of the MXene particles inside the polymer matrix. It was possible to incorporate MXenes in all studied systems, however, in the case of CHS-epoxy 200V 55 a sedimentation of MXenes during the storage appeared. From the macroscopic point of view the prepared free-standing films seemed homogenous. Even in the case of small MXenes loading the films were completely black. As follows from the analysis by optical and scanning electron microscopes, the particles distribution is better for the epoxy then for the polyurethane-acrylate system. However, isolated 3D MXene particles were visible in all cases and no 2D platelets were detectable, which means that no of the systems used support spontaneous exfoliation of MXenes.

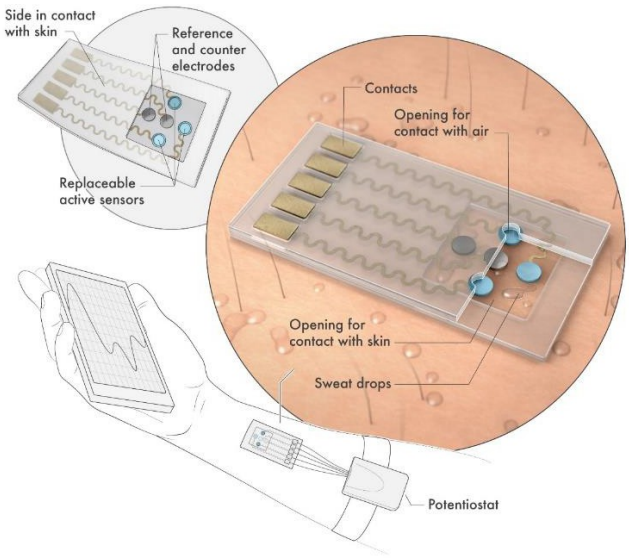
Acknowledgement
This work was financially supported by grant No. M-ERANET-18-414-Nano2Com from Slovak Academy of Sciences and from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 777810.

Poster	**A MXene-based wearable biosensor system for high-performance in-vitro perspiration analysis**
No. 14	**Yongjiu Lei**, Wenli Zhao, Yizhou Zhang, Qiu Jiang, Jr-Hau He, A.J. Baeumner, Otto Wolfbeis, Zhong Lin Wang, Khaled N. Salama and Husam N. Alshareef
	Materials Science and Engineering, King Abdullah University of Science and Technology (KAUST), Saudi Arabia

A stretchable, wearable, and modular multifunctional sweat biosensor incorporating MXenes is demonstrated for the first time. A novel MXene/Prussian blue ($Ti_3C_2T_x$/PB) composite is developed for durable and sensitive detection of biomarkers in sweat. Due to the metallic conductivity and hydrophilic nature of MXene, distinctly improved electrochemical activity is achieved using the $Ti_3C_2T_x$/PB composite which outperforms previously reported Graphene/PB and CNTs/PB composites used for the measurement of hydrogen peroxide. A unique modular design enabled a simple exchange of the specific sensing electrode to target the desired analytes. Furthermore, an implemented solid-liquid-air three-phase interface design led to superior sensing performance and stability. Typical electrochemical sensitivities of 35.3 μA mM^{-1} cm^{-2} for glucose and 11.4 μA $mM^{-1}cm^{-2}$ for lactate were achieved using artificial sweat. During in-vitro perspiration monitoring of human subjects, the physiochemistry signals (glucose and lactate level) could be measured simultaneously with high sensitivity and good repeatability, outperforming traditionally reported graphene/PB- and CNTs/PB-based biosensors.

This work was published in Small, DOI: 10.1002/smll.201901190.

A MXene-based wearable biosensor system for high-performance in-vitro perspiration analysis



Poster

No. 15

Surface structure of MXene nanosheets investigated by scanning tunneling microscopy

Zhongpeng Lyu, Rina Ibragimova and Hannu-Pekka Komsa

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To date, most studies and applications of 2-dimensional transition metal carbides and nitrides (MXenes) are sensitive to the composition and distribution of terminal groups on their surfaces [1]. The surface composition of MXenes are mainly obtained using X-ray photoelectron spectroscopy (XPS) and electron energy loss spectroscopy (EELS), or Raman spectroscopy [2-4]. However, none of these methods give direct information about the surface structure, e.g., the distribution of terminal groups, surface vacancies, or grain boundaries.
Scanning tunneling microscopy (STM) is a powerful tool to study the surface structure of many 2D materials including graphene, transition-metal dichalcogenides, boron nitride, black phosphorus, etc. In practice, clean surfaces are essential to obtain high quality STM images. However, high reactivity of the surface of MXenes makes it extremely difficult to obtain a clean surface, especially under ambient atmosphere. To the best of our knowledge, there are only two papers showing STM images of MXene nanosheet [5,6]. Unfortunately, the reported images look very different and no detailed discussion of the distribution of the surface terminal groups was given.
In this work, we have first synthesized several MXene samples ($Ti_3C_2T_x$, Ti_2NT_x, V_2CT_x) with different degrees of surface defects under various etching and intercalation conditions. Then we performed STM characterization of these 2D MXene nanosheets using different sample preparation/processing methods. The experimental images are compared to simulated images obtained using our recently developed MXene surface models [7].

