第二届国际二维过渡金属碳化物学术研讨会

2nd International Conference on MXenes

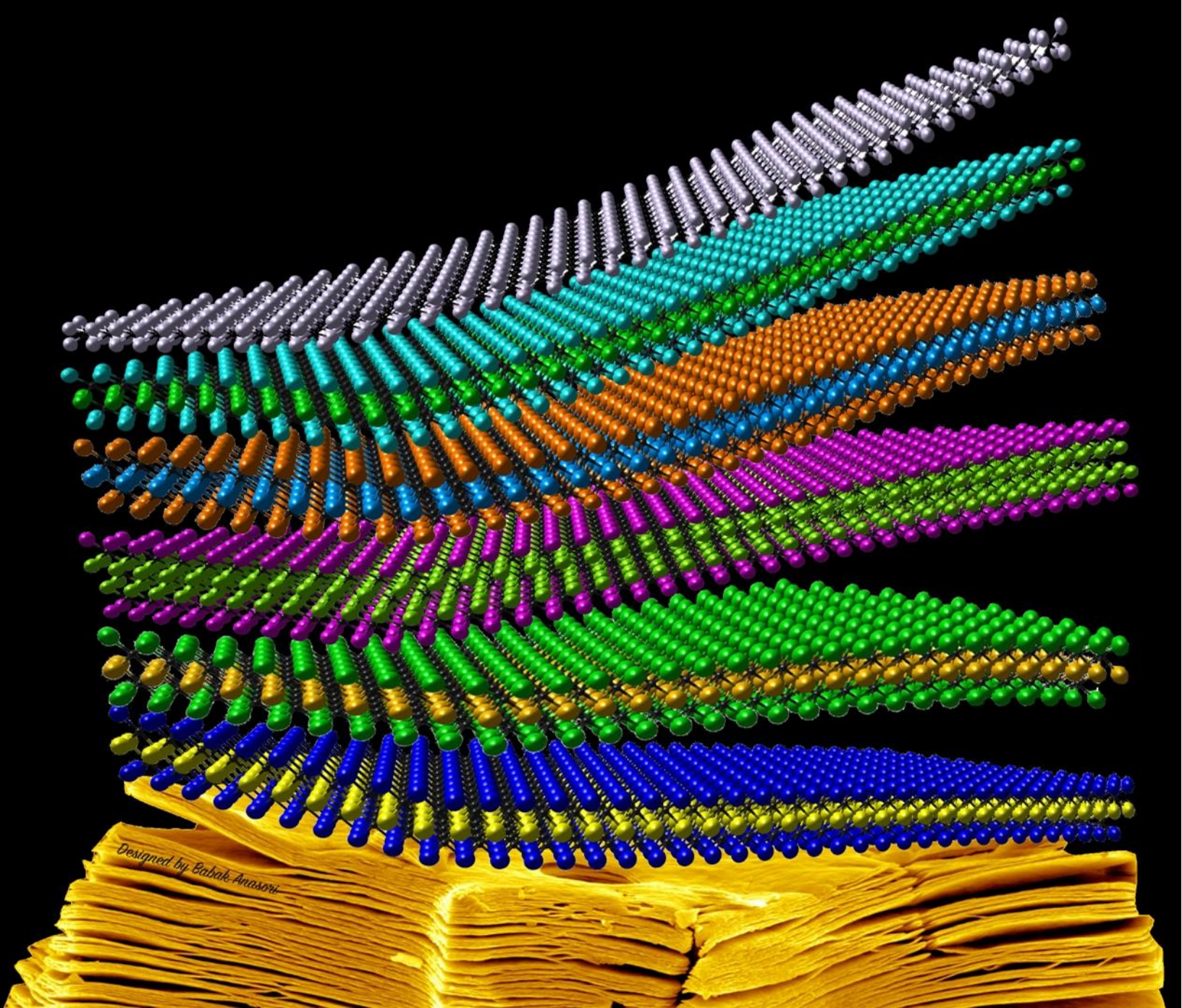
Beijing, China

May 10-12, 2019

2nd International Conference on

MXenes

May 10-12, 2019 Beijing, China



2nd International Conference on MXenes

Proceedings

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Beijing University of Chemical Technology

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Beijing, China

May 10-12, 2019

INVITATION

Dear Colleagues,

You are warmly invited to attend the 2nd International Conference on MXenes to be held on May 10-12, 2019 in Beijing, China. The conference is hosted and organized by Beijing University of Chemical Technology.

Two-dimensional (2D) materials became the focus of material research in the past decade owing to their unique chemical, electronic, optical, mechanical, and thermal properties that are different from their bulk counterparts. These unique properties are, in part, the result of quantum confinement effect in the atomically-thin 2D layers and are strongly dependent on the layer thickness and composition. Moreover, the properties of 2D materials are highly tunable by chemical doping, strain engineering, and external fields.

While graphene still remains the most widely researched 2D material, the discovery of 2D titanium carbide (Ti_3C_2) by Drexel University researchers in 2011 added a new family of materials known as MXenes to the 2D world. In general, the term MXenes refers to a very large family of 2D transition metal carbides, carbonitrides, and nitrides with the formula $M_{n+1}X_nT_x$, where M represents an early transition metal, X is carbon and/or nitrogen, and T stands for surface termination (such as OH, O, Cl, or F).

Research on MXenes is ongoing in more than 40 countries, with China leading in the number of publications. Therefore, it's not surprising that the 1st International Conference on MXenes for Energy was organized at Jilin University in 2018. It attracted about 200 researchers. The 2nd International Conference on MXenes is expected to have twice the number of attendees and will also cover all areas of applications of MXenes, including but not limited to energy storage and generation, electromagnetic interference shielding, antennas, transparent conductors, gas and pressure sensors, water purification, gas separation membranes, photo- and electrocatalysis, medicine and plasmonics. Due to a large variety of transition metals and surface functionalities, MXenes' properties can be tuned by selecting combinations of transition metals, X elements, and controlling their surface chemistries. There are endless and quickly expanding opportunities for producing MXenes with desirable properties.

Leading Chinese and foreign researchers working on MXenes will be giving plenary and invited talks at the conference. We hope that this conference will provide a forum for scientists from all over the world, both theorists and experimentalists, to meet and share information about synthesis, fundamental properties and applications of this quickly expanding family of 2D materials.

We are looking forward to seeing you in Beijing!

Sincerely yours,

Prof. Yury Gogotsi (conference chair)
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Posters

MXenes at the Frontier of the 2D Materials World

Yury Gogotsi

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Abstract:

The family of 2D transition metal carbides and nitrides (MXenes) has been expanding rapidly since the discovery of Ti_3C_2 in 2011[1]. Approximately 30 different MXenes have been synthesized, and the structure and properties of numerous other MXenes have been predicted using density functional theory (DFT) calculations [2]. 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) offer the potential for synthesis of dozens of new distinct structures. This presentation will describe the state-of-the-art in the synthesis of MXenes. Delamination into single-layer 2D flakes and assembly into films and 3D structures, as well as their properties will be discussed. Synthesis-Structure-Properties relations of MXenes will be addressed on the example of Ti_3C_2 and recently developed MXenes. The versatile chemistry of the MXene family renders their properties tunable for a large variety of applications [3]. Oxygen or hydroxyl- terminated Menes, 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 [5], but applications in plasmonics, electrocatalysis, biosensors, water purification/desalination and other fields are equally exciting. In particular, electromagnetic shielding and antenna applications of MXenes will be addressed.

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[1] M. Naguib, et al., Two-Dimensional Nanocrystals Produced by Exfoliation of Ti_3AlC_2, *Advanced Materials*, **23**, 4248 (2011).
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Biography:

Dr. Yury Gogotsi is Distinguished University Professor and Charles T. and Ruth M. Bach Professor of Materials Science and Engineering at Drexel University. He also serves as Director of the A.J. Drexel Nanomaterials Institute. He received his MS (1984) and PhD (1986) from Kiev Polytechnic and a DSc degree from the Ukrainian Academy of Sciences in 1995. His research group works on 2D carbides, nanostructured carbons, and other nanomaterials for energy, water and biomedical applications. He is recognized as Highly Cited Researcher and Citations Laureate by Thomson-Reuters/Clarivate Analytics (h-index exceeding 100). He has received numerous awards for his research including the European Carbon Association Award, S. Somiya Award from the International Union of Materials Research Societies, Nano Energy award from Elsevier, International Nanotechnology Prize (RUSNANOPrize), R&D 100 Award from R&D Magazine (twice). He has been elected a Fellow of the American Association for Advancement of Science (AAAS), Materials Research Society, American Ceramic Society, the Electrochemical Society, International Society of Electrochemistry, Royal Society of Chemistry, NanoSMAT Society, as well as Academician of the World Academy of Ceramics and Fellow of the European Academy of Sciences. He also served on the MRS Board of Directors and is acting as Associate Editor of ACS Nano.

2D transition metal carbide (MXene) thin film for EMI shielding

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Abstract:

MXenes are a family of 2D transition metal carbides, nitrides, and carbonitrides with the general formula $M_{n1}X_nT_x$ (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), 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 the atom-scale thickness, because it is hard to make uniform atom-thick film. In this presentation, we present the EMI shielding behavior of MXene thin film with atom-level thickness, which were prepared through a self-assembly method. It reveals that MXene is very good for ultra-thin film shielding applications.

Biography:

Chong Min Koo recieved his BS degree from Hanyang University in 1997 and Ph.D. degree from Chemical Engineering Department of Korea Advanced Institute of Science and Technology in 2003. He performed a postdoctoral fellowship in Minnesota University for two years (2003-2005) and works for LG Chemicals in two years (2005-2007). He is currently serving as a center head of Materials Architecturing Research Center, Korea Institute of Science and Technology (KIST), and a professor of KU-KIST Graduate School of Science and Technology, Korea University. He won the several awards including LG Group Best Research and Development Award (2007), KIST Best Researcher Award (2016, 2017), Songgok Award (2017), Young Scientist Award in the Korean Society of Industrial and Engineering Chemistry (2017), Best publication award in Korea Polymer Society (2018) and Best Korean Scientist Award from KRF (2018). His research interest covers 2D nanomaterials like transition metal carbides (MXene) and graphene and their polymer nanocomposites for EMI shielding, thermal conduction, actuators and energy storage device applications.

MXene as Charge Storage Host

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Abstract:

The development of efficient electrochemical energy storage (EES) devices is an important sustainability issue to realize green electrical grids. The metal carbide/nitride nanosheets termed MXene discovered in 2011 are a promising class of electrode materials for advanced EES devices because of their compositional versatility for materials exploration, high electrical conductivity for high current charge, and a layered structure of stacked nanosheets for ultrafast ion intercalation. However, general design strategies of MXenes for EES applications have not been established because of the limited understanding of the electrochemical mechanisms of MXenes. In this talk, we will present our current understandings of the MXene electrodes, as well as their applications to some EES devices such as sodium-ion batteries, lithium-ion batteries, and aqueous hybrid capacitors.[1-5]

References:

[1] X. Wang, *et al.*, M. Okubo, A. Yamada, *Nat. Commun.*, **2015**, *6*, 6544.
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Biography:

Dr. Masashi Okubo is an associate professor in the Department of Chemical System Engineering, School of Engineering, the University of Tokyo.

Dr. Okubo received a Ph.D. in coordination chemistry from the University of Tokyo in 2005. After serving as a postodoctral fellow, an assistant professor, and a senior researcher at Universite Pierre et Marie Curie, National Institute of Advanced Industrial Science and Technology for 9 years, he joined the faculty at the University of Tokyo, where he is now. His research group focuses on the design and development of novel materials for electrochemical energy storage devices including batteries and capacitors. He has published over 80 scientific papers in international journals.

He was awarded the Young Scientist Award from Minister of Education, Culture, Sports, Science and Technology in 2017, the Young Scientist Award from Japan Society of Coordination Chemistry in 2016, and the Young Investigator Award (Gold Prize) in 5th International Conference on Advanced Capacitors in 2016.

As a faculty member at the University of Tokyo, he was awarded the Dean's Award 2018 from School of Engineering, the University of Tokyo for his significant contributions and achievements in research category.

Nanohybrids with MXenes as Building Units for Renewable Energy

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Abstract:

MXenes, a kind of novel 2D transition metal carbides/nitrides, have attracted interests recently with great potential in vast fields. Compared to other 2D materials, the MXenes feature with wide chemical and structural diversity, and balanced-combination of myriad merits such as high conductivity, good mechanical stability, excellent hydrophily and rich surface chemistry enabled that can be engineered by grafting chemical groups. Together with ultralow work function and electronegative surface, the MXenes can also tailor the electronic and chemical structure of the guest phases via synergistic interactions. These advantages make the MXenes highly promising as building units for fabrication of high performance materials for electrochemical energy storage and conversion. In this report, we first demonstrate the great potential of MXenes with superior conductivity and density to soft carbon for construction of electrodes with high volumetric energy density, high power output and long life for Li storage. Then, we present the structural and electronic engineering strategies for developing highly active MXene-based 2D electrocatalysts with different chemical properties for electrocatalytic splitting of water. Finally, we show the possibility for engineering 3D MXene architecture with kinetics-favorable structure, enhanced surface area and aggregation-resistant properties, which is potentially an ideal building unit for making high-performance electrocatalysts.

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Biography:

Dr. Jieshan Qiu is CheungKong Distinguished Professor at College of Chemical Engineering, Beijing University of Chemical Technology (BUCT), China. Before moving to BUCT in May 2018, he was a professor at Dalian University of Technology (DUT), China, and Director of Liaoning Key Lab for Energy Materials & Chemical Engineering at DUT, China. He mainly works on functional materials and chemical engineering, with a focus on the methodologies for synthesis of advanced functional materials and their uses in catalysis, energy conversion and storage (batteries, fuel cells, supercapacitors, etc.), and environment protection. He has received over 20 awards, including the 1st-class Award for achievements in basic research from the Education Ministry of China, for two times. Currently, he is the Associate Editor of ***ACS Sustainable Chemistry & Engineering***, and the ***CIESC Journal*** published by the Chemical Industry and Engineering Society of China. He has served as the editor of the journal ***Carbon*** from 2006 to 2010, and the founding editor of the journal ***FlatChem*** (2015-2016) published by Elsevier. He is the Vice Chairman and Fellow of the Chinese Society of Micro-Nano Technology since October 2015. He has filed over 90 patents, and published over 650 papers in peer-reviewed journals including ***Adv. Mater., Adv. Funct. Mater., Adv. Energy Mater., Nano Energy, ACS Nano, Angew. Chem. Int. Ed.,*** etc., of which 50 are highlighted as hot paper and/or cover of the journals, and 190^{+} are published in journals with IF over 7. His papers have been cited for over 20000 times, with h-index of 67 (Web of Sci.).

Rational Design of MXenes for 2D Magnetic and Electrode Materials

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Abstract:

Recent experimental success in the realization of two-dimensional magnetism has invigorated the search for low-dimensional material systems with tunable magnetic anisotropy that exhibit intrinsic long-range ferromagnetic order. In this talk, I will present a rational design approach for studying and engineering magnetism in MXenes. I will also discuss MXenes as high capacity electrode materials [1], investigations into the effects of MXene surface structure on electronic properties [2], and a recently developed model for applying machine learning to accelerate MXene synthesis [3]. Using a crystal field theory model and first-principles simulations, we demonstrate intrinsic ferromagnetism, high magnetic moments, high Curie temperatures, and intrinsic semiconducting and half-metallic transport behavior in nitride [4] and ordered double-transition-metal MXenes [5]. We report that modifying the surface termination and transition metal in monolayer M_2NT_x nitride MXenes gives rise to a rich diversity of noncollinear spin structures and finely tunable magnetocrystalline anisotropy [6]. We predict that manipulating the strength of the spin-orbit interaction and electron localization via the chemical degrees of freedom can induce sufficient anisotropy to counteract thermal fluctuations that suppress long-range magnetic order. Further, surface engineering and applied electric fields enable robust switching and stabilization of magnetic behavior in MXenes [7]. Our work suggests that MXenes offer a promising avenue for achieving both high capacity electrode materials and practical spintronic devices.

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Biography:

Vivek Shenoy is the Eduardo D. Glandt President's Distinguished Professor in the School of Engineering and Applied Sciences at the University of Pennsylvania with appointments in the Departments of Materials Science and Engineering, Bioengineering and Mechanical Engineering. Shenoy is the principal investigator and director of the NSF-funded Science and Technology Center for Engineering Mechanobiology established in 2016. Dr. Shenoy's research focuses on developing theoretical concepts and numerical methods to understand the basic principles that control the behavior of both engineering and biological systems. He has used rigorous analytical methods and multiscale modeling techniques, ranging from atomistic density functional theory to continuum methods, to gain physical insight into a myriad of problems in materials science and biomechanics. Dr. Shenoy's honors include a National Science Foundation CAREER Award (2000), the Richard and Edna Solomon Assistant Professorship (2002-2005) and the Rosenbaum Visiting Fellowship from the Isaac Newton Institute of Mathematical Science, University of Cambridge and the George H. Heilmeier Faculty Award for Excellence in Research (2019). He serves as the editor of the Biophysical Journal and is a fellow of the American Institute for Medical and Biological Engineering (AIMBE).

Two-dimensional MXenes for Efficient Energy Storage and Conversion

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Abstract:

The ever increasing demand of renewable energy has driven the development of new materials for the new-generation energy conversion and storage. Among all the candidature materials, 2D transition metal carbides, carbonitrides and nitrides (often referred to as MXene) have drawn intensive attention owing to their excellent conductivity and unique catalytic capability in various functional applications. Specifically, our research shows that MXene can be applied as host materials for anchoring single atoms to be used in electrochemical hydrogen generation [1] and carbon dioxide conversion [2]. MXene-based composite materials have been successfully applied as high performance electrode materials for new-generation of rechargeable batteries including sodium-ion batteries [3-5], lithium-sulfur batteries [6, 7], and lithium-iodine batteries [8]. Moreover, the rational design of the MXene architecture can also enable highly efficient desalination of saline water [9]. The 2D MXene-based materials are promising candidates for efficient energy storage and conversion.

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Biography:

Professor Guoxiu Wang is the Director of the Centre for Clean Energy Technology and a Distinguished Professor at University of Technology Sydney (UTS), Australia. Professor Wang is an expert in materials chemistry, electrochemistry, energy storage and conversion, and battery technologies. Currently, he serves as a regional editor for **Polyhedron**, an Associate Editor for **Frontiers in Energy Research**, an editorial board member for **Scientific Reports** (Nature Publishing Group) and **Energy Storage Materials** (Elsevier). His research interests include lithium-ion batteries, lithium-air batteries, sodium-ion batteries, lithium-sulfur batteries, supercapacitors, hydrogen storage materials, fuel-cells, 2D materials such as graphene and MXene, and electrocatalysis for hydrogen production. Professor Wang has published more than 460 refereed journal papers with an h-index of 94. His publications have attracted over 30,000 citations.