1. Anasori, B., Lukatskaya, M. R. & Gogotsi, Y. 2D metal carbides and nitrides (MXenes) for energy storage. *Nat. Rev. Mater.* **2**, 16098 (2017).
2. Halim, J. *et al.* X-ray photoelectron spectroscopy of select multi-layered transition metal carbides (MXenes). *Appl. Surf. Sci.* **362**, 406–417 (2016).
3. Karlsson, L. H., Birch, J., Halim, J., Barsoum, M. W. & Persson, P. O. Å. Atomically Resolved Structural and Chemical Investigation of Single MXene Sheets. *Nano Lett.* **15**, 4955–4960 (2015).
4. Hu, T., Hu, M., Gao, B., Li, W. & Wang, X. Screening Surface Structure of MXenes by High- Throughput Computation and Vibrational Spectroscopic Confirmation. *J. Phys. Chem. C* **122**, 18501–18509 (2018).
5. Soundiraraju, B. & George, B. K. Two-Dimensional Titanium Nitride (Ti2N) MXene: Synthesis, Characterization, and Potential Application as Surface-Enhanced Raman Scattering Substrate. *ACS Nano* **11**, 8892–8900 (2017).
6. Hemmat, Z. *et al.* Tuning Thermal Transport Through Atomically Thin Ti 3 C 2 T z MXene by Current Annealing in Vacuum. *Adv. Funct. Mater.* **29**, 1805693 (2019).
7. Ibragimova, R., Puska, M. J. & Komsa, H.-P. pH-Dependent Distribution of Functional Groups on Titanium-Based MXenes. *ACS Nano* **13**, 9171–9181 (2019).

Poster

No. 16

Superfast high-energy storage hybrid device composed of MXene and Chevrel-phase electrodes operated in saturated LiCl electrolyte solution

Fyodor Malchik[1], Netanel Shpigel[1], Mikhael D Levi[1], Tyler S. Mathis[2], Yury Gogotsi[2], and Doron Aurbach[1]

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Development of high power devices with improved energy density is a highly desired target for advanced energy storage applications. Herein we propose a new strategy of triply-hybridized supercapacitive energy storage device composed of hybrid battery-supercapacitor negative electrode [Mo_6S_8 (Chevrel-phase)/Ti_3C_2 (MXene)] coupled with positive nanoporous carbon electrode, integrated with novel yet unexplored saturated (14 M) aqueous solution of LiCl. The electrochemical stability window of this electrolyte solution (2.70 V) significantly exceeds cell voltage (2.05 V) in the asymmetrical (hybrid vs. carbon) cell containing 14 M LiCl solution having far superior characteristics to that of conventional 21 m LiTFSI aqueous solution. Also potential window of MXene electrode prolongated till 1.45 V using proposed 14 M LiCl solution which is up to now is highest reported electrochemical window for MXene in water solution.

Note that the integration of Mo_6S_8 particles with the Ti_3C_2 flakes result in optimized hybrid electrode, in which the MXene sheets simultaneously serve as a conductive binder and as a source of the capacitive charge storage. The studied hybrid systems show excellent high energy and power densities (in the scales relevant to capacitive aqueous systems) and can be applied in a practical device which operates in an energy and power range between the batteries and supercapacitors.

Research is focused on a deep electroanalytical analysis of a peculiar redox/capacitive heterogeinety of hybrid electrodes, establishing a variety of additivity rules for both differential and integral equilibrium and kinetic characteristics of the charging processes in hybrid electrodes solving the puzzle of potential distribution of specific electrochemical energy stored in the hybrid electrode. A careful 3-level hybridization design of the asymmetric supercapacitive storage device enabled the integration of battery and supercapacitor materials to get free-standing binderless electrodes with high power and energy densities. The proposed 14M LiCl solution highly suitable for different types of aqueous-based supercapacitive devices combined with profound analysis of the properties of hybrid electrodes will pave the way for rational design of energy delivery in hybrid electrodes as a function of the electrode potential over time.

Poster

No. 17

Polymeric composites with 2D nanoparticles MXenes

Mária Omastová[1], Michal Procházka[1], Simona Procházková[2], Anastasiia Stepura[1], Oleksiy Gogotsi[3] and Matej Micusik[1]

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Two-dimensional (2D) materials such as graphene, metal oxides and hydroxides, dichalkogenides, boron nitride, MoS_2 and the others are currently the most intensive studied materials that have great potential for future applications in many technological areas. The current intense interest in these materials is due to the unique properties resulting from their dimension. They offer highly specific surface areas as well as electronic structures that can achieve new interesting features.

MXenes are a new class of 2D inorganic materials, first described in 2011 [1]. Different MXenes are prepared from different MAX phases of the formula $M_{n+1}AXn$, where M is the most common transition metal, A is an element of the 13 or 14 group of the periodic table of elements, X is usually C and/or N. By etching of the A layers from MAX phase, MXene are formed with the formula $M_{n+1}X_nT_x$ where T is a functional group e.g., -O, -F, -OH. They can be also used for polymeric composites preparation, which will certainly find interesting application, as electromagnetic interference shielding [2], antistatic materials, etc.

MAX phase Ti_3AlC_2, particle size 40 µm (MRC, Ukraine) was used for MXene preparation. Polymethylmethacrylate (PMMA) Plexiglas® 7N, was used as the polymeric matrix for preparation of composites by solution casting method.

XPS analysis confirmed etching the aluminium layer out of the Ti_3AlC_2 MAX phase. The intensity of Al signal decreased from 12.9 at.% to 0.0 at.%. Results also showed cleaning MXene from oxidized parts, which are in precursor MAX phase in a larger amount, and in prepared MXene this signal decreased significantly.

PMMA pellets were dissolved in acetone and stirred, MXene powder was added and stirred 2 hours under reflux. The prepared composite was poured on the Petri dish with a Teflon foil. PMMA composites with MXenes content from 2.5 wt.% to 10.0 wt.% were prepared.

Electrical properties of prepared composite were measured by Broadband Dielectric Spectrometer (BDS). BDS measurements showed increasing of conductivity with increasing content of MXene in polymeric composites. Conductivity of composites is depending on conductivity of fillers. Experimental condition of MAX phase etching and methods of MXene preparation significantly influence the final electrical conductivity of this filler. The higher the MXene conductivity, the higher the final conductivity of polymeric composites, which can be suitable in antistatic materials application.

1. M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum, Adv. Materials, 23 (37), 4248-4253 (2011).
2. F. Shahzad, M. Alhabeb, C.B. Hatter, B. Anasori, S. Man Hong, C.M. Koo, Y. Gogotsi. Science 353, 1137−40 (2016).

Acknowledgements

This work is part of project which received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 777810, and from agency VEGA 02/0010/18 (Slovakia).

Poster

No. 18

Study of MXene nanoparticles aging

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MXenes are a new class of 2D inorganic materials, first described in 2011 [1]. Since that time, they have been attracting attention because of their interesting properties, such as high conductivity and electromagnetic radiation absorption. MXenes can be used as nanofillers to different polymeric materials and can improve their properties. However, for using new materials it is necessary to know their stability under different conditions. This work is focused on the analysis of oxidation processes on MXenes during ageing under standard laboratory conditions.

MXene $Ti_3C_2T_x$ was prepared by the modified minimally intensive layer delamination (MILD) method [2]. Shortly, MAX phase Ti_3AlC_2 powder, with the particle size of 40 µm (MRC, Ukraine) was stirred 24 hours in LiF + HCl solution. After etching reaction, the suspension was centrifuged several times at 3500 rpm and washed with de-ionized water until the pH of the supernatant was 6. After last centrifugation the precipitate was collected as MXene pasta and stored in Eppendorf's vials. XPS (X-ray photoelectron spectroscopy) and TEM (transmission electron microscopy, including energy-dispersive X-ray spectroscopy and selected area electron diffraction) were then performed in different time periods.

The TEM/EDX measurement confirmed the elemental composition of MXene with Ti, C, O and F peaks domination. The relative concentration of oxygen with respect to titanium increased with time from 1.1 in "freshly" prepared MXenes to 2.4 after 4 months ageing in air. TEM micrographs proved that the overall morphology of MXene particles did not change with time. The XPS analysis confirmed the chemical composition of MXene samples with small amount of TiO_2 in "freshly" prepared samples, while after keeping the samples for one month in air the TiO_2 content increased more than two times.

Study of MXene samples ageing under standard laboratory conditions showed increased oxidation of the $Ti_3C_2T_x$ structure, which might lead to a change of MXenes properties.