Optimization of $Ti_3C_2T_x$ MXene and Its Application in Li-S battery

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Abstract:

MXenes have shown promise in the potential applications of ion batteries and supercapacitors like carbon-based materials. The fast adsorption and intercalation capabilities ensure their superiorities on the application of high-power energy storage devices. However, stacking problem still exists in these materials, which can significantly decrease their performance with increased thickness and mass loading. We have developed several strategies to try to solve this problem. $Ti_3C_2T_x$/PDA composite film electrode was rationally designed and successfully synthesized by one-step in situ polymerization of dopamine on the surface of the $Ti_3C_2T_x$ nanosheets. We also developed a simple and effective strategy to intercalate conductive polymer (PEDOT) as spacer between $Ti_3C_2T_x$ sheets. Without the additives, we employed the 3D architecture of a $Ti_3C_2T_x$ aerogel to restrict the restacking of 2D $Ti_3C_2T_x$ nanosheets and developed a foam-morphology. These samples exhibit improved performance compared with the untreated ones. For example, The $Ti_3C_2T_x$/PEDOT hybrid film electrode exhibits a high volumetric capacitance of 1065 F cm^{-3} at 2 mV s^{-1}. An asymmetric supercapacitor based on it and reduced graphene oxide delivers a maximum energy density of 23 mWh cm^{-3} and power density of 7659 mW cm^{-3}, much superior to the previous $Ti_3C_2T_x$-based supercapacitors. Furthermore, the thickness-dependent diffusion mechanism with different types of hydrated ions has also been revealed by combining the experimental and DFT calculated results.

In consideration of the superior adsorption abilities, we used $Ti_3C_2T_x$ as the host material of sulfur to tackle the poor cycling stability and inferior rate capability of Li-S battery. The S/$Ti_3C_2T_x$ composite with a carbon nanotube thin film interlayer could deliver a high initial discharge capacity of 1458 mAh g^{-1} at a current density of 0.1 A g^{-1} and an ultralow capacity decay of 0.04% per cycle at 0.8 A g^{-1} for over 1500 cycles was achieved. More importantly, a reversible capacity of 608 mAh g^{-1} was obtained at a high current density of 8.2 A g^{-1} (≈5 C), demonstrating superior rate capability. These results suggest that the S/$Ti_3C_2T_x$ composite is a promising sulfur cathode material.

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Biography:

Xitian Zhang is currently a professor and vice president at Harbin Normal University. He obtained his bachelor degree from Jilin University at 1987. After that, he received his master degree in 1989 from the Changchun Institute of Physics, Chinese Academy of Sciences and his doctorate from the Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences in 2002. From 2002 to 2005, he was a postdoctoral fellow at the Chinese University of Hong Kong (CUHK) and joined the CUHK as an assistant professor from 2005 to 2007. He has published over 120 SCI indexed research papers up to now. His research interests are centered on design and synthesis of energy storage materials and focus on seeking the advanced strategies to improve the electrochemical performance of new energy materials.

Synthesis and Surface Modification of High Pressure MAX Phase

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Abstract:

Two-dimensional titanium carbide $Ti_3C_2T_x$ MXene, as metallic-like graphene, arouses great attentions in energy storage and conversion in terms of the chemical/physical properties dependence of its unique surface structures and active Ti element[1, 2]. The existence of low valence Ti in $Ti_3C_2T_x$ MXene makes it act as an effective reductant to some oxidant agents, such as Ag(I), Au(II), Fe(III), Cr(VI), and Mn(VII)[3-5]. This special self-reductive role offers a prerequisite to tailor the chemical properties of MXene. Namely, some new MXene/metal or oxides composites are expected to be synthesized in a way in which the surfaces are covered by metal or oxides nanoparticles. Herein, a new MXene/$Na_{0.55}Mn_{1.4}Ti_{0.6}O_4$ hybrid ws synthesized by direct reduction of $NaMnO_4$ aqueous solution using $Ti_3C_2T_x$ MXene's self-reduction properties[6]. Owing to its two electrochemically active redox couples, namely, Mn^{4+}/Mn^{3+} (3.06 V) and Mn^{2+}/Mn (0.25V), the MXene/$Na_{0.55}Mn_{1.4}Ti_{0.6}O_4$ hybrid can be employed as both anode and cathode electrode materials for LIBs. This MXene/$Na_{0.55}Mn_{1.4}Ti_{0.6}O_4$-based symmetrical LIBs exhibites an average voltage of 2.8 V and the highest energy density of ~ 393.4 Wh kg^{-1}, among all symmetric full cells reported so far. This novel work will open a new pathway for the MXene applications in symmetric battery fields.

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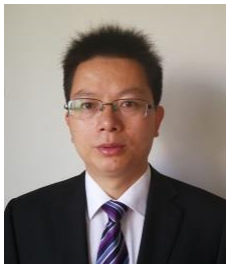
Biography:



Qiuming Peng is a professor of College of Materials Science & Engineering and Metastable material science and technology SKL, Yanshan University. He received his Ph.D. degree in 2008 from ChangChun Institute of Applied Chemistry, CAS. He was a Alexander von Humboldt Fellow in GKSS Research Centre in 2009-2011. He has published more than 140 peer-reviewed papers in the international journals with citation over 2140 times and H-index of 32.

MXenes for Energy Storage: from Active Materials to Electrodes

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Abstract:

MXenes, a new family of two-dimensional (2D) transition metal carbides and nitrides, are receiving intense interests in energy storage and conversation due to their unique characteristics. The rich chemistry and tunable surface termination, metallic conductivity and surface hydrophilicity make MXene an attractive candidate electrode material for supercapacitors and secondary batteries. Meanwhile, due to their hydrophilic 2D layer structure, MXene sheets can fabricate into freestanding and flexible films, which are regarded as a promising candidate for flexible electrodes. In this presentation, we will show our recent work on the application of MXenes in energy storage, including MXene-based active materials and MXene-bonded electrodes for batteries and supercapacitors. A series of MXene-based nanocomposites including Mn_3O_4/MXene, SnO_2/MXene, TiO_2/MXene and P/MXene are prepared. In these nanocomposites, the MXene nanosheets can not only provide efficient pathways for fast transport of electrons and Li ions, but also buffer the volume change of the metal oxides or P during lithiation/delithiation, making the nanocomposites exhibit high capacity, excellent cycle and rate performances as anodes for LIBs. In addition, we propose a novel strategy to employ 2D MXene as a multifunctional conductive binder for electrode fabrication for batteries and supercapacitors. By a simple vacuum-assisted filtration, MXene-bonded freestanding flexible activated carbon, silicon, small sulfur electrodes are fabricated for supercapacitors, sodium ion batteries and Li-S batteries, respectively. Different from the conventional insulate binders such as PVDF and PTFE, the MXene acts as conductive binder, active material and flexible backbone, and can also buffer the volume change of the active materials. As a result, the MXene-bonded electrodes present much superior electrochemical performances to the conventional PVDF/PTFE-bonded electrodes, indicating a promising electrode fabrication for energy storage.

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Biography：

Dr. Bin Xu is a professor in College of Materials Science & Engineering and State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology. He is also a Vice-Director of Beijing Key Laboratory of Electrochemical Process and Technology for Materials. He received his Ph.D. degree in 2006 from Beijing Institute of Technology. He served as a visiting professor in Drexel University in 2016-2017. He leads a group of researchers working on carbon and MXene-based materials for energy storage, including supercapacitors and batteries. Prof. Bin Xu has published more than 90 peer-reviewed papers in international journals with citations over 4000 times and H-index of 35.

MXene based materials for high-performance micro-supercapacitors and batteries

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Abstract:

MXenes, as an emerging novel class of two-dimensional materials, have been widely explored as a great promising electrode material for energy storage, such as supercapacitors and batteries. Herein, we reported the assembling of MXene-based micro-supercapacitors based on ionic liquid pre-intercalated MXene films with high voltage of 3 V and high energy density of 43 mWh cm^{-3}. We also demonstrated the fabrication of alkalized Ti_3C_2 (a-Ti_3C_2) MXene nanoribbons with expanded interlayer spacing, ultrathin thickness, narrow widths of nanoribbons and open macroporous structures, which was prepared via continuous shaking treatment of pristine Ti_3C_2 MXene in aqueous KOH solution. Benefitting from the expanded interlayer spacing of a-Ti_3C_2, narrow widths of nanoribbons as well as 3D interconnected porous frameworks for enhanced ion reaction kinetics and improved structure stability, the resulting a-Ti_3C_2 anodes showed excellent sodium/potassium storage performance. Further, ultrathin nanoribbons of sodium/potassium titanate were successfully synthesized by simultaneous oxidation and alkalization process of Ti_3C_2 MXene. In addition, we constructed 3D a-Ti_3C_2 frameworks as S/polysulfides host and 2D delaminated Ti_3C_2 MXene (d-Ti_3C_2) nanosheets as interlayer on polypropylene (PP) separator, respectively, resulting in an all-MXene based integrated cathode for Li-S batteries without metal current collector.

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Biography:

Dr. Wu received Ph.D. degree in materials science from Institute of Metal Research (IMR), Chinese Academy of Sciences (CAS) in 2011. Then he worked as a postdoctor at Max-Planck Institute for Polymer Research in Germany from 2011 to 2015. Since June 2015, he joined DICP, CAS and became a full Professor, and was appointed group leader of 2D Materials & Energy Devices.

His current scientific interests include graphene, two-dimensional nanomaterials, and advanced nanocarbon based materials for energy and environmental applications. He has published 80 peer-reviewed papers (IF>10, 40 papers) in Energy Environ. Sci., Nat. Commun., Adv. Mater., J. Am. Chem. Soc., ACS Nano, Angew. Chem. Int. Ed., which have been cited more than 16000 times with Web of Science, H-index=39. He has received many awards and honors, such as the National Natural Science Award (2nd class, 2017), Liaoning Provincial Science and Technology Award (1st class, 2015), Recruitment Program of Global Expert (1000 Talent Plan), etc. He is a member of National Technical Committee 279 on Nanotechnology of Standardization Administration of China, CIGIU International Standardization Technical Committee, Technology Committee for Inner Mongolia Institute of Graphene Materials, etc. Additionally, Dr. Wu is currently severing as guest editors and editorial board of Journal of Energy Chemistry and Chinese Chemical Letters, guest editor of Energy Storage Materials, and corresponding expert (Clean Energy) of journal Engineering, International Advisory Board of Materials Research Express, and Editorial Board of *Journal of Physics:* Energy.

Two-Dimensional MXene and Their Composites: Synthesis and Applications

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Abstract:

MXenes, a new family of two-dimensional (2D) early transition metal carbides and carbonitrides, have been receiving a significant research interest by virtue of their excellent electrochemical energy storage properties, high electrical conductivity, and superior mechanical properties. The precursor MAX phases Ti_3AlC_2 and Ti_2AlC, as well as some bimetal composites with high purity have been successfully obtained by hot pressing method [1-4]. MXenes are successfully prepared by etching Al from precursor MAX in HF [5]. To obtain MXene with few and/or single layer, the etching time is lengthened [6]. Another mature synthesis route to layered MXene is HCl/LiF etching, which is assisted by mild sonication [7]. Also, we focus on the surface modification of MXene and MXene-based composites, with probable synergistic effect in agglomeration prevention, facilitating electronic conductivity, improving electrochemical stability and enhancing pseudocapacitance [8-11]. Here, we summarize the development and progress of our work in synthesis of various MXene and modifications to MXene-based composites, focusing on their performances and applications as mediator-free biosensors, Li-ion batteries, supercapacitors and photocatalysts.

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Biography:

Dr. Jianfeng Zhu, is the professor, doctoral supervisor and dean at School of Materials Science and Engineering, as well as executive dean at Institute of Silicate Cultural Heritage, Shaanxi University of Science and Technology. He is also a director of Key Laboratory of Green Preparation and Functionalization of Inorganic Materials, an academic leader in Material Science and a leading talent of young and middle-aged technological innovation in Shaanxi Province. His main research areas are green preparation of ceramic materials and functional materials for new energy storage and environmental purification. He has published more than 150 papers in domestic and international famous academic journals, in which over 120 papers were indexed by SCI and EI. More than 100 national invention patents have been authorized and 15 patents have been transferred and applied. He also has presided over 10 projects including the National Natural Science Foundation, the Shaanxi Natural Science Foundation, the Shaanxi Major Science and Technology Coordination and key industrial projects of Petrochina or other enterprises. He has won 2 first prize and 4 second prizes for science and technology at the provincial and ministerial level.

$Ti_3C_2T_x$ MXene for Energy Storage Applications

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Abstract:

MXenes are two-dimensional (2D) early transition metal carbides and nitrides, which are usually produced by selective etching of the A group element from MAX phases [1,2]. Thanks to their unique properties, MXenes have shown great potential as electrode materials in energy storage devices [3-6]. In this presentation, we will first show new strategies to boost the electrochemical performance of MXenes materials. Ultra-high rates performance, exceeding those of conventional EDLCs, could be achieved in sulfuric acid electrolyte thanks to the control of the electrode architecture with 1500 F cm^{-3} and 350 F g^{-1} for the volumetric and gravimetric capacitance, respectively [7]. Differently, in non-aqueous electrolyte - which offer increased voltage window and thus improved energy density - MXene electrodes performance was so far limited to few tens of F g^{-1}. For instance, only 70 F g^{-1} could be achieved in a 3V in EMI-TFSI neat ionic liquid (IL) electrolyte [8,9]. However, our recent results have shown that MXene electrodes can be successfully operated in non-aqueous Li^+-containing electrolytes with capacitance beyond 200 F g^{-1}, by controlling the architecture [10] or the surface functional groups. This opens new opportunities for MXene materials for energy storage applications.

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Biography:

Patrice Simon is currently Distinguished Professeur of Materials Sciences at Université Paul Sabatier, Toulouse, France. He also serves as Deputy director of the French network on electrochemical energy storage (RS2E, see http://www.energie-rs2e.com/en).

He received his PhD in 1995 from Ecole Nationale Supérieure de Chimie - Toulouse. He was appointed as Assistant Professor in Electrochemistry at Conservatoire National des Arts et Métiers in Paris, and joint Université Paul Sabatier in 2001.

His research activities are focused onto the modification of the material/electrolyte interfaces in electrodes for electrochemical energy storage devices (batteries and electrochemical capacitors). Patrice Simon is currently senior member (2017) of the Institut Universitaire de France and member of the French Academy of Technologies (2018). He received several awards for his work such as the CNRS Silver medal (2015), the Russnanoprize (2015), the Brian Conway Prize from the International Society of Electrochemistry (2018). He was distinguished as Citation Laureates 2018 by Clarivates Analytics.

Smaller is better: MXene particulates for energy storage

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Abstract:

Ti_3AlC_2, a typical layered ternary carbide belonging to a big family referred as to MAX phases, has shown much promise in various applications. Especially, its derivative, $Ti_3C_2T_x$ MXene, have been regarded as promising candidates in the field of electrochemical energy storage. Researchers have long committed to obtain small-grain-sized Ti_3AlC_2 powder, owing to that small-sized Ti_3AlC_2 with higher surface areas always leads to high catalysis efficiency and sintering activity of Ti_3AlC_2 itself and shortens ions diffuse distance and provides lager electroactive surface area for $Ti_3C_2T_x$ MXene. However, among the reports so far, the synthesis of Ti_3AlC_2 with small size is difficult to achieve. Here, we present a new method to obtain submicron Ti_3AlC_2 grains grown in molten salt *for the first time*. Importantly, small-sized $Ti_3C_2T_x$ MXene prepared by etching as-fabricated Ti_3AlC_2 exhibited high gravimetric capacitance as supercapacitor electrode.

The significances are as bellow.

(1) To the best of our knowledge, submicron Ti_3AlC_2 grains were synthesized by molten salt method for the first time. The synthesis temperature is about 300 ℃ lower than other synthesis methods which means obtaining submicron-sized Ti_3AlC_2 powders become easier.

(2) Submicron-sized $Ti_3C_2T_x$ MXene was obtained by etching the Ti_3AlC_2 synthesized in molten salt. As-prepared $Ti_3C_2T_x$ exhibited a better electrochemical performance than that obtained by etching bulk porous Ti_3AlC_2. As far as we know, it is the highest record for the multilayer $Ti_3C_2T_x$ MXene without any modification treatment.

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Biography:

Dr. Xiaohui Wang is currently a professor at the Institute of Metal Research (IMR), Chinese Academy of Sciences (CAS). He was born in Henan, China in 1976. He received a B.S. in chemistry from Zhengzhou University in 1997. He obtained his Ph.D. in materials science and engineering in 2003 from IMR, CAS, with a focus on the synthesis, structure and properties of layered machinable and electrically conductive Ti_2AlC and Ti_3AlC_2 MAX ceramics. He then spent almost two years for plasma processing of nanomaterials at the NIMS (Tsukuba, Japan, under Dr. T. Ishigaki) where he explored spherical nanosized TiO_2 with tunable Fe(III) dopant concentrations, and established the relationship between the dopant concentration and photocatalytic properties under UV and/or visible irradiations. He then spent over two years as a postdoctoral fellow at the Tohoku University (Sendai, Japan, under Prof. T. Kyotani) where he developed an electrochemical approach to selectively fill magnetic particles into one-end-opened carbon nanotubes at the bottom, and carbon-coated anodic aluminum oxide films with brilliant and tunable colors based on the template method. He joined IMR in 2007, and became a full Professor in 2015. His current research interests include MAX phases-derived MXenes for energy storage, and $LiFePO_4$ nanomaterials for high-rate lithium-ion batteries.

Nanocomposites Based on MXenes for Energy Storage

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Abstract:

To tackle the problems such as the restacking of the nano-layer structure and the moderate capacity of the MXenes for energy storage applications, we worked on the construction of MXene based nanocomposites for Li-ion batteries (LIBs), supercapacitors (SCs) and Li-S batteries. Firstly, we developed a facile route to the synthesis of CNTs@MXene nanostructures, in order to overcome the problems of re-stacking and collapse of MXenes. At a high rate, the capacity of as-prepared CNTs@MXene anodes exceeds commercial graphite and most reported MXenes systems in LIBs. Secondly, a three dimensional (3D) SnO_2@C/d-Ti_3C_2 (S-TCS) network architecture was fabricated by employing a sol-gel method to anchor the core-shell SnO_2@C onto the d-Ti_3C_2 xerogel framework. Typically, 3D S-TCS delivers reversible specific capacity of 520 and 492 mA h g^{-1} at the current density of 1.0 and 2.0 A g^{-1}, respectively, after 1000 times charge-discharge cycles. Thirdly, binder-free Ti_3C_2 MXene-carbon nanotubes (Ti_3C_2-CNTs) composite films were successfully deposited onto graphite substrate by electrophoretic deposition (EPD). The as-prepared Ti_3C_2-CNTs electrode exhibited enhanced specific capacitance, with excellent cycling stability. Finally, we will report our latest progress on the research of MXenes for energy storage at the conference.