1. M. Naguib, M. Kurtoglu, V. Presser, J. Lu, J. Niu, M. Heon, L. Hultman, Y. Gogotsi, M. W. Barsoum, Adv. Materials, 23 (37), 4248-4253 (2011).
2. M. Alhabeb, K. Maleski, B. Anasori, P. Lelyukh, L. Clark, S. Sin, Y. Gogotsi. Chem. Mater. 29, 18, 7633-7644 (2017).

Acknowledgements
The research was funded by projects No. M-ERANET-18-414-Nano2Com from Slovak Academy of Sciences, No. 1.1.1.5/ERANET/18/02 from Latvian State Education Development Agency, and APVV SK-BY-RD-19-0011 (Slovakia).

Poster

No. 19

Silanization as an efficient way of protecting MXenes against oxidation

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MXenes are a novel family of 2D nanomaterials that, because of their hydrophilicity and excellent electrical conductivity, are being considered for a broad range of potential applications in nanoelectronic and energy storage systems, among others. Their main disadvantage is their short shelf-life related to their high susceptibility to oxidation. In this work, we show that silanization is a possible solution to this problem. By grafting siloxane bonds to MXenes via hydroxyl groups we stabilized the structure against environmental and thermal oxidation. Pristine and silanized $Ti_3C_2T_x$ were characterized by Raman, XRD, AFM, TGA, XPS and water contact angle techniques. The increased thermostability of MXenes was confirmed via *in situ* XRD and Raman measurements in the 20°C to 600°C temperature range. Moreover, the morphology and composition of the reference (as-obtained), after 300°C and after 600°C, MXene samples were analyzed using SEM, AFM and XPS. All the results confirmed that silanized $Ti_3C_2T_x$ are stable up to ≈ 280°C, without any sign of decomposition of oxide formation. This enhanced stability suggests they can be used in hydrothermal processes. Additional biological investigations showed that silanization did not influence their cytotoxicity. It follows that silanized MXenes can be safely used in biomedical applications.

Acknowledgments
The research was financially supported by National Science Center Poland – Sonata 7 project (2014/13/D/ST5/02824), „Podpora mobility na UP"(CZ.02.2.69/0.0/16_027/0008482) and the European Research Council – ERC-COG programme (683024). Authors are grateful to Maria Cecilia Pérez for SEM measurements.

Poster

No. 20

Mo_4VC_4: a two-dimensional MXene with five atomic layers of transition metals

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MXenes have a general formula of $M_{n+1}X_n$, typically described as n=1-3, where M is a transition metal (Ti, Nb, V, Mo, etc.) and are interleaved with layers of C and/or N (shown as X). Here, we report on the synthesis and characterization of the first MXene Mo_4VC_4), with 5 atomic layers (n=4), as well as its precursor, Mo_4VAlC_4. TEM and XRD showed the structure of this phase is $P6_3/mmc$ similar to other MAX phases. However, this structure has a twinned set of M-layers, unique in the MAX/MXene family. Compositionally studied *via* EDS and XPS, the MXene composition was determined to be $Mo_{4.10}V_{0.90}C_{2.99}$. HRSTEM, Raman spectroscopy, and DFT indicate that the crystal structure contains a solid solution of Mo and V. DFT calculations also indicate that other n=4 transition metal MAX phases ($M'_4M''AlC_4$) may be possible, suggesting that more $M_5C_4T_x$ MXenes can potentially be synthesized. In addition, UV-vis-NIR spectroscopy, temperature-dependent resistivity measurements, and thermogravimetric analysis provide additional characterization on the optical, electronic, and thermal properties of this new Mo_4VC_4 MXene. This study provides a new subfamily of MXenes with five atomic layers of transition metals, allowing for wider range of compositions for more control over properties.

Poster

No. 21

Stability of MXenes dispersions – oxidation and use for air purification

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$Ti_3C_2T_x$ type of MXenes was prepared from MAX phase Ti_3AlC_2 and consequent removal of the Al element by treatment with HF acid and LiF/HCl mixture. The dispersibility and the chemical stability of the prepared MXenes in water and ethanol media were investigated. In terms of homogeneity, the HF etched materials appeared more stable in water, while the MXenes obtained by etching with LiF/HCl exhibited long-term (more than three months) stability in ethanol. The results were related to the creation of different functional groups (T_x) in each type of MXenes and their compatibility with the solvent. Regarding the chemical stability, more intensive oxidation to anatase TiO_2 was observed in water than in ethanol that was attributed to the presence of dissolved oxygen. Various modifiers such as alkali ions (Li^+, K^+, Na^+), 2D carbonaceous materials (Graphene, Graphene Oxide) and nanoparticles (Cobalt ferrite, Carbonyl iron) were tested to prevent the undesired process of oxidation. It was found that in presence of the Na^+, K^+ and Graphene Oxide, TiO_2 was not formed within a 3-months period of time. On the contrary, for the pure MXene and the rest of modifiers spontaneous Anatase formation was observed.

Also, deliberate oxidation by treatment at 500 ^oC for 1 h was carried out to transform the $Ti_3C_2T_x$ to TiO_2. The obtained material exhibited Anatase crystalline structure, 2D MXene-like morphology, specific surface area (SSA_{BET}) of 55 m^2/g as well as increase of the oxygen content and the formation of Ti-O bonds. The 2D TiO_2 material was tested for photocatalytic removal of air pollutants NOx revealing better activity than the reference photocatalyst Evonik-Degussa P25 under UV light. The outcome was attributed to the anatase formation, the higher SSA_{BET} and possibly for influence of a residual conductive MXene substrate.

Acknowledgments
The research has been supported by "2D-NanoSMART" project and ISN foundation.

Poster	**Synthesis of a thermoresponsive hybrid MXene with switchable conductivity**
No. 22	**Minh Hai Tran**
	Eduard-Zintl-Institute of Inorganic and Physical Chemistry, TU Darmstadt, Germany

The surface chemistry and structure of MXenes play an important role for the properties and applications of these exciting 2D materials. After chemical exfoliation the surface of the 2D carbides are functionalized by a mixture of F-, O-, and OH-groups. Here, we take advantage of the hydroxyl terminated surface using the OH-groups as a linker for organic molecules. More specifically, we graft PDMAEMA onto the MXene surface through self-initiated photoiniferter polymerization (SIPIP). The product is a new “smart” hybrid MXene material with switchable materials properties. PDMAEMA is a well-known thermo-responsive polymer with a relatively low critical solution temperature (LCST) of around 35° C. Successful bonding between the MXene surface and PDMAEMA is shown by IR and X-ray photoelectron spectroscopy, thermal analysis and electron microscopy. We further demonstrate a reversible change of conductivity of thin films of this hybrid material using temperature as an external stimulus.

Poster No. 23	**MXene-derived ferroelectric crystals**
	Shaobo Tu, Fangwang Ming, Junwei Zhang, Xixiang Zhang and Husam N. Alshareef
	Materials Science and Engineering, King Abdullah University of Science and Technology (KAUST), Saudi Arabia

This study demonstrates the first synthesis of MXene derived ferroelectric crystals. Specifically, we have successfully synthesized high aspect ratio potassium niobate ($KNbO_3$) ferroelectric crystals using two-dimensional Nb_2C MXene and KOH as the potassium and niobium source, respectively. Material analysis confirms that a $KNbO_3$ orthorhombic phase with Amm2 symmetry was obtained. Additionally, ferroelectricity in $KNbO_3$ was confirmed using standard ferroelectric, dielectric, and piezoresponse force microscopy (PFM) measurements. The $KNbO_3$ crystals exhibit a saturated polarization of ~ 21 μC/cm^2, a remnant polarization of ~17 μC/cm^2, and a coercive field of ~50 kV/cm. Our discovery illustrates that the two-dimensional nature of MXenes can be exploited to grow ferroelectric crystals.

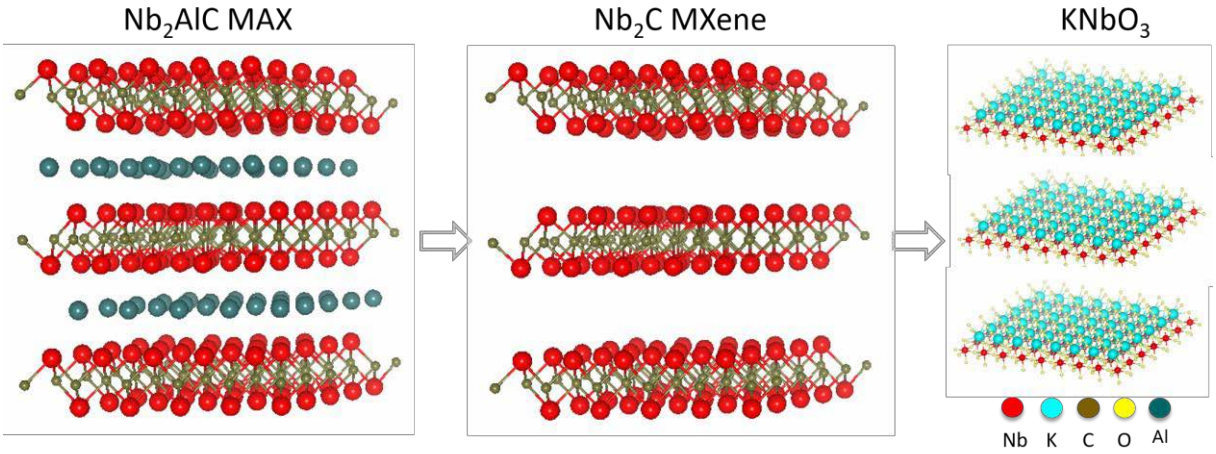

Figure 1. Crystal structures of the initial Nb_2AlC MAX phase, Nb_2C MXene after etching out Al, and MXene-derived $KNbO_3$ ferroelectric crystals (M-$KNbO_3$).