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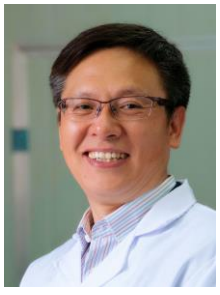
Biography:



Prof. Sun served as a research associate at IMR after gaining his Ph.D degree in 1992. In March 1993, he joined the Institute of Physical Chemistry, the University of Vienna, as a guest researcher. In August 1994, he joined the Toyohashi University of Technology, Japan, under the support of Daiko Foundation, and later obtained a fellowship from the Japan Society for the Promotion of Science (JSPS). In April 1997, he joined the Tohoku National Industrial Research Institute (reorganized to AIST), as a research officer, a permanent position.), and was later promoted to a senior research scientist and served as an associate to the director of the International Affairs Division. He also worked at Drexel University, USA, in February 2004 for one year, on his sabbatical leave from AIST. In 2013, he was selected by The Recruitment Program of Global Experts, generally called 1000-Talents Program, and joined the School of Materials Science and Engineering, Southeast University. His research interests cover the research and development of metallic materials, intermetallic compounds, ceramics and composites, including their synthesis, characterization and applications. In the past decade, he devoted most of his energy to the MAX phase materials, a family of ternary compounds, which combines the best attributes of metals and ceramics. Recently, he is leading his group on the research and development of materials, including MXene and other low dimensional materials, for the application in energy storage and conversion. He has authored over 200 SCI indexed papers and applied over 40 patents. http://smse.seu.edu.cn/sun/

Ab initio study of Transition Metal Carbides

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Abstract:

In this talk, I will present our recent progress on the theoretical research of two-dimensional transition metal carbides (MXenes). Our main findings include: (1) Vacancy-mediated lithium adsorption and diffusion on MXenes. We highlighted that compared with other well-studied 2D materials (such as graphene, 2D MoS_2), MXenes are more likely to contain vacancies with defect formation energies as low as 0.96 eV. The vacancy defect will enhance the adsorption of Li in the region near the defect through acting as a potential trap, which may cause the first cycle irreversibility for lithiation/delithiation process in MXene LIBs. Nevertheless, Li tends to migrate on defect-free surface of MXene with energy barrier of 0.096-0.115 eV and thus this potential trap has a minor influence on the charge-discharge rate of MXene LIBs. (2) Abnormally strong electron-phonon scattering induced unprecedented reduction in lattice thermal conductivity of 2D Nb_2C. In most materials, the electron-phonon (e-p) scattering is far weaker than phonon-phonon (p-p) scattering, and the e-p scattering is usually proportional to the e-p coupling strength. Here, we report strong e-p scattering but low e-p coupling strength in 2D Nb_2C by first-principles calculations. By calculating the phonon transport property of 2D Nb_2C, we show that this strong e-p scattering can result in great reduction in the lattice thermal conductivity. (3) Prediction of new 2D molybdenum barbides as high capacity anodes for Lithium-ion batteries and Sodium-ion batteries.

Biography：

Dr. Zhimei Sun is a Cheung Kong Scholar Chair Professor, currently working at the School of Materials Science and Engineering, Beihang Univerisity, China. She received her doctor degree from the Institute of Metal Research, Chinese Academy of Sciences in 2002; From 2002 to 2007, Dr. Sun had worked at RWTH Aachen University (Germany) and Uppsala University (Sweden); From 2007 to 2013, she had worked as a professor in Xiamen University; In August 2013, she joined the faculty of Beihang University. Dr. Sun has been working in the research fields of semiconductor materials and high-performance structural materials by both computational simulations and experiments.

Operando spectroscopic study of MXene-based energy materials

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Abstract:

As a fascinating new layered structure, MXenes have captured much attention as energy storage material due to their tunable chemical components and distinctive structural/electronic properties. The key to enhance its storage capacity is the controllable engineering of the interlayer spacing and not much have been achieved in this regard. Meanwhile, the dynamitic working process of MXene-based energy devices is still not clear. In this talk, we will present a concept of engineering of interlayer spacing and coordination of MXenes via atomic metal ion for realizing excellent storage capacity. Combining with ex-situ tests, an operando XAFS and Raman studies to in-situ probe the dynamic process in MXene electrodes will be discussed, along with the general structural self-reconstruction in electrocatalysis.

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Biography：

Prof. Li Song received his Ph.D. in 2006 from Institute of Physics, CAS. After four years as Humboldt fellow at University of Munich and postdoctoral researcher at Rice University, he became an associate professor at Shinshu University. He was promoted as professor at University of Science and Technology of China in 2012 by CAS Hundred Talent Program and Recruitment Program of Global Experts. His current research interests are synchrotron radiation study of low dimensional nanostructures and energy-related devices. In the past five years, he has published more than 60 SCI papers in *Adv. Mater.*, *Adv. Energy Mater.*, and other periodicals journals. More details can be found from his research ID http://www.researcherid.com/rid/B-1950-2010.

Printable MXene-based Nanocomposites for Wearable Electronics

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Abstract:

In recent years, the trend toward miniaturization and wearable electronics has pushed forward the field of stretchable and printable electronics and microscale energy storage units. The development of wearable strain sensors with simultaneous large stretchability (strain >55%) and high sensitivity (gauge factor >100) remains a grand challenge to this day. Moreover, the fabrication of fully printable, flexible micro-supercapacitors (MSCs) with high energy and power density remains a significant technological hurdle. To overcome these grand challenges, the 2D material MXene has garnered significant attention for its application, among others, as a printable functional material for high performing sensing and electrochemical energy storage devices. In this work, we demonstrate that strain sensors based on printable MXene-based nancomposite can simultaneously achieve ultrahigh sensitivity and large stretchability while performing well in linearity, reliability, long-term durability, and monotonicity. The bioinspired sensor demonstrated a gauge factor >200 over a range of working strains up to 83% and achieved a high gauge factor exceeding 8700 in the strain region of 76−83%. This successful combination of high sensitivity and large stretchability is attributed to (1) the microscale hierarchical architecture derived from the amalgamation of 2D titanium carbide (MXene) $Ti_3C_2T_x$/1D silver nanowire "brick" and poly(dopamine)/Ni^{2+} "mortar" and (2) the synergistic toughing effects from interfacial interactions of hydrogen and coordination bonding, layer slippage, and molecular chain stretching. Furthermore, we developed a facile and in situ process to homogeneously anchor hydrous ruthenium oxide (RuO_2) nanoparticles on $Ti_3C_2T_x$ MXene nanosheets. The resulting RuO_2@MXene nanosheets can associate with silver nanowires (AgNWs) to serve as a printable electrode with micrometer-scale resolution for high performing, fully printed MSCs. The fully-printed MSCs from the MXene-based nanocomposite inks demonstrated record volumetric capacitances of 864.2 F cm^{-3} at 1 mV s^{-1}, long-term cycling performance, good rate capability (304.0 F cm^{-3} at 2000 mV s^{-1}), outstanding flexibility, remarkable energy (13.5 mWh cm^{-3}) and power density (48.5 W cm^{-3}).

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Biography:

Jiajie Liang received his B.S. degree in chemistry from Nankai University in 2006. He obtained his Ph.D. degree in polymer chemistry and physics from Nankai University in 2011 under the supervision of Prof. Yongsheng Chen. He worked as a postdoctoral researcher in Prof. Qibing Pei's group at the University of California, Los Angeles, from 2011 to 2016. Thereafter, he joined Nankai University as a full professor and started to build the Lab for Printed and Wearable Electronics at the School of Materials Science & Engineering. He has published more than 50 papers including in top journals such as ***Nat. Photonics, Nat. Commun., Adv. Mater., ACS Nano, Adv. Funct. Mater.,*** and ***Adv. Energy. Mater.*** with citation over 6,000 times.

Capture and Catalytic Conversion of Polysulfides by in-situ Built TiO_2-MXene Heterostructures for Lithium-sulfur Batteries

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Abstract:

Lithium-sulfur (Li-S) batteries have attracted scientific attention owing to their superior energy density and low cost [1]. However, the shuttling behavior caused by the mobility of soluble polysulfide intermediates (LiPSs) and sluggish redox kinetics significantly degrades the capacity, rate capability and cycling life of Li-S batteries [2]. According to the previous works, 2D conductive MXene nanosheets cathode hosts can improve the performance of Li–S batteries by chemically entrapping polysulfides in the sulfur cathode [3]. In this presentation, I will present a novel catalyst design to kinetically propel polysulfide-involving redox reactions with high efficiency by in-situ crafting a unique TiO_2-MXene heterostructure. The TiO_2 nanocrystals on MXene sheets act as capturing centers to immobilize LiPSs, while the hetero-interface ensures rapid diffusion of anchored LiPSs from TiO_2 to MXene for fast conversion. As a result, the Li-S batteries with an interlayer composed of TiO_2-MXene heterostructures and graphene deliver high sulfur utilization and stable cycling performance [4]. Impressively, the capacity decay is only 0.028% per cycle over 1000 cycles at 2C, and even with the high sulfur loading over 5 mg cm^{-2}, the capacity retention of ~ 93% after 200 cycles at 0.5 C is achieved.

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Biography：

Prof. Quan-Hong Yang is a chair professor of School of Chemical Engineering and Technology, Tianjin University and the winner of National Science Fund for Distinguished Young Scholars. He received his BEng from Tianjin University in 1994 and his PhD on New Carbon Materials from Institute of Coal Chemistry, Chinese Academy of Sciences in 1999. He continued his carbon studies as research fellows in Institute of Metal Research, Chinese Academy of Sciences, CNRS France, Tohoku University and Southampton University. He joined Tianjin University as a full professor in 2006, and was promoted to a chair professor in 2016. His research focuses on nanocarbons and other low dimensional materials, and their applications in energy storage and environmental protection. He has published over 200 peer-reviewed papers with citations over 12,000 times and H-index of 60. He is the Clarivate Highly Cited Researcher and among 2018 Most Cited Chinese Researchers. He holds over 30 patents about nanocarbons and batteries. He received National Award for Technological Invention (2nd class, 2017), Nature Science Award of Tianjin (1st class, 2013), the Science and Technology Progress Award of Tianjin (1st class, 2012) and the Brian Kelly Award (British Carbon Group, 2004). He serves as Associate Editor for Energy Storage Materials and the members of the editorial boards for ten journals including Carbon and Science China Materials.

Salt-Assisted Synthesis of Two-Dimensional Metal Oixdes and Nitrides

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Abstract:

Two-dimensional (2D) materials have demonstrated excellent chemical, optical, electrical and magnetic characteristics and offer great potential in numerous applications. Therefore, corresponding synthesis technology of 2D materials with high-quality, high-yield, low-cost and time-saving is desired. This presentation will focus on the recent research progress in my group about the salt-assisted synthesis of 2D materials and their applications. We will discuss the properties of crystal and molten salts, provide examples of 2D materials synthesis (such as transition metal oxides, transition metal dichalcogenides, transition metal nitrides, transition metal phosphides) based on salt-templated method and molten salt method with their applications in energy storage and conversion. Importantly, the underlying mechanisms of salts with different states on the formation of 2D morphology are introduced to aid in rational synthetic route design.

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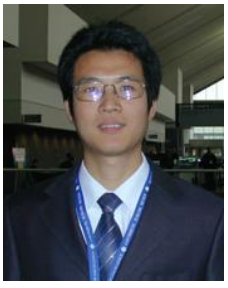
Biography：



Jun Zhou is a professor in Wuhan National Laboratory for Optoelectronics (WNLO) at Huazhong University of Science and Technology (HUST). He received his Bachelor Degree (2001) and PhD degree (2007) from the Sun Yat-sen University. During 2005-2006, He was a visiting student at school of materials science and engineering, Georgia institute of technology (GT). During 2007-2009, he served as a research scientist in the Wallace H. Coulter department of biomedical engineering and school of materials science and engineering of GT. He has published over 150 peer reviewed journal papers which have been cited over 12000 times. He has awarded 2018 highly cited researcher by Clarivate Analytics, the National Natural Science Award of Chinese government (second prize) for the Year of 2016, and the Excellent Doctoral Dissertation of China for the Year of 2009. He also has been awarded Excellent Youth fund of National Natural Science Foundation of China on year of 2013, enrolled in National Program for Support of Top-notch Young Professionals for the Year of 2014, Youth project for “Cheung Kong Scholars programme” of Ministry of Education Department of China for the Year of 2015. His research focuses on materials and devices for environmental microenergy conversion.

Fabrication and Properties of Actuators based on MXenes

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Abstract:

Electrochemical actuators are devices that convert electrical energy directly into mechanical energy, and are widely used in artificial muscles, micro-medical devices, sensors and other fields. With the development of science and technology, numerous materials have emerged for actuators, such as conductive polymers, carbon nanotubes, and graphene. Yet, the development of flexible, portable and stable electrode materials is a major challenge in the field of electrochemical actuators.

In this presentation, we report for the first time an actuator device using flexible MXenes as electrode material.[1] Device with response voltage of 0.6 V and the frequency of 0.001 Hz exhibits high performance with the curvature reaching 0.037 mm^{-1} and strain value up to 0.19 %. The actuation mechanism is investigated using *in-situ* XRD. This research provides a proof of concept for MXenes in new applications and promotes the development of electrochemical actuators.

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[1] D. Pang, M. Alhabeb, X. Mu, Y. Gogotsi*, Y. Dall'Agnese*, Y. Gao*. *In preparation*.

Biography:

Yu Gao is an Associate Professor at Key Laboratory of Physics and Technology for Advanced Batteries (Ministry of Education) at the Jilin University. He received his Ph.D. in Physical Chemistry from Jilin University in 2012. At 2012 he got the position of junior researcher, 2016 - Associate Professor in Department of Physics of JLU.

His research interests lie in the design, synthesis and characterization of novel nanomaterials for energy storage and conversion applications.

Yohan Dall'Agnese is an Assistant Professor at the Institute for Materials Discovery at the University College London. He received his Ph.D. in Materials Science and Engineering from Paul Sabatier University and Drexel University in 2016. Prior to joining UCL, he held an Associate Professor position at Jilin University, and a Postdoctoral appointment in the Faculty of Textile Science and Technology at Shinshu University.

His research interests lie in the design, synthesis and characterization of novel nanomaterials for energy storage and conversion applications.

Assembling 2D MXenes into supercapacitor electrodes with high energy and power densities

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Abstract:

Two-dimensional (2D) transition metal carbides/nitrides (MXenes) have shown promise for a range of applications due to their unique physical and chemical properties. The high electrical conductivity, 2D and layered structure, and rich surface chemistry of MXenes have sparked great interest in their properties as electrode materials for energy storage devices. However, similar to other 2D materials, the applications of MXenes in batteries and supercapacitors is dependent on their assembly into electrode structures with high electrical and ionic conductivities. The main focus of this talk is our group's recent research on the assembly of MXene flakes into electrode structures with high energy and power densities. We have found that the electrochemical properties of MXene electrodes are highly dependent on the size of MXene flakes used in their fabrications. Controlling the flake size in the electrode structures leads to significant improvements in their specific capacitance and rate capability. These properties are also improved by assembling MXene flakes into porous 3D structures. A method for fabrication of 3D MXene aerogels with ordered structures and the effects of ordering on the electrochemical properties of the aerogels will be discussed. Furthermore, our recent studies on preparation of MXene inks and 3D printing of MXene based devices will be presented. In addition, our work on increasing the chemical and electrochemical stability of MXene electrodes through unconventional assembly methods will be discussed.

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Biography:

Majid Beidaghi is an Assistant Professor of Materials Engineering at the Department of Mechanical Engineering at Auburn University. He obtained his Ph.D. in Materials Engineering from Florida International University in 2012. Then, he joined A. J. Drexel nanomaterials Institute and the Department of Material Science and Engineering at Drexel University to work as a Postdoctoral Researcher Associate from 2012 to 2015. He received the Ralph E. Powe Junior Faculty Enhancement award in 2017. The current research in Beidaghi's research group focuses on the synthesis of advanced materials and the development of manufacturing methods for applications such as energy storage (batteries and supercapacitors), sensors, and separation membranes.

Pillared Structure Design of MXene with Controlled Interlayer Spacing for Electrochemical Energy Storage

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Abstract:

Two-dimensional transition metal carbide materials (termed MXenes) have attracted huge attention in the field of electrochemical energy storage. Herein, with inspiration from the unique structure of pillared interlayered clays, we attempt to fabricate pillared Ti_3C_2 MXene via a facile liquid-phase alkali metal ion and cationic surfactant pre-pillaring and Sn^{4+} pillaring method. The interlayer spacing of Ti_3C_2 MXene can be controlled according to the size of the intercalated prepillaring agent (alkali metal ion, cationic surfactant). Due to the "pillar effect" of Sn between layers of Ti_3C_2, the nanocomposites exhibit excellent electrochemical performance as the electrodes for lithium-ion batteries and lithium-ion capacitors.

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[4] J.M. Luo, J.H. Zheng, J.W. Nai, **X.Y. Tao**, ***** *Adv. Funct. Mater.*, 2018, DOI:10.1002/adfm.201808107.

Biography：

Prof. Xinyong Tao, received his ph. D degree in Department of Materials Science and Engineering, Zhejiang University in 2007. Then, he did postdoctoral research at University of South Carolina from 2007 to 2008 and went to Stanford University as a visiting scholar from 2014 to 2015. He joined the Department of Materials Science and Engineering, Zhejiang University of Technology as professor at 2008. His research interests focus on the preparation and energy storage properties investigation of carbon-based functional materials, advanced lithium secondary battery and new energy storage materials. He has authored and co-authored about 200 peer-reviewed journal articles and has earned over 6400 citations with a personal h-index of 45. He was selected as "New century excellent talents in university", "Qianjiang specially-appointed professor", "New century 151 talent project (Level 1)" and acquired 2017 China National Funds for Excellent Young Scientists.

Advanced micro-supercapacitors based on MXenes

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Abstract:

Flexible micro-supercapacitors (FMSCs) show promising candidates for portable and on-chip energy storage due to their miniaturization, lightweight and high-security.[1] As an emerging class of two dimensional materials, MXenes have gain ground in the fabrication of high performance MSCs recently.[2] Herein, we have fabricated a series of micro-supercapacitors through varying processing procedure of $Ti_3C_2T_x$ powders prepared by a typical chemical etching method of MAX (Ti_3AlC_2) phase. For instance, highly conductive and flexible freestanding MXene films were obtained through vacuum filtration, FMSCs based on this films show high volumetric capacitance and energy density up to 183 F cm^{-3} and 12.4 mWh cm^{-3}.[3] Besides, conductive MXene ink have been successfully prepared through vigorous ultrasonication treatment of $Ti_3C_2T_x$ dispersion. With this conductive MXene ink, a paper-based FMSC was elaborately designed through spaying method, in which interdigitated MXene electrodes serve the dual function of active materials and current collector. This paper-based FMSCs exhibit high areal capacitance of 23.4 mF cm^{-2} and outstanding cyclic stability with 92.4% capacitance retention after 5,000 cycles.[4] On the other hand, the $Ti_3C_2T_x$ MXene ink was spin-coated on silicon wafer to fabricate on-chip micro-supercapacitors, thus MXene based on-chip supercapacitors with high electrochemical performance can be achieved.

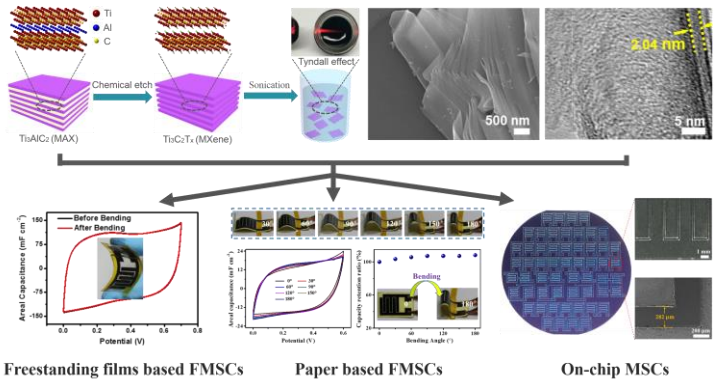

Figure 1 Preparation of $Ti_3C_2T_x$ MXene and corresponding micro-supercapacitors.

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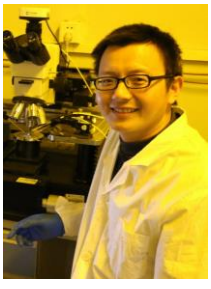
Biography:



Weiqing Yang received his Ph.D. in Materials Science and Engineering from Sichuan University in 2011. He was a post-doctorate research fellow at Georgia Institute of Technology from 2013 to 2014 under the supervision of Prof. Z. L. Wang. He is now a distinguished Young Scholars Professor of Southwest Jiaotong University in Sichuan province, Chengdu. His main research interest includes advanced nanoenergy materials and functional devices. He has published more than 140 papers in the famous journals such as Advanced Materials, Nano Letter, ACS Nano et.al. His works were reported by more than 20 famous media such as Newscientists, CCTV, et.al.