[1] B. Anasori, M. R. Lukatskaya, Y. Gogotsi, Nat. Rev. Mater. 2017, 2,16098.
[2] M. Naguib, J. Halim, J. Lu, K. M. Cook, L. Hultman, Y. Gogotsi, M. W. Barsoum, J. Am. Chem. Soc. 2013, 135, 15966.
[3] I. Grinberg, D. V. West, M. Torres, G. Gou, D. M. Stein, L. Wu, G. Chen, E. M. Gallo, A. R. Akbashev, P. K. Davies, J. E. Spanier, A. M. Rappe, Nature 2013, 503, 509.

Poster

No. 24

Two-dimensional titanium carbide (MXene) in accommodating lens design

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Intraocular lenses (IOLs) have been used to treat cataracts since the 1940s and have undergone significant changes in the type and design of materials used in order to improve patient visual and clinical outcomes (1). Despite these developments there still remain several deficiencies linked to IOL failure to mimic the accommodative properties of the natural lens. Accommodation refers to the ability of the lens to produce changes in optical power providing continuous focus for objects at varying distances. A range of approaches have been used in the development of accommodating IOLs (AIOLs). However, current, clinically available IOLs do not possess the refractive properties of the natural lens (2). The 2D transition-metal carbides and nitrides (MXenes) have a number of characteristics including transparency, high conductivity, flexibility, reactive surface chemistry and hydrophilicity that lend themselves to optoelectronic IOL design (3,4). The aim of this study was to develop and characterise a biocompatible, transparent, conductive MXene $Ti_3C_2T_x$ coating for use in optoelectronic IOL design to act as a transparent conductive electrode (TCE) aiming to actuate controlled changes in dioptic power.

$Ti_3C_2T_x$ was synthesised via liquid exfoliation of the precursor MAX phase with lithium fluoride and hydrochloric acid. The physical characterisation of $Ti_3C_2T_x$ was performed using X-ray powder diffraction (XRD), X-ray photoelectron spectroscopy (XPS), UV-Vis spectroscopy and dynamic light scattering (DLS) size analysis. $Ti_3C_2T_x$ was spin coated on to hydrophobic acrylate IOLs. Optical measurements of modulation transfer function and power were made. Device performance was optoelectronically evaluated through spectral transmittance and conductivity using UV-Vis spectroscopy and a four-point probe technique. A figure of merit (FOM) was established through the ratio of electronic to optical conductivities allowing a universal comparison to other optoelectronic devices. Coating biocompatibility was assessed using a human lens epithelial B-3 cell line with the CellTiter 96® AQueous One Solution Cell Proliferation Assay (MTS) and the CytoTox96 non-radioactive cytotoxicity assay (LDH). A monocytic THP-1 cell line was used to assess oxidative stress using the dichloro-dihydro-fluorescein diacetate (DCFH-DA) assay and stimulation of inflammation by enzyme linked immunosorbent assay (ELISA) for cytokines IL-6, IL-8 and TNF.

Etching $Ti_3C_2T_x$ in the presence of a fluoride salt produced delaminated colloidal solutions confirmed with XRD, XPS and UV-Vis with flakes of sizes ranging from 0.6 to ~8 μm measured with DLS. The optical quality of the spin coated device was evaluated for contrast

and resolution and showed no significant difference when measured before and after coating with $Ti_3C_2T_x$ demonstrating no impact on the device's ability to act as an IOL. The optoelectronic performance evaluation found the sheet resistance to range from 0.3-1.0 $K\Omega sq^{-1}$ with % transmittance ranging from 50-80% respectively and a FOM was calculated. MTS and LDH results indicated that the MXene coating supported viable cell growth and did not induce cell necrosis. The DCFH-DA results showed no production od ROS in response to the coating. The ELISA results indicate no production of cytokine IL-6, IL-8 and TNF in the presence of the MXene coating.

The study showed that $Ti_3C_2T_x$ could be synthesised and spin coated as a thin film onto a hydrophobic lens polymer with high transmittance and good conductivity. The coating did not negatively impact cell viability or induce oxidative stress and inflammatory pathway activation. Thus, indicating suitability for use in accommodating IOL design.