Tailoring of MXene composition, structure and surface chemistry

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Abstract:

Since their discovery in 2011 [1], 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 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 the state of the art available tailoring of the MXene properties owing to 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.

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Biography：

Dr. Per O.Å. Persson is a Professor of Thin Film Physics at the Department of Physics Chemistry and Biology, Linköping University (LiU), where he received his PhD in 2001. His research focus on the atomic level understanding of structure and chemistry in low-dimensional materials using advanced electron microscopy and spectroscopy methods.

Dr. Persson has been appointed as Special Researcher as well as Infrastructure Fellow by the Swedish Research Council (Basic Science) and the Swedish foundation for Strategic Research, respectively, in electron microscopy atomic level structural and chemical characterization.

New MAX phases and MXenes through A Replacement Approach

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Abstract:

Nanolaminated materials are important because of their exceptional properties and wide range of applications. Here, we demonstrate a general approach to synthesize a series of novel MAX phases and Halide ion-terminated MXenes originating from the replacement reaction between the MAX phase and the late transition metal halides. The approach is a top-down route that enables the late transitional element atom (Such as Zn, Cu etc.) to occupy the A site in the pre-existing MAX phase structure. For example, using this replacement reaction between Zn element from molten $ZnCl_2$ and Al element in MAX phase precursors (Ti_3AlC_2, Ti_2AlC, Ti_2AlN, and V_2AlC), novel MAX phases Ti_3ZnC_2, Ti_2ZnC, Ti_2ZnN, and V_2ZnC were synthesized. When employing excess $ZnCl_2$, Cl terminated MXenes (such as $Ti_3C_2Cl_2$ and Ti_2CCl_2) were derived by a subsequent exfoliation of Ti_3ZnC_2 and Ti_2ZnC due to the strong Lewis acidity of molten $ZnCl_2$. These results indicate that A-site element replacement in traditional MAX phases by late transition metal halides opens the door to explore novel MAX phases that are not thermodynamically stable at high temperature and would be difficult to synthesize through the commonly employed powder metallurgy approach. Moreover, the etching effect of Lewis acid in molten salts provides a clean and safe chemistry for the delamination of MAX phase to obtain MXene when compared with the commonly used HF-etching process. As evidenced by means of high-resolution scanning transmission electron microscopy (STEM), corresponding image simulations and first principles calculations, it is found that Cl atoms form a highly stable and ordered termination structure, without presence of other termination species. *In situ* (S)TEM heating experiments show that the Cl terminations are stable up to 600 °C, above which they desorb.

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Biography:

Dr. Qing HUANG is a Professor in the Engineering Laboratory of Nuclear Energy Materials, Ningbo Institute of Industrial Technology, CAS. He has worked as a post-doctoral research fellow at National Institute for Materials Science (2005-2008) and Chemical Engineering and Materials Science Department, UC-Davis (2008-2010). He was then joined Ningbo Institute of Industrial Technology, CAS as a professor (2010.4-Present), and been appointed as CAS Hundred-Talent Program Fellow (2010.12). His main research interests include structural materials for nuclear applications; structure-function integrated ceramics; novel layered multi-element materials, as well as their derivants-2D MXene.

Multifunctional MXene/Polyimide Aerogels

Hao-Bin Zhang

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Abstract:

2D transition metal carbides and nitrides (MXenes) have gained extensive attention recently due to their superb electrical conductivity, versatile surface chemistry, layered structure and intriguing properties [1-4]. The assembly of MXene sheets into macroscopic architectures is an important approach to harness their extraordinary properties [5-6]. However, it is difficult to construct a freestanding, mechanically flexible, and 3D framework of MXene sheets owing to the weak inter-sheet interactions. Herein, we developed an interfacial enhancement strategy to construct superelastic and lightweight 3D MXene architectures by bridging the individual MXene sheets with polyimide macromolecules. The resultant aerogel exhibits superelasticity with large reversible compressibility, excellent fatigue resistance (1000 cycles at 50 % strain), 20 % reversible stretchability, and high electrical conductivity of ≈ 4.0 S m^{-1}. The outstanding mechanical flexibility and electrical conductivity make the aerogel promising for damping, microwave absorption coating, and flexible strain sensor. More interestingly, an exceptional microwave absorption performance with a maximum reflection loss of −45.4 dB at 9.59 GHz and a wide effective absorption bandwidth (< −10 dB) of 5.1 GHz are achieved, as well as high sensitivity and excellent long-term stability as a smart flexible strain sensor. Additionally, the thermal stability and thermal insulation performances of the porous MXene/PI aerogel are also explored. Thus, this work provides a new methodology for constructing 3D highly porous MXene materials and would expand the potential applications of MXene materials greatly.

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Biography：

Hao-Bin Zhang is a professor in College of Materials Science & Engineering at Beijing University of Chemical Technology. He received his Ph.D in Polymer Chemistry & Physics from Ningbo Institute of Material Technology & Engineering (CAS) in 2010. He has published 48 peer-reviewed SCI research papers including *Adv. Mater.*, *Adv. Funct. Mater.*, *ACS Nano*, and *Small*. All the papers have been cited for over 3000 times and the most cited paper has got over 500 citations, and 5 papers are listed as the ESI highly cited papers and one Hot paper. He is the principal investigator of 6 grants funded by National Science Foundation of China and others institutions. His research focuses on synthesis and modification of 2D nanomaterials (Graphene/MXenes), electrically/thermally conductive polymer nanocomposites, and high-performance EMI shielding materials.

MXene/Polymer Hybrid Materials for Flexible AC-Filtering Electrochemical Capacitors

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Abstract:

Energy storage devices are limited by the trade-off between the transport properties and charge storage ability of materials. Electrolytic capacitors are kinetically fast, operating at kilohertz frequency, but limited by low capacitance. Electrochemical capacitors (ECs) provide high capacitance, yet their sluggish kinetics limit frequency response to a few hertz. Here, we devise strongly interacting, porous MXene/conducting polymer hybrids for large-scale flexible alternating current filtering symmetric ECs with high areal and volumetric capacitances of 0.56 mF cm^{-2} and 24.2 F cm^{-3} at 120 Hz, respectively. The high capacitance was maintained up to 1,000 V s^{-1} and originates from synergy of MXene/polymer hybrids. The operation of tandem ECs that filter a pulsating voltage from 60 to 10,000 Hz is demonstrated with device flexibility and durability over 30,000 cycles. These MXene hybrid-based ECs are expected to bridge the performance gap between high capacitance and the high-frequency response toward the form-factor-free miniature and scalable devices.

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Biography:

Prof. Ho Seok Park is an associate professor of Chemical Engineering at the Sungkyunkwan University (SKKU), an adjunct professor of the Samsung Advanced Institute for Health Science & Technology (SAIHST) and SKKU Advanced Institute of Nano Technology (SAINT), and SKKU Young Fellow. He received his Ph.D. from Korea Advanced Institute of Science & Technology (KAIST) in 2008 and worked as a Postdoctoral Researcher in the Department of Biological Engineering at Massachusetts Institute of Technology (MIT) from 2008 to 2010. His current research interests focus on energy and chemical storage materials and devices based on 2D and carbon nanomaterials. He has published ~150 peer-reviewed papers on top journals, such as Nat. Mater., Joule, Energy & Environmental Science, JACS, ACS Nano, Nano Lett., Adv. Mater., Adv. Energy Mater., Adv. Funct. Mater., and Nano Energy, and being taking editorial board member or associate editor in "Batteries & Supercaps" (Wiley), "Materials", "Carbon Letters", and "Macromolecular Research".

Atomic Defects in MXene Using Scanning Transmission Electron Microscopy

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Abstract:

MXene materials, transition metal carbides or nitrides, have recently gained interest as a developing class of 2D materials with applications geared towards energy storage, catalysis, and electronic devices. To better understand the physiochemical and electronic properties, detailed atomic resolution structural analysis of monolayer MXene was investigated using a combination of aberration-corrected scanning transmission electron microscopy (STEM), electron energy loss spectroscopy, and density functional theory (DFT). Large area $Ti_3C_2T_x$ MXene flakes, were synthesized and the type and concentration of atomic scaled defects were analyzed [1]. Ti vacancies and Ti vacancy clusters were found to be the most prevalent defects. The concentration of Ti vacancies depend on the synthesis conditions. Moreover, using in situ STEM, we observed growth in MXene layers around Ti vacancies. We obtained direct insight into the homoepitaxial Frank-van der Merwe atomic layer growth mechanism and demonstrate how the process can be exploited to obtain new transition metal carbides (TMC) phases that is synthesized on surfaces of Ti_3C_2 MXene substrates with the substrate being the source material [2]. This work could lead to the development of bottom-up synthesis methods, such as CVD and MBE, for controllable synthesis of larger-scale and higher quality single-layer TMC.

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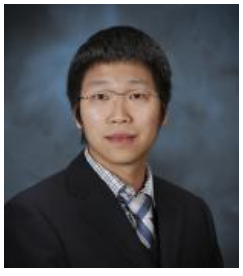
Biography:



Xiahan Sang is a professor at Wuhan University of Technology. He received a B. E. degree from Wuhan University in 2005, a Master's degree from Institute of Metal Research, Chinese Academy of Science in 2008, and obtained his Ph.D. in Materials Science from University of Pittsburgh in 2012. He was a postdoc at North Carolina State University from 2013 to 2015. His work involves TEM and STEM based technique development and applications in materials sciences including accurate and precise electron density measurement from quantitative CBED, drift-free and distortion free atomic resolution images using revolving STEM, and in situ S/TEM using gas cell, liquid cell, and heating stages.

Computational Synthesis of MXenes

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Abstract:

MXenes, an emerging family of two-dimensional materials, has attracted many attentions due to its extraordinary physical properties and potential applications in electrochemical energy storage devices [1]. Currently, MXenes are prepared through top-down method by selectively etching A elements away from MAX phases in hydrofluoric acid solution. The size and quality of MXenes are highly dependent on the parent MAX phases and the synthetic conditions, which hampers the practical applications of MXenes. In this talk, we report our recent findings on theoretical development of bottom-up method for large-scale preparation of MXenes. We will first show that hexagonal titanium carbide monolayer can be grown on Ti_3C_2 MXene [2]. Then we will show that various hexagonal transition metal carbides and nitrides can be grown on corresponded metal surfaces, which can be viewed as MXenes sitting on the surfaces. Our results can potentially lead to the development of a bottom-up synthetic method for large-scale MXenes.

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Biography:

Prof. Yu Xie received his doctor degree from Jilin University at 2010. After postdoc research in ETH Zurich, Oak Ridge National Laboratory, and Rice University, he became the professor in College of Physics at Jilin University in 2018. His interests are mainly focused on computational design and discovery of new energy materials and the application of machine learning in materials sciences. His publications encompass more than 30 research papers, including Nature, PRL, JACS, ACS Nano, Adv. Energy Mat., with a total citation over 3000 times and H-index of 27.

Two-Dimensional Nanomaterials for Electrocatalysis

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Abstract:

The global demand for energy has increased rapidly. Many advanced technologies for clean and sustainable energy conversion have become the subjects of extensive studies. Recently, 2D materials have displayed great potential in electrocatalysis due to their unique physical, chemical, and electronic properties.[1] Their low-cost and high performance demonstrate their potential as next generation electrocatalysts to replace precious metal catalysts. At the same time, there are tremendous opportunities in advancing electrochemical surface science at the atomic level by merging theoretical and experimental methodologies, which has led to many breakthroughs in the study and development of advanced 2D electrocatalysts. Recently, our group presented some works in the electrocatalytic application of 2D materials by combining experimental and simulation studies.[2] A special emphasis is placed on the development of design principles and determination of activity sites and catalytic mechanisms. Various 2D material-based electrocatalysts such as MXene, C_3N_4, MoN, Mo_5N_6 are applied for fuel cells, water splitting and CO_2 reduction etc.[3-5] Various engineering strategies for 2D materials and their influence on the intrinsic catalytic activities are discussed.

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Biography:

Dr. Shi-Zhang Qiao is currently a professor (Chair of Nanotechnology) at School of Chemical Engineering of the University of Adelaide. His research expertise is in nanostructured materials for new energy technologies including electrocatalysis, photocatalysis, fuel cell and batteries. He has co-authored more than 360 papers in refereed journals (over 37,000 citations with h-index 99). He has filed several patents and has attracted more than 12.0 million dollars in research grants from industrial partners and Australian Research Council (ARC).

Prof. Qiao was honored with a prestigious ARC Australian Laureate Fellow (2017), ExxonMobil Award (2016), ARC Discovery Outstanding Researcher Award (DORA, 2013) and an Emerging Researcher Award (2013, ENFL Division of the American Chemical Society). He has also been awarded an ARC ARF Fellowship and an ARC APD Fellowship.

Prof. Qiao is a Fellow of Institution of Chemical Engineers (FIChemE), a Fellow of Royal Society of Chemistry (FRSC) and a Fellow of Royal Australian Chemical Institute (FRACI). He is currently an Associate Editor of *Journal of Materials Chemistry* A, and is a Thomson Reuters/Clarivate Analytics Highly Cited Researcher (Chemistry, Materials Science).

Transition metal decorated Mo_2C MXene for enhancing fuel cell's performance

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Abstract:

Pt-based catalysts are still the promising catalysts for fuel cells, but their large-scale usage suffers from high cost, low abundance, poor stability, poor oxygen reduction reaction (ORR) reactivity on the cathode and CO poisoning on the anode. By using density functional theory, we select a representative MXene, Mo_2C, to screen the best supported metal monolayer on Mo_2C (M_{ML}/Mo_2C, M = Cu, Pd, Pt, Ag and Au) as catalysts towards ORR [1], aiming to find a promising catalyst to replace Pt/C catalysts used in the proton exchange membrane fuel cells (PEMFCs). We propose that Au_{ML}/Mo_2C is a promising ORR candidate with good stability, enhanced durability, comparable or even better ORR activity than the commercial Pt/C catalysts. Besides, to improve the CO tolerance of the anode Pt/C catalysts, we study Mo_2C-based single atom catalysts (SACs) [2], single cluster catalysts (SCCs) [3] and single metal monolayer catalysts (SMCs) [4]. We speculate that Zn/Mo_2CO_2 SAC and Cu_3/Mo_2CO_2 SCC can be used as good catalysts for CO removal. Considering the influence of H_2 fuels, we suggest that Ag_{ML}/Mo_2C can be used as a good catalyst for CO removal in H_2 feeds. It can be used not only as a filter membrane connected to the anode of fuel cells for separating H_2 and CO, but also as an efficient catalyst with high selectivity and activity for preferential oxidation of CO in the H_2 feeds. We hope our present studies could advance the development of fuel cells and inspire more applications about MXene catalysts.

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Biography:

Zongxian Yang, distinguished professor/Dean of College of Physics and Materials Science, Henan Normal University, China. He obtained Ph.D in 1998 at Fudan University majoring in Condensed Matter Physics. He worked as a postdoc and visiting professor in California State University (Northridge), University of California (Irvine), University of Western Ontario, and University of Ottawa in the years from 1999 to 2005.

Research field: Density functional studies on the physical and chemical properties of novel materials, especially the novel catalysts for energy and environment, e.g. the highly efficient electrode catalysts for fuel cells.

High-performance Electrocatalytic Conversion of N_2 to NH_3 Using Oxygen-vacancy-rich TiO_2 In-situ Grown on Ti_3C_2Tx MXene

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Abstract:

To achieve the energy-effective NH_3 production via the ambient-condition electrochemical N_2 reduction reaction (NRR), it is vital to ingeniously design an efficient electrocatalyst assembling the features of abundant surface deficiency, good dispersibility, high conductivity and large surface specific area (SSA) via a simple way. Inspired by that the MXene is with thermodynamically metastable marginal transition metal atoms, we prepared the oxygen-vacancy-rich TiO_2 nanoparticles (NPs) in-situ grown on the $Ti_3C_2T_x$ nanosheets ($TiO_2/Ti_3C_2T_x$) via a one-step ethanol-thermal treatment of the $Ti_3C_2T_x$ MXene. The oxygen vacancies acted as the main active sites for the NH_3 synthesis. The highly-conductive interior untreated $Ti_3C_2T_x$ nanosheets could not only facilitate the electron transport but also avoid the self-aggregation of the TiO_2 NPs. Meanwhile, the TiO_2 NPs generation could enhance the SSA of the $Ti_3C_2T_x$ in return. Accordingly, the as-prepared electrocatalyst exhibited a NH_3 yield of 32.17 μg h^{-1} $mg^{-1}_{cat.}$ at -0.55 V vs. RHE and a remarkable Faradaic efficiency of 16.07% at -0.45 V vs. RHE in 0.1 M HCl, placing it one of the most promising NRR electrocatlysts. Moreover, the density functional theory calculations confirmed the lowest NRR energy barrier (0.40 eV) of TiO_2 (101)/$Ti_3C_2T_x$ compared with $Ti_3C_2T_x$ or TiO_2 (101) alone.

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Biography:

Yuanhong Xu is currently a Professor of College of Life Sciences, Qingdao University, China. She also serves as an executive vice-president of the College. She received her Ph. D in analytical chemistry from Changchun Institute of Applied Chemistry (CIAC), Chinese Academy of Sciences (2009) with Prof. Erkang Wang. She then worked as assistant professor and associate professor from Mar. 2009 to Spe. 2014 in CIAC. During the period from May 2010 to May 2011, she obtained the "Humboldt Research Fellowship for Postdoctoral Researchers" and did postdoctoral research in Prof. Hermann Wätzig's group at TU Braunschweig, Germany. She joined Qingdao University in Oct. 2014. Her current scientific interests are in designing two-dimensional micro-/nano-materials for biosensors, fluorescent imaging and catalysis. She has published over 90 papers in peer-reviewed journals to an H-index of 25.

Property-driven Biomedical Applications of MXenes

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Abstract:

MXenes high electrical conductivity, electrochemical performance, surface functionality, ability to intercalate different ions and molecules into their gallery, and their biocompatibility make them a great candidate for different biomedical applications. In this talk, we present two recently explored biomedical applications of MXenes, as electrodes in neuroelectronic devices and as sorbents for urea removal from dialysate. For the former application, with collaboration with University of Pennsylvania, we have shown $Ti_3C_2T_x$ neural electrodes have remarkably low impedance and superior in vivo neural recording performance in comparison with standard metal microelectrodes. Specifically, when compared to gold microelectrodes of the same size, $Ti_3C_2T_x$ electrodes exhibit a 4-fold reduction in interface impedance with higher signal-to-noise ratio. Additionally, in neuronal biocompatibility studies, neurons cultured on $Ti_3C_2T_x$ are as viable as those in control cultures, and they can adhere, grow axonal processes, and form functional networks. In the second part of this talk, we present our recent work on urea adsorption of MXenes, with collaboration with University of Brighton. Since the early years of MXenes, several studies demonstrated MXene strong capability of intercalating different molecules and ions. By taking advantage of this property, we show $Ti_3C_2T_x$ can adsorb urea from dialysate reaching 94% removal efficiency at the initial urea concentration of 30 mg/dL, with the maximum urea adsorption capacity of 21.7 mg/g at 37 ºC. $Ti_3C_2T_x$ showed good hemocompatibility; it did not induce cell apoptosis or reduce the metabolizing cell fraction, indicating no impact on cell viability at concentrations of up to 200 µg/mL.