1. Findl O. Intraocular Lens Materials and Design. Achiev Excell Cataract Surg. 2009;95–108.
2. Haripriya A, Sonawane H, Thulasiraj RD. Changing techniques in cataract surgery: how have patients benefited? Community eye Heal. 2017;30(100):80–1.
3. Tang H, Hu Q, Zheng M, Chi Y, Qin X, Pang H, et al. MXene–2D layered electrode materials for energy storage. Prog Nat Sci Mater Int. 2018;28(2):133–47.
4. Kang KM, Kim DW, Ren CE, Cho KM, Kim SJ, Choi JH, et al. Selective Molecular Separation on Ti_3C_2Tx Graphene Oxide Membranes during Pressure Driven Filtration: Comparison with Graphene Oxide and MXenes. ACS Appl Mater Interfaces. 2017;9(51):44687–94.

Poster

No. 25

3D printing of freestanding MXene architectures for current collector-free supercapacitors

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Additive Manufacturing (AM) technologies appear to be a paradigm for the scalable manufacture of electrochemical energy storage (EES) devices, where complex three-dimensional (3D) architectures are typically required but hard to achieve using conventional techniques. The combination of these technologies and innovative material formulations that maximize surface area accessibility and ion transport within electrodes while minimizing space are of growing interest. Herein, we formulate aqueous inks composed of atomically thin (1-3 nm) 2D $Ti_3C_2T_x$ with large lateral size of about 8 μm possessing ideal viscoelastic properties for extrusion-based 3D printing of freestanding, high-specific surface area architectures. The MXene inks were 3D printed into interdigitated electrodes to determine the viability of manufacturing energy storage devices. The 3D printed device with active material loading of about 8.5 mg cm^{-2} achieved areal capacitance as high as 2.1 F cm^{-2} at 1.7 mA cm^{-2} and gravimetric capacitance of 242.5 F g^{-1} at 0.2 A g^{-1} with retention of above 90 % capacitance for 10000 cycles. It also exhibited a high energy density of 0.0244 mWh cm^{-2} and power density of 0.64 mW cm^{-2} at a current density of 4.3 mA cm^{-2}. We anticipate that the sustainable printing and design approach developed in this work can be applied to fabricate high performance bespoke multi-scale and multi-dimensional 3D architectures of functional and structural materials for integrated devices in energy, catalysis and transportation applications.

Poster

No. 26

Strategies for enhancing the electrochemical activities of MXenes *via* chemical doping with nonmetallic electron donors

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An effective chemical and structural doping approach has been described to enhance the electrochemical activities of MXenes (such as Ti_2CT_x and V_2CT_x) by chemical doping with nonmetallic (nitrogen and/or phosphorous) impurities. In this presentation, the substitutional and interstitial doped models of MXene structures were constructed with different doped sites, and then their dopant surface formation energies (eV/Å^2) and chemical structural properties were performed to study the electrochemical active sites, energy storage and hydrogen production performances. Our results have identified that an N atom preferentially substitute for the defect site C atom and/or interstitial site of edge region (defect) of MXene (in case of Ti_2CT_x); however, a P atom preferentially situate the vacancy sites of transition metal and/or in-planar of MXene (V_2CT_x). In addition, it was confirmed that the chemical structure of the dopants in MXenes can be controlled according to the reactant concentration, reaction time and temperature in the chemical doping processes. As a results of this, we have studied which chemical formation or structure affects electrochemical activities. Furthermore, it is demonstrated that the doping with nonmetallic impurities indicates the Gibbs free energy (ΔG_H) of nearly zero depending on their chemical compositions. Especially, dopants interstitial doping shows a prominent potential due to the appearance of a new channel for carrier migration as well as redox sites for energy density in energy storages. It should be pointed out that proper doping form should be controlled, so that reasonable electrochemical properties can be achieved.

[1] Y. Yoon et.al., ***Adv. Energy. Mater***., 8(15), 1703173, **2018**
[2] Y. Yoon et.al., ***J. Mater. Chem. A***., 6(42), 20869, **2018**
[3] Y. Yoon et.al., ***Adv. Funct. Mater***., 29(30) 1903443, **2019**

Poster

No. 27

Simulation on mechanical behaviour of polymer/MXene nanocomposites

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The aim of this study is to identify a suitable methodology based on finite element (FE) homogenization approach for prediction of mechanical behaviour of polymer/MXene nanocomposites.

Polyvinyl alcohol (PVA) reinforced with MXene 2D nano flakes was analysed. The main mechanical properties of the polymer are: Young's modulus of 0.91 GPa; tensile strength of 32 MPa; tensile elongation (at break) 13.7 %. The mechanical properties of MXene nanosheets were predicted by simulation on classical molecular dynamics (MD) [1] and only elastic properties were obtained experimentally by nanoindentation with the tip of an atomic force microscope [2]. According to MD simulation the modulus of the most important MXene material (Ti_3C_2) is 0.502 TPa, but experimentally was obtained modulus of 0.33 ± 0.03 TPa. For this investigation these MXene properties were used: Young's modulus of 0.33 TPa; tensile strength of 20 MPa; tensile elongation (at break) 4.5 %.

The FE analysis of mechanical behaviour of PVA/MXene composite was based on the micro-macro homogenization strategy. The analysis was performed by FE code DIGIMAT™ and ABAQUS. The effects of MXene nano flake shape, aspect ratio, clustering, and volume fraction on the elastic and strength properties of nanocomposite under static loading conditions were investigated.

FE model for mechanical properties simulation of PVA/MXene composite was proposed. The results demonstrated good agreement with experimental data.

1. V. N Borysiuk, V. N. Mochalin1 and Y. Gogotsi "Molecular dynamic study of the mechanical properties of two-dimensional titanium carbides $Ti_{n+1}C_n$ (MXenes)". Nanotechnology, No. 91, pp 1-10, 2015.
2. Lipatov, H. Lu, M. Alhabeb, B. Anasori, A. Gruverman, Y. Gogotsi, and A. Sinitskii, "Elastic properties of 2D Ti_3C_2Tx MXene monolayers and bilayers". Science Advances, Vol. 4, pp 1-7, 2018.

Acknowledgements
This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 777810.

Poster

No. 28

Synthesis and characterization of scandium and lutetium containing two dimensional carbides

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Two-dimensional (2D) materials have attracted intense attention in nanoscience and nanotechnology due to their outstanding properties. Among these materials, the emerging family of 2D transition metal carbides, carbonitrides, and nitrides (referred to as MXenes) stands out because of the vast available chemical space for tuning materials chemistry and surface termination, offering opportunities for property tailoring. Specifically, semiconducting properties are needed to enable utilization in optoelectronics, but direct band gaps are experimentally challenging to achieve in these 2D carbides. In addition, it is still a challenge to synthesize rare earth (RE)-based MXenes from selective etching of traditional MAX phases in the corrosive fluoride-containing solution. Structural design of a layered precursor that can be etched and establishment of mild and compatible etching chemistry could be key issues. Here, we demonstrate the fabrication of 2D hydroxyl-functionalized and carbon-deficient scandium carbide, namely, ScC_xOH, by selective etching of a layered parent $ScAl_3C_3$ compound. The 2D configuration is determined as a direct band gap semiconductor, with an experimentally measured band gap approximated at 2.5 eV. Furthermore, this ScC_xOH-based device exhibits excellent photoresponse in the ultraviolet−visible light region (responsivity of 0.125 A/W at 360 nm/10 V, and quantum efficiency of 43%). As inspired by this work, we further demonstrate the fabrication of 2D lutetium containing carbide, namely LuCOH, by selective etching of an alternative $LuAl_3C_3$ precursor, using an alternative organic base as etchant. Since many lanthanide series of metals can form similar layered compounds, more 2D RE-based carbides could be realized in the near future, which will further enlarge the family and enrich the applications of MXenes.

Poster

No. 29

Atomic defects in monolayer ordered double transition metals carbide ($Mo_2TiC_2T_x$) MXene

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Transition metal carbides (MXenes) with formulas $M_{n+1}C_n$ (n = 2 and 3) are emerging as a new family of two-dimensional (2D) materials providing great potential in electronic applications and CO_2 conversion catalysts. It was investigated that the electronic and electrochemical properties of $Ti_3C_2T_x$ MXenes can be tuned by replacing the two outer titanium layers with molybdenum layers. Similar to other 2D materials, intrinsic defects form in MXene flakes during the etching and delamination and the formation of defects in MXenes can influence the performance of these materials.

Here, we systematically study the effect of the different types of structural defects in on the structural stability, electronic behavior, and electrochemical properties of ordered $Mo_2TiC_2T_x$ terminated with specific surface functions of fluorine, oxygen or hydroxide. The calculated defect formation energies imply that the formation of defects are dependent on the surface terminations, where the O-terminated MXenes demand more energy than F- and OH-terminated MXenes. We found that the defect formation is more feasible in outer molybdenum layers than inner titanium layer. Electronic properties of MXene can be affected depending on the type of defects. Our results predicted that the CO_2 molecule adsorbs on the defected surfaces through a spontaneous and exothermic process that is critical to its capture while the perfect surface weakly attracts the molecule through a nonspontaneous and endothermic process. Thus, our study predicts that the electronic and electrochemical properties of $Mo_2TiC_2T_x$ can be tuned by forming the specific defects towards promising applications.

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