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Biography:

Babak Anasori is currently a Research Assistant Professor in the Department of Materials Science and Engineering and the A.J. Drexel Nanomaterials Institute at Drexel University. He received his PhD at Drexel University in 2014 in Materials Science and Engineering. His current research focuses on synthesis and characterizations of MXenes and their composites, as well as study of MXenes in energy storage, electronics, and biomedical applications. He has co-authored over 90 refereed publications, most of which are on MXenes, with more than 5000 citations and *h*-index of 36. He has received several national and international awards for his research and artistic way of presenting science including NSF/*Science* Visualization Challenge in 2011 and 2013, Diamond ranking in ACerS Graduate Excellence in Materials Science (GEMS) in 2012, and Materials Research Society (MRS) Postdoctoral Award in 2016. Babak has originated and organized multiple international student competitions including NanoArtography, and Science in Video (SciVid) in the MRS Fall Meetings.

Design of Pentagonal Monolayers for diverse applications

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Abstract:

Recently, MXenes, transitional-metal carbides/nitrides monolayers with a general formula of $M_{i+1}X_i$ ("M" is transition metal element, "X" is C or N, and i is 1 or 2), have attracted extensive attention because of their versatile properties for broad applications into nanodevices, energy storage, catalysis, electromagnetic interference (EMI), etc. In this talk, we will present our design on a new family of two-dimensional (2D) monolayers, pentagonal transitional-metal borides/carbides (penta-TMBs and penta-TMCs) and chalcogenides (penta-TMXs, X= S, Se, and Te) for multi-functional applications on the basis of density functional theory (DFT). (1) We found that all of the stable 2D penta-TMBs/TMCs are metallic, and 2D WB and HfC are ferromagnetic metals. We showed penta-TMBs and penta-TMCs show highly catalytic performance in HER. (2) We proposed that 2D *pentagonal* CrX (X = S, Se or Te) monolayers (penta-CrX) can be applicable into electronics, spintronics and photocatalysis. The penta-CrX monolayers are antiferromagnetic and semiconducting. The penta-CrS and penta-CrSe monolayers show good redox potentials versus normal hydrogen electrode, and their band gaps are comparable to the energy of photon in the visible light region, indicating their capable of maximal utilization of solar energy for water splitting. (3) We found that penta-NbX changes from metal to semiconductor as X changes from S/Se to Te. We show that penta-NbTe is a direct band-gap semiconductor with ultra-high carrier mobility (in the order of ~10^4 $cm^2V^{-1}s^{-1}$) and metallic penta-NbS is catalytically active for hydrogen evolution reaction.

Biography:

Dr. Hui Pan is an associate professor in the Institute of Applied Physics and Materials Engineering and head of Department of Physics and Chemistry in the Faculty of Science and technology at the University of Macau. He got his PhD degree in Physics from the National University of Singapore in 2006. From 2008 to 2013, he had worked at National University of Singapore as Research Fellow, Oak Ridge National Laboratory (USA) as Postdoctoral Fellow, and Institute of High Performance Computing (Singapore) as Senior Scientist. He joined the University of Macau as an assistant professor in 2013. In his research, a combined computational and experimental method is used to design novel nanomaterials for applications in energy conversion and storage (such as solar cells, water-splitting, Li batteries, supercapacitors, hydrogen storage, and fuel cells), electronic devices, spintronics, and quantum devices. He has published more than **130** papers in international peer-reviewed journals. The total citation is more than **6300**. Additionally, he is the author of 5 book chapters, and the inventor of **4** USA and **3** China patents. His present h-index is **39**.

Two-dimensional MXenes for Biomedical Applications

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Abstract:

The fast progress of nanomedicine provides an alternative but highly efficient strategy for the theranostics of diverse diseases. The nanomaterials with abundant compositions and nanostructures are the bases in theranostic nanomedicine. Different from traditional zero-dimensional spherical nanoparticles, two-dimensional (2D) nanomaterials exhibit the unique physiochemical properties for satisfying the strict requirements of biomedical applications. Especially, we have successfully demonstrated that 2D MXene (Ti_3C_2) nanosheets are featured with high photothermal-conversion property of near infrared (NIR)-triggered photothermal tumor hyperthermia. The 2D Nb_2C MXene nanosheets have been shown to be featured with high photothermal-conversion efficiency at the second NIR biowindow (NIR-II), which also exhibited high tissue-penetrating capability for the therapy of deep-seated tumor. Importantly, 2D Ta_4C_3 MXene nanosheets could be used not only for tumor-photothermal therapy, but also for diagnostic imaging because of the high atomic number of Ta element in CT imaging. Especially, the photothermal performance of these 2D MXene nanosheets could also be used for the intriguing photoacoustic imaging. We also demonstrated that the photothermal performance of 2D MXene nanosheets triggered the generation of radials for the synergistic cancer therapy after the coating of a mesoporous silica layer onto the surface of 2D MXenes and the encapsulation of AIPH initiators. The biocompatibility and biosafety have also been systematically evaluated both in vitro and in vivo.

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Biography：

Prof. Yu Chen received his Ph.D. degree at Shanghai Institute of Ceramics, Chinese Academy of Sciences (SICCAS). He is now the full professor in SICCAS. His research includes the design, synthesis and biomedical applications of mesoporous silica/organosilica, 2D biomaterials (graphene, metal oxides, TMDCs, and MXenes) and 3D-printing bio-implants, including drug delivery, molecular imaging, nanocatalytic medicine, sonodynamic therapy, cardiac therapy, gene therapy and tissue engineering. He has published more than 160 scientific papers in nanomedicine field with a total citation of more than 10000 times (h-index: 53). He has been awarded with the National Science Foundation for Excellent Youth Foundation, National High Level Talents Special Support Plan (Ten Thousand Plan, Young Talents) and Program of Shanghai Subject Chief Scientist. He was also listed in the “Highly Cited Researchers 2018”.

MXene Membranes for Separation

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Abstract:

The abundant research in atomically thin graphene has triggered enormous studying of other two-dimensional (2D) layered materials such as transition metal dichalcogenides, layered double hydroxides, zeolites and metal−organic frameworks (MOFs). Previous studies have demonstrated that these 2D materials exhibited superior advantages in fabricating separation membranes. MXenes, a new class of 2D transition metal carbides and/or nitrides, was discovered recently. MXenes are derived from the MAX phases and with similarity to graphene. Till now, the most studied MXene is $Ti_3C_2T_X$, which was delaminated successfully in 2011. $Ti_3C_2T_X$ MXene is normally produced by selectively etching the Al layer between the Ti_3AlC_2 phases and making the surface of Ti_3C_2 terminated by oxygen, hydroxyl, and/or fluoride groups (T_X). Owing to its flexibility, superior structural stability, high electrical conductivity and hydrophilic surfaces, MXene has been widely used in super capacitors, lithium-ion batteries, oxygen-evolution reaction, and heavy metal adsorption. However, there so far no report on the inorganic MXene-based membranes till now, except the paper by Gogotsi et al. for ion sieving. Herein, we propose two kinds of 2D lamellar membranes with $Ti_3C_2T_X$ MXene nanosheets, and its application in water purification and selective gas separation. For the application in water purification, the modified MXene membrane supported on anodic aluminum oxide (AAO) substrate shows excellent water permeance and favorable rejection rate in nanofiltration process. For the application in selective gas separation, the MXene membrane without any support shows superior selectivity for H_2/CO_2 separation and extremely high H_2 permeability. And both of the selectivity and the permeability are higher than the most studied graphene oxide membranes. More systematic studies are required to evaluate the applicability of MXenes for other related separation applications.

Biography:

Dr. Haihui Wang is a professor at the South China University of Technology, China.

Dr. Wang received Ph.D (2003) from Dalian Institute of Chemical Physics, Chinese Academic Science. He was an Alexander von Humboldt Fellow and research associate (2005-2007) at Leibniz University of Hannover, Germany (2003-2007). In 2007 Dr. Wang joined the School of Chemistry & Chemical Engineering at South China University of Technology as a full professor. He was an ARC (Australia Research Council) Future Fellow Professor at School of Chemical Engineering in The University of Adelaide from March, 2015 to Nov. 2016. He published over 220 refereed papers in chemical engineering and materials science SCI journals; he also holds 36 patents; his papers have received more than 6500 citations (with H-index of 47).

Dr. Wang received several awards, including Excellent Presidential Award, Chinese Academy of Sciences (2003), The Alexander von Humboldt Fellow (2003), New Century Excellent Talents in Universities of China (2007), Award from Fok Ying Tung Education Foundation, Hongkong (2008), Pearl River Scholar for Distinguished Professor (2011). He got Distinguished Young Scientist Foundation, National Nature Science Foundation of China (2012), the highly reputable and supports young scholars who have made outstanding achievements in fundamental research. He was awarded as Cheung Kong Chair Professor (Ministry of Education). He was awarded as Fellow of The Royal Society of Chemistry in 2016.

Dr. Wang's services to the scientific community include serving as a referee for over 20 journals and 5 funding agencies. He was chair of the first Sino-German Symposium on Inorganic Membrane with Nano Design (2010, Guangzhou) and Co-Chair of the Second Sino-German Symposium on Inorganic Membrane for Clean Energy and Clear Environment (2012, Hannover).

Ti_3C_2 MXene Sensor with High Selectivity for NH_3 Detection at Room-temperature

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Abstract:

MXene, a two-dimensional (2D) transition metal carbide/nitride/carbonitride material shows unique physical and chemical properties due to its unique two-dimensional layer structure and surface terminal functional groups (-OH, -O, -F).The conductive properties of MXenes can be changed by the type and amount of surface termination groups, thus theoretically, MXene can be applied as gas sensors. By theoretical calculation, several research groups concluded that MXenes are promising materials for gas sensing. By now, all the theoretical calculations were carried out on M_2C MXenes (M = Ti, V, Nb, Mo, Sc, etc.). No calculations were done on the most common MXene, Ti_3C_2. This is because that M_2C MXenes have simple structure compared with Ti_3C_2 MXene. Recently, there are some reports on the experimental research the gas-sensing of MXenes. However, all the experiments were carried on Ti_3C_2 MXene. This is because that Ti_3C_2 MXene is easy to made and stable compared with other MXenes. In this study, we reported the preparation and properties of Ti_3C_2-MXene sensors for NH_3 detection at room-temperature. Ti_3C_2 MXene was prepared by etching off Al atoms from Ti_3AlC_2. Then the Ti_3C_2 MXene was delaminated and coated on the ceramic tube surface to make sensors with different structure. Thereafter the sensors were used to detect various gases (NH_3, H_2S, NO, CH_4, ethanol, acetone, methanol and deionized water) with the concentration 500 ppm at room temperature. It was found that, for gas detection, the Ti_3C_2 sensors have high selectivity to NH_3 compared with other gases. The sensitivity of the Ti_3C_2 sensor to NH_3 was 6.13%, and the second highest sensitivity was 1.5% to ethanol gas. The humidity tests, stability tests and different concentration cycle tests of NH_3 showed that the Ti_3C_2 MXene gas sensor has good performances for NH_3 detection. In addition, it is more in line with actual needs to use a static gas sensing system without being exposed to clean air to recover the base resistance of the sensor.

Biography:

Aiguo Zhou, PhD, Professor of School of Materials Science and Engineering, Henan Polytechnic University, Jiaozuo, China. He obtained BS degree in Ceramics Engineering from Wuhan University (Wuhan, China) in 1997, MS degree in Materials Science from Tsinghua University (Beijing, China) in 2003, PhD degree in Materials Engineering from Drexel University (Philadelphia, PA, USA) in 2008. He work at Henan Polytechnic University since 1997. Now he is Taihang Scholar of university, leader of Innovative Research Team (in Science and Technology) in the University of Henan Province. He obtained prize for Young Faculty from Fok Ying Tung Education Foundation at 2012. Since his study at Tsinghua and Drexel, he do the research on ternary carbides/nitrides MAX phases. His research is focused on the synthesis and mechanical properties of MAX phases. Since 2011, he started to research MXenes. His research on MXenes is focused on the preparation of novel MXenes from MAX phases and the application of MXenes in the field of gas adsorption/sensoring.

A Wearable Transient Pressure Sensor Made with MXene Nanosheets for Sensitive Broad-Range Human−Machine Interfacing

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Abstract:

Flexible and degradable pressure sensors have received tremendous attention for potential use in transient electronic skins, flexible displays, and intelligent robotics due to their portability, real-time sensing performance, flexibility, and decreased electronic waste and environmental impact. However, it remains a critical challenge to simultaneously achieve a high sensitivity, broad sensing range (up to 30 kPa), fast response, long-term durability, and robust environmental degradability to achieve full-scale biomonitoring and decreased electronic waste. MXenes, which are two-dimensional layered structures with a large specific surface area and high conductivity, are widely employed in electrochemical energy devices. Here, we present a highly sensitive, flexible, and degradable pressure sensor fabricated by sandwiching porous MXene-impregnated tissue paper between a biodegradable polylactic acid (PLA) thin sheet and an interdigitated electrode-coated PLA thin sheet. The flexible pressure sensor exhibits high sensitivity with a low detection limit (10.2 Pa), broad range (up to 30 kPa), fast response (11 ms), low power consumption (10^{-8} W), great reproducibility over 10 000 cycles, and excellent degradability. It can also be used to predict the potential health status of patients and act as an electronic skin (E-skin) for mapping tactile stimuli, suggesting potential in personal healthcare monitoring, clinical diagnosis, and next-generation artificial skins.

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Biography:

Prof. Dr. Pengbo Wan is a Full Professor of Materials Science and Engineering. He is supported by the "Hundred Talent Program (BUCT)" (Supervisor: Prof. Xi Zhang and Prof. Liqun Zhang). He was a Postdoc. Researcher of Harvard University in Prof. David A. Weitz's group. He received his B.S. degree (2006) at Wuhan University and his Ph.D. degree (Supervisor: Prof. Xi Zhang) at Tsinghua University (2011). After working as a Research Fellow at Nanyang Technological University (Singapore) with Prof. Xiaodong Chen, he joined Beijing University of Chemical Technology (BUCT) in 2013. His research interests include transparent conducting films, hydrogels, flexible electronic sensors, wearable electronics, and supramolecular assembly.

Electromagnetic absorption properties of MXene-based materials

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Abstract:

Electromagnetic wave (EM) absorption materials with broader effective absorption bandwidth (EAB), lightweight, and thin thickness are highly desirable in areas of wearable device and portable electronics. There are still many obstacles to simultaneously satisfy the above critical requirements required by new high-performance EM absorption materials. In the present work, MXenes as a new kind of flexible material with high electric conductivity and excellent hydrophilicity, which has been proven to be a promising EM shielding materials, is considered to be the ideal EM absorbing agent. Different approaches have been proposed to develop the MXene based EM absorbing materials. For example, to prepare reduced graphene oxide (RGO)/$Ti_3C_2T_X$ hybrids foam with hollow core–shell architectures and controllable complex permittivity via self-assembly and sacrificial template processes, RGO is grafted flatly on the outer surface of the $Ti_3C_2T_X$ spheres-core, forming a unique heterostructure. The RGO/$Ti_3C_2T_X$ foam possesses excellent EM absorption performance superior to all reported foam-based counterparts, the EAB covers the whole X-band at 3.2 mm while the density is merely 0.0033 g cm^{-3}, and its specific EM absorption performance (*SMAP* = *RL* (dB)/*Thickness* (cm)/*Density* (g cm^{-3})) value exceeds 14299.2 dB cm^{-2} g^{-1}. The key developments and future challenges in this field are summarized.

Biography:

Xiaowei Yin is a Professor of Materials Science at the School of Materials Science and Engineering of Northwestern Polytechnical University (NPU), Xi'an, China. He earned his Ph. D. degrees at NPU in 2001. During 2002 and 2004, he worked as a post-doctor in Faculty of Materials Engineering, Israel Institute of Technology (Technion), supported by Lady Davis fellowship. During 2005-2006, he worked in Department of Materials Science, University of Erlangen-Nurernberg, supported by Alexander von Humboldt fellowship. His publications were cited by SCI for more than 4500 times, H-index: 38. He obtained the support of China National Funds for Distinguished Young Scientists in 2017. He was selected into National High-Level Talent Special Support Plan of China in 2018.

A preliminary study on MXene optoelectronics

Han Zhang

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Abstract:

MXene, as a novel 2D crystal material, possessing excellent optoelectronic properties, such as tunable bandgap, low optical attenuation, broadband nonlinear optical responses, fast carrier dynamics, high electronic conductivity, that may promote the fabrications of advanced electro-photonics devices has gathered remarkable attention recently. Herein, we will briefly summary several preliminary investigations in our group on the optoelectronic properties of MXene and their applications. We have systematically investigated the broadband nonlinear optical responses of MXene, and have demonstrated their use for ultrafast photonics, all-light signal processing, and photo-detecting. Taking advantage of additive manufactures, we have printed MXene patterns on varies substrates, including silica glass, transparent flexible PET, silicon wafer, side-polished fiber, optical mirrors, etc., and have found wide applications of these directly printed optoelectronic devices. On the other sides, we also touched the bio-photonics applications of MXene for biological sensing, photo-thermal medical treatment and more. Hopefully, we wish our preliminary studies on MXene optoelectronics may offer some inspirations for the researchers in the communities of 2D materials and nonlinear optics.

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Biography：

Prof. Han Zhang was born in Wuhan, China, in 1984. He received his BS degree from Wuhan University in 2006 and PhD from Nanyang Technological University in 2010. He is currently a director of the Shenzhen Key Laboratory of 2D Materials and Devices, and the Shenzhen Engineering Laboratory of Phosphorene and Optoelectronics, Shenzhen University. To date, he has published over 203 scientific publications and 38 patents. His current research focus is the ultrafast and nonlinear photonics of two-dimensional materials. His publications have received >18000 citations, with an H-index of 66. He was also selected as the highly cited researcher by Clarivate Analytics at 2018 and has been awarded/enrolled with ‘the Second Prize of Natural Science Award, Ministry of Education (Rank the second) ' and ‘China’s Top 10 Optical Breakthroughs', ‘NSFC Key Project' and ‘NSFC outstanding young scholar fund' etc.

Atomistic Insight into of Photoelectrochemical Reaction Mechanism on MX(B)ene

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Abstract:

Density functional theory investigations of M_3C_2 transition metal carbides from the d2, d3, and d4 series suggest promising N_2 capture behaviour, displaying spontaneous chemisorption energies that are larger than those for the capture of CO_2 and H_2O in d3 and d4 MXenes.[1,2,3] The chemisorbed N_2 becomes activated, promoting its catalytic conversion into NH_3.[4,5] The first proton–electron transfer is found to be the rate-determining step for the whole process, with an activation barrier of only 0.64 eV vs. SHE for V_3C_2. Whilst MXenes from the d2 series (M = Ti, Zr, and Hf) have demonstrated active behaviour for the capture of CO_2, the Cr_3C_2, and Mo_3C_2 MXenes exhibit the most promising results (at DFT computational level plus explicit PBE/DFT-D3 dispersion corrections) for their application in selective CO_2 conversion into CH_4. Cr_3C_2 MXene is especially promising owing to its low expected over-potential. Moreover, spontaneous reaction energies are predicted for the early hydrogenation steps towards the formation of OCHO• and HOCO• radical species. Our results provide novel insights into the computer-aided search for high-performance catalysts and the understanding of reaction mechanisms for CO_2 reduction.

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Biography:

Neng Li obtained his Ph.D. in Physics from the Huazhong University of Science & Technology in 2011. He later accepted a Research Assistant Professor position at Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences in 2011. After that, he held a post-doctoral position at UMKC under the supervision of Prof. Wai-Yim Ching from 2012 to 2014, and then he joined the State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology in 2014 as a full Professor. He is a visiting Professor in **University of Cambridge** from 2016-2017. He was awarded the "Huo Yingdong Education Foundation Higher Education Youth Teacher Fund" in 2018, and was elected "Peacock Talent People" plan, which is the high-level researcher project in Shenzhen City, China. He is interested in the modeling of defective, nanostructured, and low-dimensional materials and their enenrgy enviormental applications using ab initio method. He has authored or coauthored **more than 80 scientific papers** and attended more than 50 international conferences as invited speakers, oral speaker and over poster. **His H-index is 26**. Outside of research and university teaching he is an enthusiastic supporter of efforts to bring science, technology, engineering, mathematics educational and entertainment content into the lives of young students from elementary age to junior undergraduates.

MXene/carbon nanotube composites for high-perfornce lithium-ion capacitors

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Abstract:

Lithium-ion capacitors (LICs) are designed to have a high energy density without significantly sacrificing their high power density. However, the kinetics imbalance between the faradaic anode and the capacitive cathode in LICs leads to a poor rate capability and low cycling life, thus greatly limiting their practical applications. Recently, a novel family of two-dimensional (2D) materials called MXenes has been discovered, which consist of early transition metal carbides and/or carbonitrides. MXenes have a very good application prospect in the field of electrochemical energy storage due to their metallic conductivity, high volumetric capacity, mechanical and thermal stability. Herein, we report the preparation of titanium carbide ($Ti_3C_2T_x$)/carbon nanotube (CNT) flexible selfsupporting composite films by vacuum filtration. The CNTs can effectively prevent $Ti_3C_2T_x$ from stacking and improve the electrochemical performance. The full-cell LIC is assembled using the $Ti_3C_2T_x$/CNT film as the anode and activated carbon as the cathode. The LIC exhibits a high energy density of 67 Wh/kg (based on the total weight of the anode and the cathode), and a good capacity retention of 81.3% after 5000 cycles. These results suggest that $Ti_3C_2T_x$/CNT films are promising as anode materials for lithium ion capacitors.

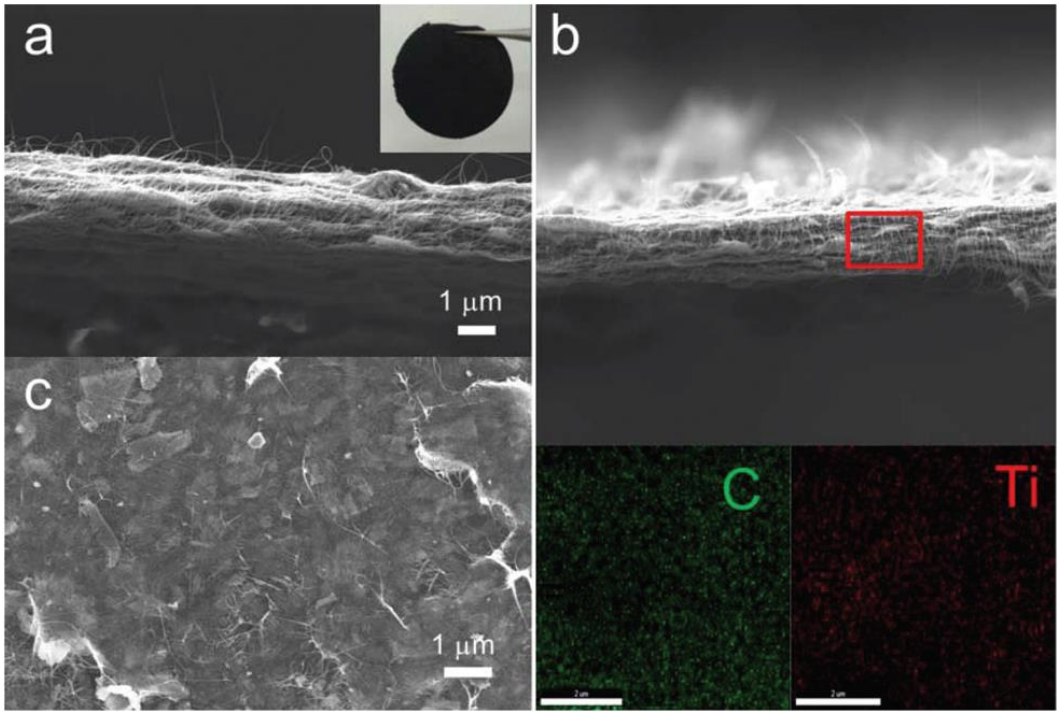

Figure 1 SEM images of the $Ti_3C_2T_x$/CNT composite film: (a) cross-section of the film, (b) EDS maps for C and Ti, and (c) surface of the film. The inset in (a) is a picture of a free-standing $Ti_3C_2T_x$/CNTs film.

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Energy Storage Devices in Textiles by Knitting MXene Yarns

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Abstract:

A growing number of devices have been integrated into textiles for applications including actuation and wireless communication. Many of these devices require power, motivating researchers to develop energy storage devices that can be seamlessly integrated into textiles. In the last five years, several works have been published on fiber and yarn supercapacitors. These devices demonstrate high capacitance and energy density at short lengths (<4 cm) but suffer from high resistance at longer lengths leading to reduced performance. For this reason, knitted electrodes are a promising architecture for textile energy storage devices because yarn electrodes are manipulated into interconnected loops, providing multiple pathways for electron transport. As such, the linear growth of resistance with yarn length can be circumvented by using knitting as a manufacturing platform for textile supercapacitors.

In this work, industrial-scale knitting technology was used to rapidly design and prototype textile supercapacitors. In order to assess the performance of this new device architecture, meters of knittable yarn electrodes were needed. $Ti_3C_2T_x$ MXene is promising material for the development of large-scale yarn electrodes due to its hydrophilicity,[1] high conductivity,[2] and high capacitance in acidic electrolytes.[3,4] Tens of meters of MXene coated-yarns were produced using an automated yarn coating device, demonstrating the ability to scale-up yarn production. The impact on electrochemical performance of knit structure and geometry was investigated in attempt to produce energy storing textiles with power and energy densities that can be used for practical applications. To our knowledge, this is the first work studying the effects of these design parameters on the performance of textile supercapacitors.

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3D porous MXene Film Synthesized by Few Layered MXene and Bacterial Cellulose for Supercapacitor Anode

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Abstract:

The urgent commercialization of various flexible electronic devices, including electronic skins, curved mobile phones, smart clothes and wearable healthcare devices, poses great challenges to new energy storage devices.[1] Supercapacitors are one of the most promising candidate to steadily power these flexible electronics under continuous mechanical deformation.[2,3] To endow supercapacitors high flexibility without compromising electrochemical performance when bended and high energy density for practical application, the key lies in electrode materials. Among them, 2D nanomaterials have the built-in advantages in achieving the highly flexible supercapacitors, because typical layer-by-layer stacked film structure contribute to their mechanical integrity and large specific surface area provides rich electrochemical active sites for receiving high capacitance. However, layered graphene,[4] although excellent conductivity, stores charges based on electrical double-layer mechanism, which delivers low energy density. Most of other 2D pseudocapacitive nanomaterials such as MnO_2 and $Ni(OH)_2$) present high electrode resistance. Recently, a new family of 2D transition metal carbides and nitrides (MXenes) are being paid more attention to. Impressively, titanium carbide ($Ti_3C_2T_x$) not only owns wonderful conductivity and flexibility but exhibits surprising pseudocapacitive properties.[5] Few layered MXene (**Figure 1**) and bacterial cellulose are found to produce highly flexible and robust mechanical properties as well as porous architecture, which is favorable to alleviate the sluggish ion diffusion in pure MXene film, there achieving high specific capacitance for supercapacitor anode.

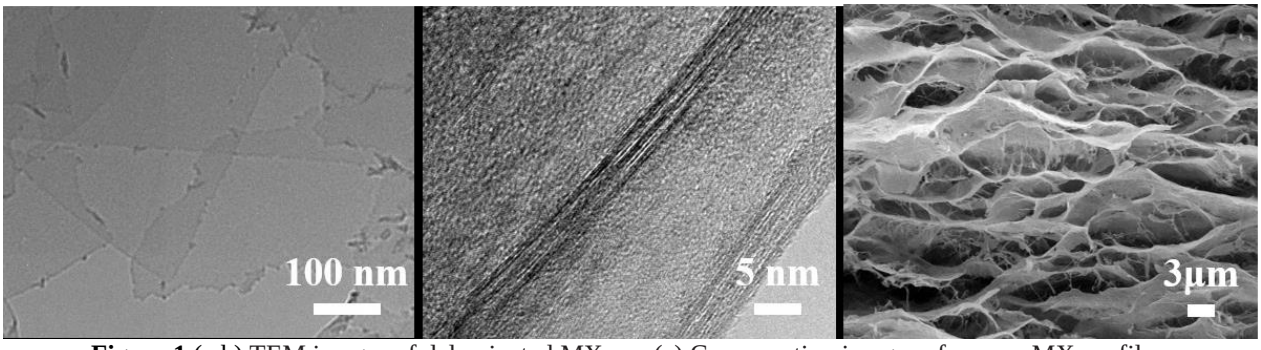

Figure 1 (a,b) TEM images of delaminated MXene. (c) Cross-section images of porous MXene film.

Reference:

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Controlled Crumpling of $Ti_3C_2T_x$ MXene for Stretchable Energy Storage

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Abstract:

Adding stretchability to MXene remains challenging due to its high mechanical stiffness and weak intersheet interaction, so the assembling techniques for mechanically-stable MXene architectures require further development. We report a simple fabrication by harnessing the interfacial instability to generate higher dimensional MXene nanocoatings capable of programmed crumpling/unfolding. A sequential patterning approach enabled the design of sequence-dependent MXene textures across multiple length scales, which were utilized for controllable wetting surfaces and high-areal-capacitance electrodes. We next transferred the crumpled MXene nanocoating onto elastomer to fabricate a MXene/elastomer electrode with high stretchability. The accordion-like MXene can be reversibly folded/unfolded and still preserve efficient specific capacitances. We further fabricated asymmetric MXene supercapacitors, and the devices demonstrated efficient electrochemical performance and large deformability (180° bendability, 100% stretchability). Our texturing techniques can be applied to large MXene families for designing stretchable architectures in wearable electronics.

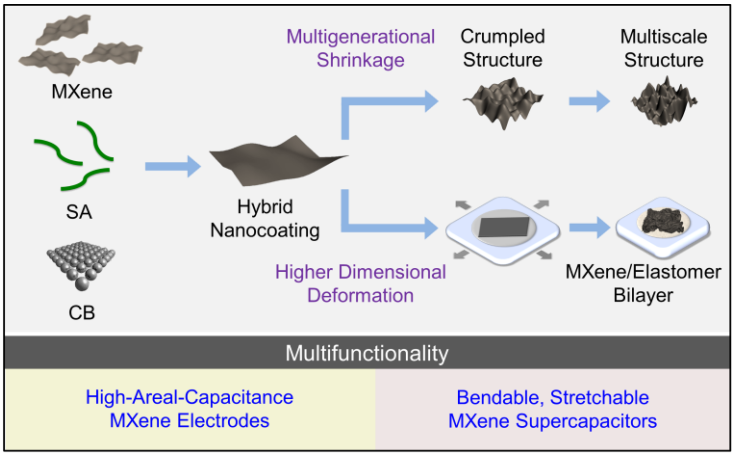

Figure 1 Controlled crumpling of MXene hybrid nanocoatings for the fabrication of high-areal-capacitance electrodes and highly bendable, stretchable supercapacitors. The planar MXene hybrid nanocoatings undergo multigenerational shrinkage processes to fabricate multiscale MXene structures, which can serve as electrochemical electrodes with high CA. The crumpled MXene nanocoating can be further transferred on soft elastomer to achieve the MXene/elastomer electrodes for bendable, stretchable supercapacitors.

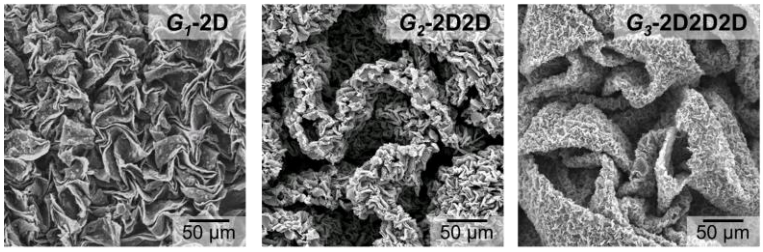

Figure 2 Top-down SEM images of G1-2D, G2-2D2D, and G3-2D2D2D MXene-CB structures. (e) EIS curves of MXene and MXene-CB electrochemical electrodes.

Electrochemical study of pseudocapacitive behavior of $Ti_3C_2T_x$ MXene material in aqueous electrolytes

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Abstract:

The family of 2D transition metal carbides, also known as MXenes, has shown great potential applying to the electrochemical energy storage devices due to its electronic, mechanical and optical properties [1]. $Ti_3C_2T_x$ is the most studied MXene for electrochemical capacitors. For example, the $Ti_3C_2T_x$ MXene electrodes prepared from filtration of delaminated samples have shown high volumetric (1500 F cm^{-3}) and areal (2F cm^{-2}) capacitance, together with high power capability in aqueous electrolytes [2].

Here, we present a multiple potential step chronoamperometry (MUSCA) technique to analyze the electrochemical behavior of pseudocapacitive $Ti_3C_2T_x$ MXene material in aqueous electrolytes. MUSCA allows for reconstruction of cyclic voltammograms with considerably lower ohmic drop contribution. As such, the voltammogram current responses from the surface and bulk processes can be precisely deconvoluted at any given potentials, especially at high scan rates. An electrochemical kinetic analysis of the $Ti_3C_2T_x$ electrode using the calculated voltammograms showed that the surface process dominates at higher scan rate while the bulk process takes over at the low scan rate in both acidic and alkaline electrolytes. By minimizing the ohmic drops, the MUSCA method is presented to be a useful tool to study the natural electrochemical behavior of pseudocapacitive electrodes and to help designing better energy storage systems [3].

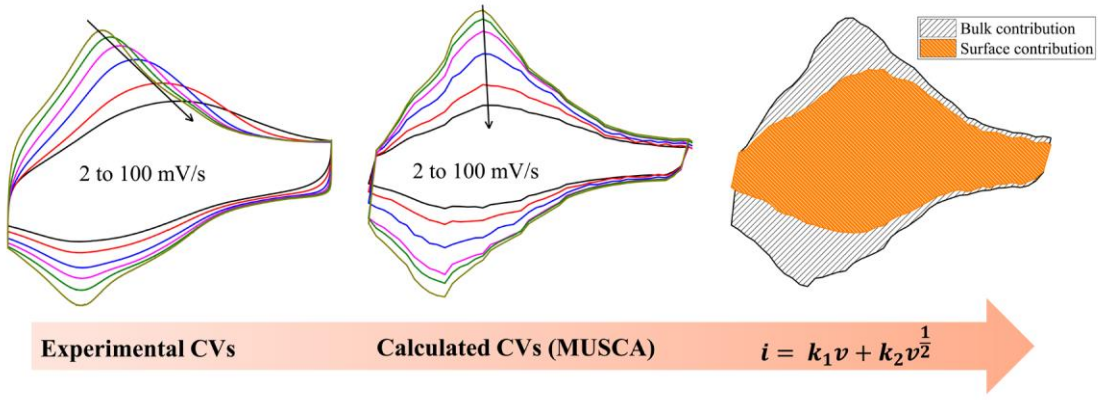

Figure 1 Graphical abstract.

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A General Atomic Surface Modification Strategy for Improving Anchoring and Electrocatalysis Behavior of MXenes in Lithium-Sulfur Batteries

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Abstract:

Multiple negative factors, including poor electronic conductivity of sulfur, dissolution and shuttling of lithium polysulfides (Li_2S_n), and sluggish decomposition kinetics of solid Li_2S, seriously hinder practical applications of lithium-sulfur (Li-S) batteries. To solve these problems, a general strategy was proposed for enhancing the electrochemical performance of Li-S batteries using surface-functionalized Ti_3C_2 MXenes. Functionalized $Ti_3C_2T_2$ (T = N, O, F, S, and Cl) showed metallic conductivity, as bare Ti_3C_2. Among all $Ti_3C_2T_2$ investigated, $Ti_3C_2S_2$, $Ti_3C_2O_2$, and $Ti_3C_2N_2$ offered moderate adsorption strength, which effectively suppressed Li_2S_n dissolution and shuttling. This $Ti_3C_2T_2$ exhibited effective electrocatalytic ability for Li_2S decomposition. The Li_2S decomposition barrier was significantly decreased from 3.390 to ~0.4 eV using $Ti_3C_2S_2$ and $Ti_3C_2O_2$, with fast Li^+ diffusivity. Based on these results, O and S terminated Ti_3C_2 were suggested as promising host materials for S cathodes. Moreover, appropriate functional group vacancies could further promote anchoring and catalytic abilities of $Ti_3C_2T_2$ to boost the electrochemical performance of Li-S batteries.

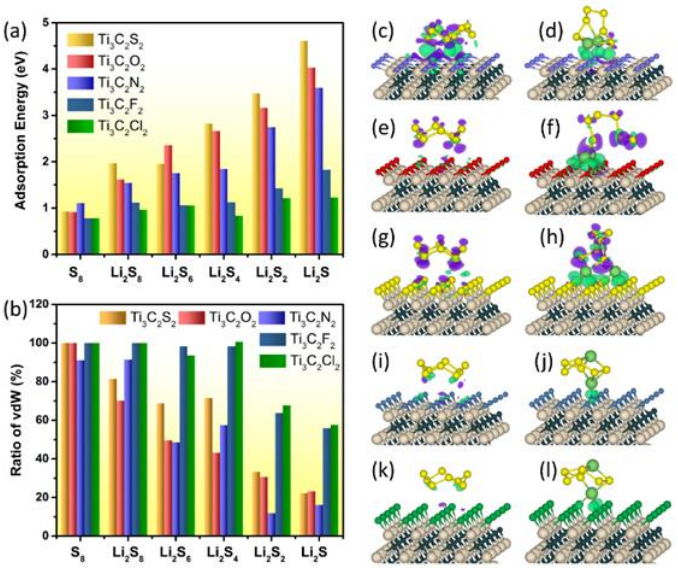

Figure 1 (a) Adsorption energies, (b) ratio of vdW interaction of S_8 and Li_2S_n on $Ti_3C_2T_2$. Charge density difference of (c, e, g, i, k) S_8 and (d, f, h, j, l) Li_2S_6 on $Ti_3C_2T_2$ (T = N, O, S, F, Cl, from top to bottom). The isosurface level is set at 0.0003 and 0.003 e $Å^{-3}$ for S_8 and Li_2S_6 adsorption, respectively.

Table 1 Calculated Li_2S, Li_2S_6 decomposition barriers and Li^+ diffusion barriers on $Ti_3C_2T_2$. (eV)

Substrate	Decomposition barrier		Li^+ diffusion barrier
	Li_2S	Li_2S_6	
$Ti_3C_2O_2$	0.411	0.211	0.236
$Ti_3C_2S_2$	0.351	0.180	0.188
$Ti_3C_2N_2$	1.101	0.434	0.573
$Ti_3C_2F_2$	0.903	1.208	0.187
$Ti_3C_2Cl_2$	1.625	1.532	0.196

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Rational Design of Free-Standing 3D Porous MXene/RGO Hybrid Aerogels as Polysulfides Reservoir for High-Energy Lithium-Sulfur Batteries

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Abstract:

Lithium-sulfur (Li-S) batteries with a high theoretical energy density are attracting increasing attention as promising candidates for next-generation energy storage systems. However, the insulating nature and undesirable shuttle effect of sulfur species dramatically impede their practical applications. Herein, a unique 3D porous $Ti_3C_2T_x$ MXene/rGO (MX/G) hybrid aerogel is rationally designed and applied for the first time as a free-standing polysulfides reservoir to improve the overall performance of Li-S batteries.[1] In this strategy, highly conductive MXene and rGO are integrated into a 3D interconnected porous aerogel structure with efficient 2D polar adsorption interfaces (**Fig 1**), enabling fast Li^+/electron transport and strong chemical anchoring ability for lithium polysulfides as well as enhanced redox reaction kinetics. The robust MX/G aerogel electrodes deliver excellent electrochemical performances including a high capacity of 1270 mAh g^{-1} at 0.1 C, an extended cycling life up to 500 cycles with a low capacity decay rate of 0.07% per cycle, and a high areal capacity of 5.27 mAh cm^{-2} (**Fig 2**).

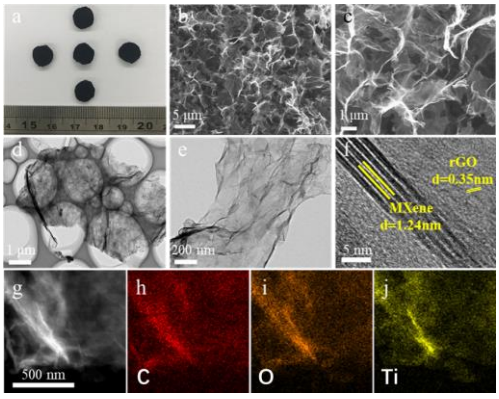

Fig 1 a) Photograph of free-standing MX/G-30 electrodes. b,c) Low-magnification and high-magnification SEM images of MX/G-30 aerogel. d,e) TEM and HRTEM images of MX/G-30 aerogel. g-j) STEM image and EDS spectrum mapping: C, O and Ti elemental distribution of MX/G-30 aerogel.

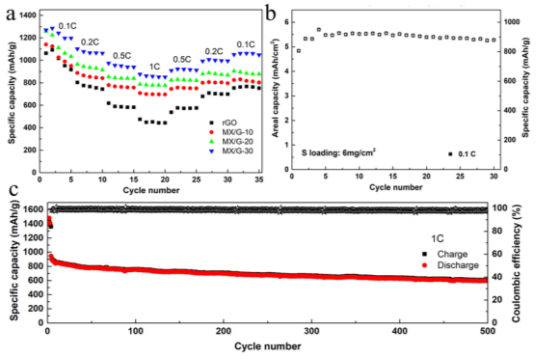

Fig 2 a) Rate performance of Li-S cells with rGO, MX/G-10, MX/G-20, and MX/G-30 electrodes, respectively. b) Cycling stability of the MX/G-30 electrode at 0.1 C rate for 30 cycles with a high sulfur loading of 6 mg cm^{-2}. c) Long-term cycling performance of Li-S cell with MX/G-30 electrode at 1 C for 500 cycles.

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High Performance Biscrolled MXene/Carbon Nanotube Yarn Supercapacitors

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Abstract:

Yarn-shaped supercapacitors (YSCs) once integrated into fabrics provide promising energy storage solutions to the increasing demand of wearable and portable electronics. In such device format, however, it is a challenge to achieve outstanding electrochemical performance without compromising flexibility. Here, MXene-based YSCs that exhibit both flexibility and superior energy storage performance by employing a biscrolling approach to create flexible yarns from highly delaminated and pseudocapacitive MXene sheets that are trapped within helical yarn corridors are reported. With specific capacitance and energy and power densities values exceeding those reported for any YSCs, this work illustrates that biscrolled MXene yarns can potentially provide the conformal energy solution for powering electronics beyond just the form factor of flexible YSCs.

The employed biscrolling technique enabled the spinning of BMX yarns containing predominantly MXene nanosheets (up to ≈98 wt%) that are trapped within CNT yarn scrolls. Importantly, this BMX yarn provided a specific capacitance as high as 1083 F cm^{-3} (3188 mF cm^{-2}), which exceeds the previously recorded performance for any yarn supercapacitor electrode.

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Design and Fabrication of high-performance binder-free flexible supercapacitor electrodes from MXene and Cellulose Nanofibers with outstanding foldable and mechanical properties

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Abstract:

MXene-based materials are promising in supercapacitors owing to their metallic conductivty and excellent electrochemical activity,[1-3] while their poor mechanical strength, flexibility and stability against deformation limit their applications in flexible and foldable electonics. In order to overcome these shortcomings, a simple and scalable strategy is developed to fabricate strong and foldable $Ti_3C_2T_x$/cellulose nanofibers (CNF) composite paper with superior electrochemical performance. $Ti_3C_2T_x$ nanoflakes are interacted with cellulose nanofibers via physical entanglement and hydrogen-bonding induced self-assembly to form an interwoven spiderweb-like structure, leading to significantly enhanced tensile strength (up to 157.3 MPa) and electrical conductivity (up to 15504 S m^{-1}). The freestanding $Ti_3C_2T_x$/CNF electrode presents an outstanding areal capacitance (1050 mF cm^{-2}) and energy density (119.9 Wh kg^{-1}), which exceeds the performance of most reported flexible supercapacitor electrodes, and retains more than 95% capacitance after 6000 cycles. Furthermore, $Ti_3C_2T_x$/CNF composite paper is highly flexible and compliant, which can be folded into complex shapes and exhibit negligible loss of conductivity and capacitance after repeated folding/defolding process. The schematic illustration of $Ti_3C_2T_x$/CNF composite paper is shown in Figure 1. These results demonstrate that $Ti_3C_2T_x$/CNF composite paper is promising for the applications of flexible, portable and wearable electronic devices.

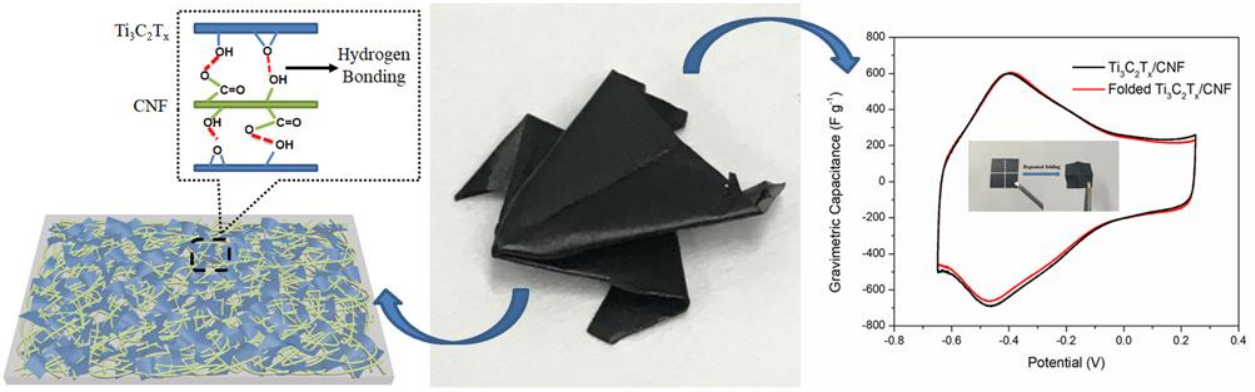

Figure 1 Schematic illustration of $Ti_3C_2T_x$/CNF composite paper.

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Preparation and Properties of MXene/Chitin Composite Paper

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Abstract:

The development of portable and wearable electronic devices puts forward higher requirements for electrode materials with high flexibility, high volumetric capacity and low cost. Recently, MXene proved to be a promising candidate material as an electrode for supercapacitor due to its superior conductivity, high density and high electrochemical activity, exhibiting higher volumetric capacity compared to most reported electrode materials.[1, 2] Herein, we report on the preparation of high flexible MXene/chitin composite paper through a facile electrostatic self-assembly between negatively charged titanium carbide MXene nanosheets and positively charged chitin nanofibers. Benefiting from the strong interaction between the chitin nanofibers and MXene nanosheets, this composite shows very good flexibility without any defects even after a few hundred foldings. It can be observed from Figure 1 that the surface of MXene/chitin is smoother than that of pure MXene film, indicating a better flexibility can be achieved by hybridizing MXene with chitin. In addition, adding chitin efficiently prevented restacking of MXene nanosheets, resulting in an enhanced electrochemical performance due to accelerated diffusion of electrolyte ions compared to pure MXene film. When using as electrode for supercapacitor, the free-standing MXene/chitin-10 wt.% composite paper displays a volumetric capacity of more than 1000 F cm^{-3} as well as good rate ability and long cycle life. Specially, the capacity of MXene/chitin-10 wt.% composite paper is as high as 324 F g^{-1} at a scan rate of 2 mV s^{-1}, increased by 15.7% compared to pure MXene film. This work may provide a new insight into the construction of flexible earth-abundant MXene and chitin-based electrodes for portable and wearable supercapacitor with high performance and low cost.

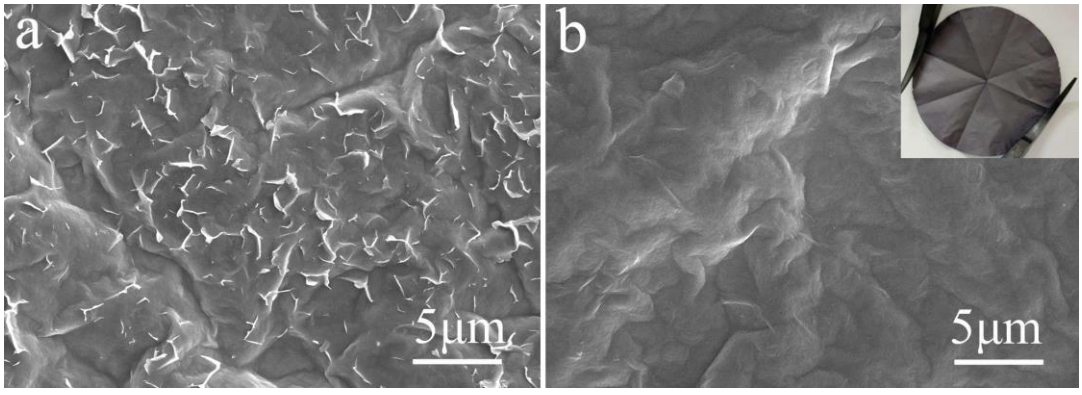

Figure 1 SEM images of (a) Ti_3C_2 film and (b) Ti_3C_2/Chitin film. The inset in (b) is a piece of folded Ti_3C_2/Chitin film.

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MXene based composite materials as the electrolytes for fuel cell

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Abstract:

This report demonstrated a new 2D nanomaterial (MXene[1-3]) as filler in the electrolyte membrane for intermediate temperature (>100℃) polymer exchange membrane fuel cells[4] and alkaline anion exchange membrane electrolyte membrane fuel cells. In the study, $Ti_3C_2T_x$ etched by LiF/HCl[5] was incorporated with polybenzimidazole(PBI) matrix. The composite membrane with 3wt% $Ti_3C_2T_x$ exhibited the proton conductivity above 2 times higher than that of pristine PBI membrane at the temperature range of 100℃-170℃, and led to substantial increase in maximum power density of fuel cells by ~30% tested at 150℃. The addition of $Ti_3C_2T_x$ improved the mechanical properties and thermal stability of PBI membranes. $Ti_3C_2T_x$ functionalized with quaternary ammonium groups were successfully achieved. Incorporation of $Ti_3C_2T_x$ etched with NH_4HF_2[6] and LiF/HCl into quaterized polysulfone based membranes. The quaterized polysulfone/NH_4HF_2-$Ti_3C_2T_x$ composite membrane exhibitd the hydroxide ionic conductivity nearly 2 times higher than that both of pristine quaterized polysulfone and quaterized polysulfone/LiF-$Ti_3C_2T_x$ membranes at the temperature range of 20-60 ºC, and also ~30% increase in peak power density at 60 ºC, indicating The NH_4^+ groups on the MXene surface further enhances the OH^- conductivity. These studies point out promising application of MXene in electrolyte membranes for fuel cells.

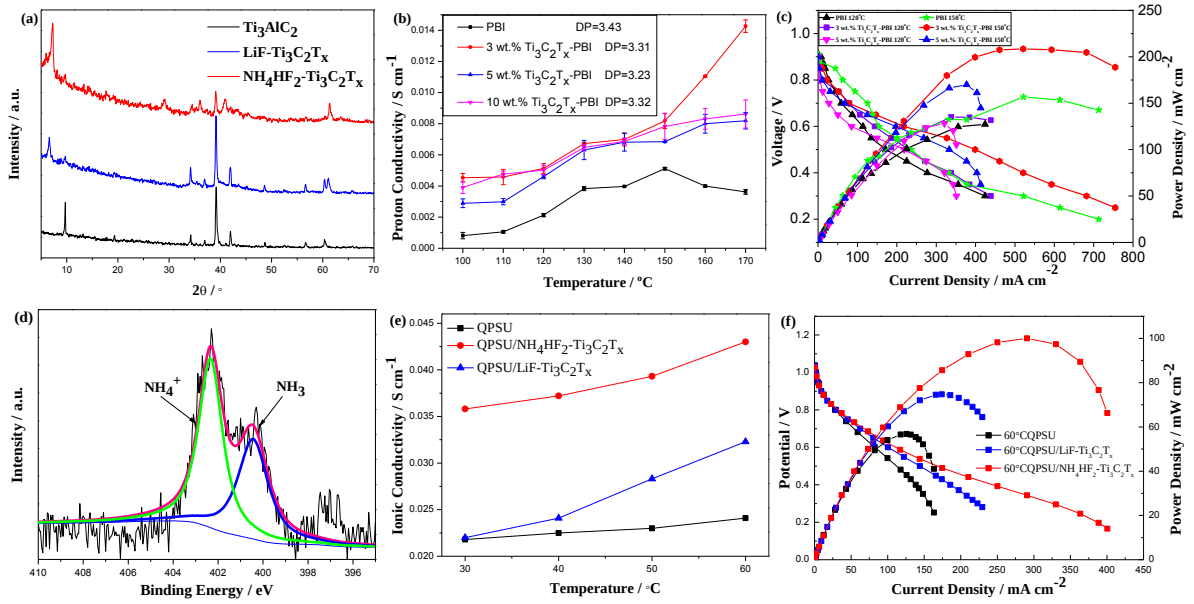

Figure 1 (a) XRD patterns of MAX and MXene; (b) The conductivities of PA doped PBI and PA doped $Ti_3C_2T_x$-PBI membranes; (c) Polarisation and power density curves of fuel cells operated at 120℃ and 150℃; (d) XPS spectra for N 1s region for NH_4HF_2-$Ti_3C_2T_x$; (e) Hydroxide ion conductivity of QPSU, QPSU/LiF-$Ti_3C_2T_x$ and QPSU/NH_4HF_2-$Ti_3C_2T_x$ membranes; (f) Polarization and power density curves of a fuel cell at 30℃ and 60℃.

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MXene-based flexible Li^+-capacitors and micro-supercapacitors

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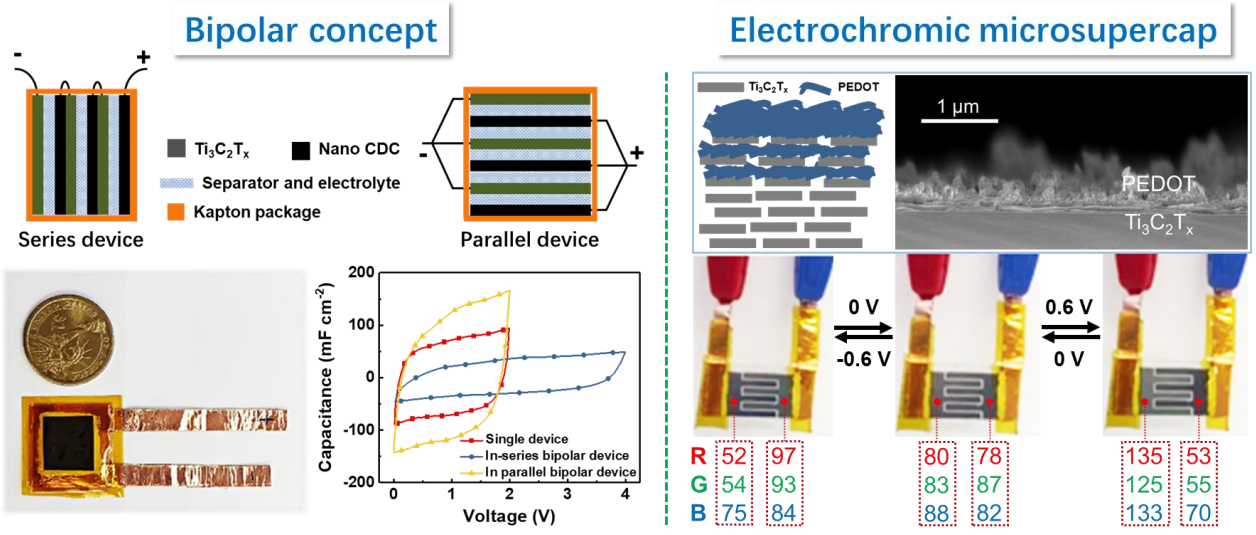
Abstract:

MXenes - two-dimensional (2D) transition metal carbides and nitrides - are an emerging class of high-rate pseudocapacitive materials that offer a combination of solution processability, fast surface redox reactions and metallic conductivity. These properties have been exploited to develop various kinds of supercapacitors. In addition, the ability of MXenes to spontaneously intercalate cations, broadens the scope for developing metal-ion capacitors beyond the protic electrolytes. To date, the stable voltage window of MXene-based supercapacitors was limited at 1.5 V in acidic aqueous electrolytes, even for asymmetric devices. We developed a $Ti_3C_2T_x$//CDC asymmetric supercapacitor with a voltage window of 2 V, by using neutral electrolyte. What is more, to maximize the electronic conductivity, we developed titanium carbide-poly(3,4-ethylenedioxythiophene) heterostructures by electrochemical deposition using a non-aqueous monomeric electrolytic bath. The electrochromic microsupercapacitor was carved using an automated scalpel technique. Hybrid microsupercapacitors showed 5-fold areal capacitance and higher rate capabilities (2.4 mF/cm^2 at 10 mV/s, retaining 1.4 mF/cm^2 at 1000 mV/s) over the pristine MXene microsupercapacitors (455 µF/cm^2 at 10 mV/s and 120 µF/cm^2 at 1000 mV/s). These studies opened new avenues for developing high-performance multifunctional energy storage devices based on MXene heterostructures.



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Novel two-dimensional Molybdenum Carbides as high capacity anodes for Lithium/Sodium-ion batteries

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Abstract:

Searching for high performance electrode materials is one of the key factors for next generation renewable energy technologies. Here, based on the structure of two dimensional (2D) transition metal carbides (MXenes) Mo_2C, we report novel 2D Mo_xC_y (x, y = 1 or 2) phases with great potentials as anode materials for both Lithium-ion batteries(LIBs) and Sodium-ion batteries(SIBs) through first principles swarm structural search. The predicted 2D MoC and MoC_2 monolayers exhibit great stabilities, metallic conductivities, and excellent electrode performances. Interestingly, the structure of MoC_2 monolayer is composed of C2 dimers without metal atoms directly exposing on the surface, suggesting that the surface functionalization occurred in MXenes can be effectively avoided, which is beneficial for maintaining good stability of the anode materials. Furthermore, MoC_2 monolayer exhibits superior LIBs and SIBs performances with high theoretical storage capacities (893.5 and 446.9 mA h/g) and small diffusion energy barriers (0.15 and 0.23 eV) for Li and Na atoms, respectively. These intriguing results demonstrate the robust applicability of the predicted monolayers as ideal anode materials for both LIBs and SIBs.

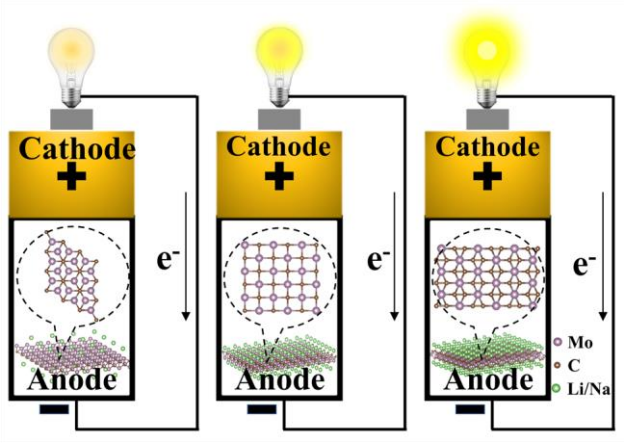

Figure 1 The structures of the Mo_2C, MoC, and MoC_2 monolayers and their potential applications as anodes for metal-ion batteries.

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Probing the Domain Architecture in 2D α-Mo_2C via Polarized Raman Spectroscopy

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Abstract:

MXenes are a group of two-dimensional (2D) materials with excellent stability and intriguing properties. Here, we conduct a systematic study on the Raman spectra of α-Mo_2C and use it to study the unique domain structure of 2D α-Mo_2C crystals grown by chemical vapor deposition (CVD). Six experimentally observed Raman modes are assigned with the assistance of phonon dispersion calculated from density functional theory (DFT). Angle-resolved polarized Raman spectroscopy indicates the anisotropy of α-Mo_2C in the b-c plane, which is further applied to study the domains of the CVD grown 2D α-Mo_2C crystals with different morphologies. Most of the α-Mo_2C flakes contain multiple domains and the c-axes of neighboring domains within the same flake tend to form a 60° or 120° angle, indicating the carbon chains in α-Mo_2C align along three equivalent directions. This is attributed to weak Mo-C bonds in this interstitial carbide and the low formation energy of the carbon chains along certain directions. Our study demonstrates that polarized Raman spectroscopy is a powerful and effective way to characterize the domain structures in α-Mo_2C, which will facilitate the further exploration of properties and applications of α-Mo_2C, as well as other MXenes.

Reference：

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Two-Dimensional Transition Metal Nitrides

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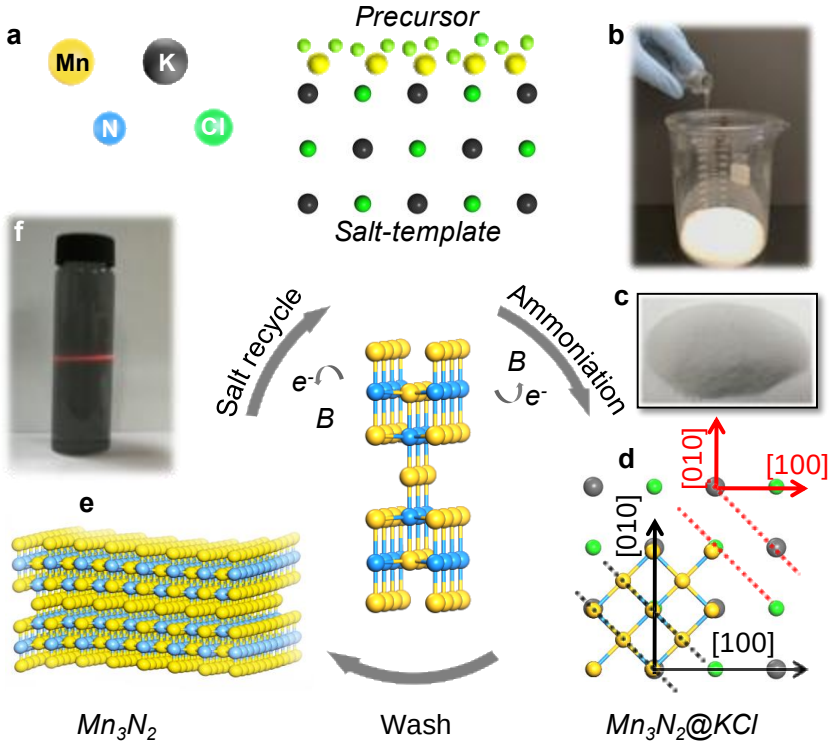
Abstract:

Two-dimensional (2D) transition metal nitrides are in high demand due to their promising physical and electrochemical properties. While more than 20 2D transition metal carbides, such as $Ti_3C_2T_x$ and other carbide MXenes have been obtained, 2D metal nitrides are limited to only a handful of synthesized materials so far. In terms of their superior conductivity and stability, the field of 2D metal nitrides is of growing significance. The bottleneck is a lack of known synthesis routes. For example, there are few bulk layered transition metal ternary nitrides known and so far only 2D Ti_4N_3 and Ti_2N (nitride MXene) have been successfully exfoliated from nitride MAX phases. Hence we recently developed a salt-templating method, which has already produced 2D MoN, V_2N, W_2N, W_2N_3 and Mn_3N_2. In this procedure, a metal-containing precursor is mixed with a salt and then treated at high temperatures under ammonia flow. A 2D metal nitride is obtained due to the lattice match between the surface of the salt and the target product. X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS) and X-ray pair distribution function (PDF) analysis confirmed the various nitrides structures. Importantly, we have proved the antiferromagnetic properties of 2D Mn_3N_2 theoretically and experimentally, which should be the first experimentally demonstrated 2D magnetic metal nitrides. We will also discuss on the energy storage properties of 2D metal nitrides and other potential applications.



The electrical properties and performance of a few MXenes that promise their application for electronic nanodevices

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Abstract:

In this work, we have examined the potential of layered transitional metal carbide (MXene) materials as satisfactory candidate for electronics by performing theoretical predictions on the physical properties as well as electron transport characteristics. According to our data, the scandium MXenes with all termination groups are determined to be semiconducting. Employing theoretical investigations, the Sc_2CF_2 and $Sc_2C(OH)_2$ MXenes both show excellent electron mobilities and thermal conductivities. However, the Sc MXene $Sc_3C_2F_2$ appear metallic which might be difficult for application in electronic devices. From our work, by alloying with Nitrogen, the band gaps of $Sc_3C_2F_2$ MXene can be well modulated and conversion from metallic MXenes to semiconductor can be achieved. The performance of $Sc_3(CN)F_2$ MXenes is thus examined. Furthermore, the chemical conversion of the OH group to Oxygen group in Sc MXenes is investigated as well, in which the mechanism is elucidated. With the properties of MXene well established, the calculation on the electron transport and optical properties of the semiconducting MXene nanoribbons is carried out and their I-V characteristics are evaluated. We demonstrate that the performance in patterned MXene nanoribbons such as Ti_2CO_2 can be tuned by appropriate designs. From the current work, the application of MXenes for the next generation nanoelectronics might be accelerated.

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Evidence for Presence of Multiferroic Order in Pure and Doped MXene

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Abstract:

New family of two-dimensional materials called MXene, with general formula Ti_3C_2Tx, is successfully fabricated after etching from its bulk powder namely MAX. We have reported theoretical and experimental results on structural, optical and multiferroic properties of undoped and doped-MXene. The lattice parameters are changed after the doping, indicating adsorption-dominant properties. The magnetization vs. temperature curves, ferromagnetic hysteresis loops and existence of exchange-bias indicate the presence of ferromagnetic/antiferromagnetic phases together, making it a multiferroic material at low and room-temperatures. The results presented here are novel and is a first report on multiferroic properties of undoped Ti_3C_2 MXene and doped-MXene showing it to be a potential candidate for future magnetic data storage applications.

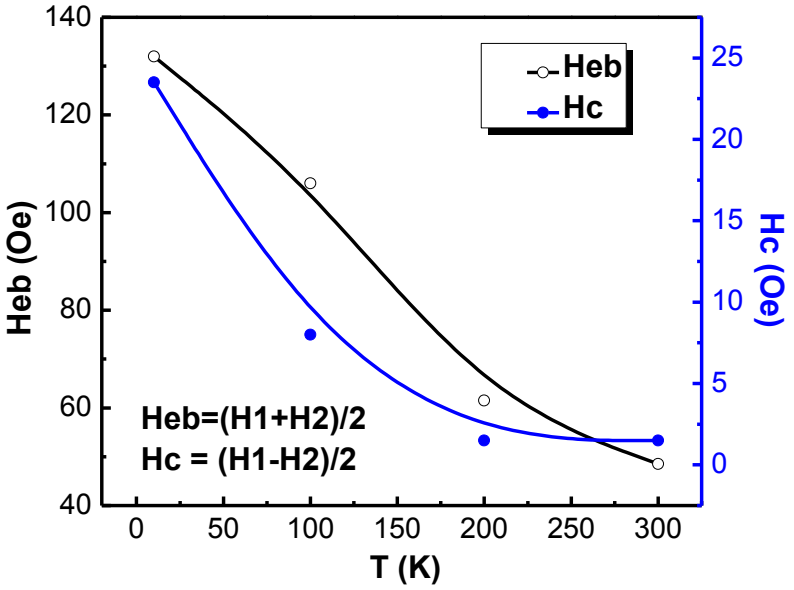

Figure 1 The trend of magnetic exchange-bias and coercivity as a function of temperature for pure and doped MXene.

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Fabrication of hierarchical MXene-based nanocomposites by various self-assembled strategies with catalytic and environmental performances

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Abstract:

MXene, a new type of two-dimensional layered transition metal carbide material differing from graphene, demonstrates intriguing chemical/physical properties and wide applications in recent years. In our recent work, some MXene-based self-assembled systems, including MXene-gold nanoparticles (MXene@AuNPs) nanocomposites by self-reduction reaction, core-shell MXene-COOH@$(PEI/PAA)_n$ structures via layer-by-layer (LbL) strategy, polymer/Fe_3O_4/MXene@Ag nanoparticle composite film fabricated by electrospinning, sulfanilic acid-modified MXene (MXene-SO3H)/dye composite films via Langmuir-Blodgett (LB) technology, and MXene-Co_3O_4 nanocomposites by simple solvothermal method, have been designed and prepared. The relative applications, such as catalytic reactions of nitro-compounds, adsorption capacities of typical dyes, and surface-enhanced Raman scattering (SERS) spectra, have been investigated in details, showing potential applications in composite catalysts and environmental fields.

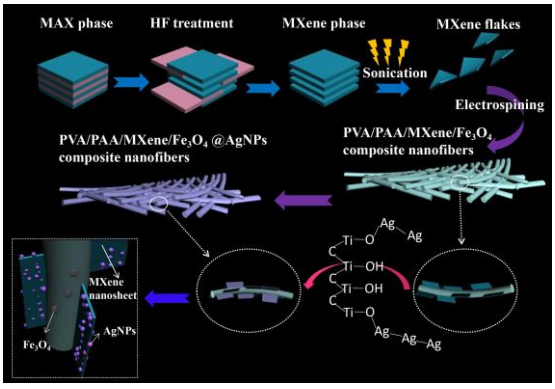

Figure 1 Schematic illustration of the preparation process of polymer/Fe_3O_4/MXene@Ag nanoparticle composite film fabricated by electrospinning. (ACS Omega 2019, 4: 1897-1906.)

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MXene (Ti_3C_2) Vacancy Confined Single-Atom Catalyst for Efficient Functionalization of CO_2

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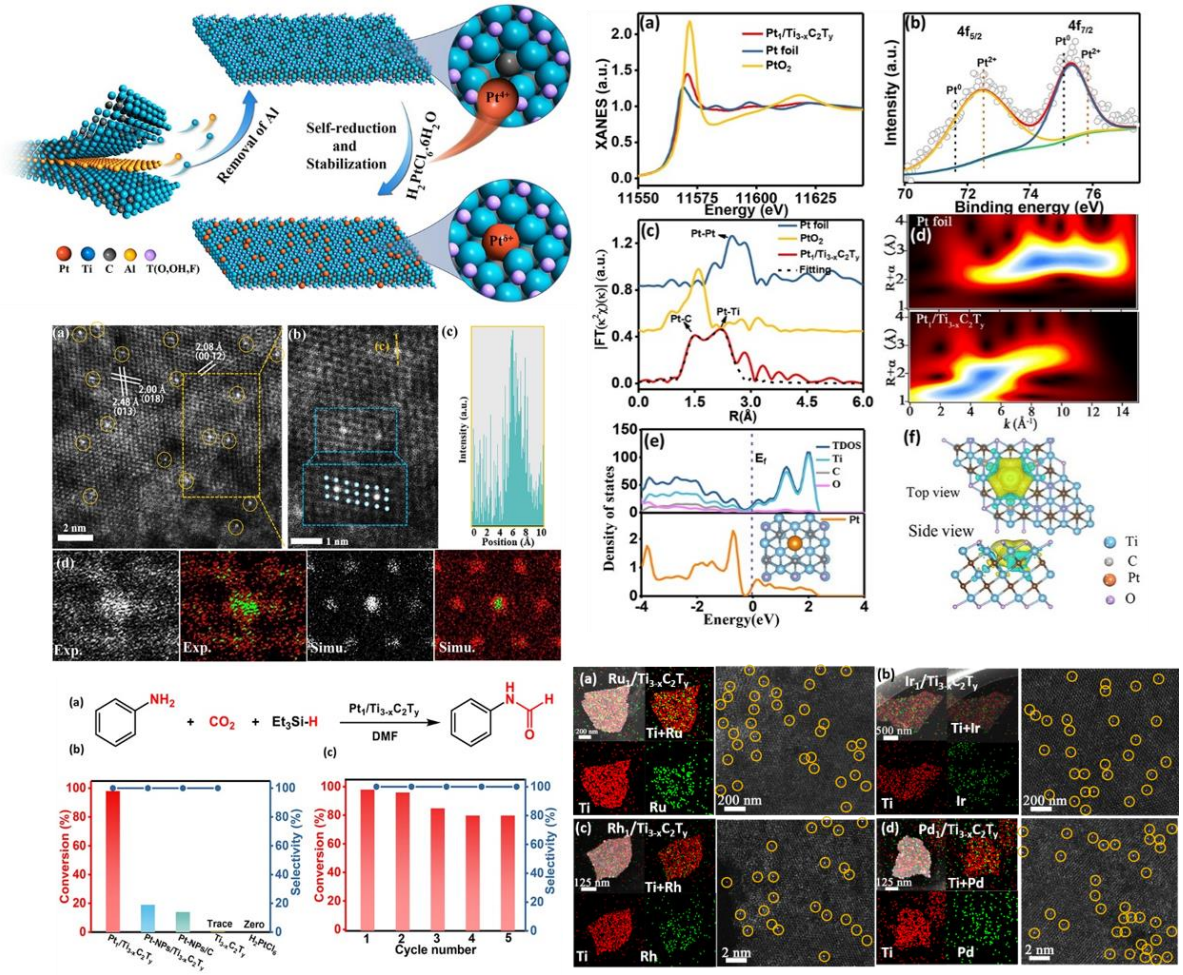
Abstract:

A central topic in single atom catalysis is to build strong interactions between single atoms and the support for stabilization. Herein we report the preparation of stabilized single atom catalysts via a simultaneous self-reduction-stabilization process under room temperature using ultrathin two-dimensional $Ti_{3-x}C_2T_y$ MXene nanosheets characterized by abundant Ti-deficit vacancy defects and high reducing capability. The single atoms therein form strong metal-carbon bonds with the $Ti_{3-x}C_2T_y$ support, and are therefore stabilized onto the sites previously occupied by Ti. The Pt-based single atom catalyst (SAC) $Pt_1/Ti_{3-x}C_2T_y$ offers a green route to utilize the greenhouse gas CO_2, via formylation of amines, as a C_1 source in organic synthesis. DFT calculations reveal that, compared to Pt nanoparticles, the single Pt atoms on $Ti_{3-x}C_2T_y$ support feature partial positive charges and atomic dispersion, which helps to significantly decrease the adsorption energy and activation energy of silane, CO_2 and aniline, thereby boosting catalytic performance. We believe that these results would open up new opportunities for the fabrication of SACs and the applications of MXenes in organic synthesis.



$Ti_3C_2T_x$ MXene film as a conductive and biocompatible material for neural stem cells

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Abstract:

Preclinical studies involving stem cells require efficient biological and physiochemical cues to regulate the development, self-renewal, and differentiation of such cells. Because of their unique planar structure, excellent conductivity, and flexible surface functionalization, MXenes show potential for modulating stem cell fate. Here, we synthesized $Ti_3C_2T_x$ MXene films with a sheet size of several hundred nanometers, and these MXene films were mounted on TCPS enriched with surface functional groups. To study the biocompatibility of this film for neural stem cells (NSCs), primary mouse NSCs were dissociated and cultured on laminin-coated $Ti_3C_2T_x$ MXene film and a cytotoxicity assay was performed. The NSCs grew well, had excellent adhesion, and retained their functional activity, and they showed extensive spreading of the structure of lamellipodia and filopodia on $Ti_3C_2T_x$ MXene film. An EdU assay and other experiments showed that the $Ti_3C_2T_x$ MXene film maintained the stemness and proliferative ability of the NSCs. With respect to their functional activity, NSCs cultured on $Ti_3C_2T_x$ MXene film were more active and synchronous than those cultured on a normal TCPS substrate, which was demonstrated by calcium imaging (Fig.2). Furthermore, $Ti_3C_2T_x$ MXene film significantly enhanced the efficiency of NSCs differentiation towards neurons, and neurons derived from NSCs cultured on $Ti_3C_2T_x$ MXene film had longer neurites and greater numbers of branch points and branch tips, leading to more complicated dendritic morphology. Moreover, the $Ti_3C_2T_x$ MXene film did not affect the maturation of NSC-derived neurons, which was evaluated by immunostaining for presynaptic protein synapsin-1 and postsynaptic protein PSD95. Finally, electrical stimulation was applied to NSCs via the $Ti_3C_2T_x$ MXene film, and this significantly enhanced the proliferative ability of NSCs. Collectively, our results show that $Ti_3C_2T_x$ MXene is an efficient kind of neural surface biomaterial for modulating various stem cell behaviors, and this expands the potential uses of the MXene family of materials and provides new strategies for stem cell studies.

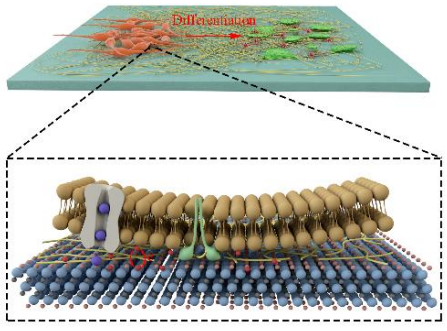

Figure 1 The schematic diagram of NSCs culture and differentiation on $Ti_3C_2T_x$ MXene film.

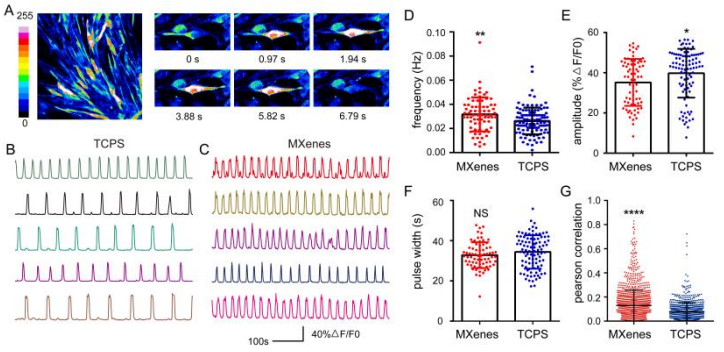

Figure 2 Spontaneous Ca^{2+} transients in NSCs cultured on TCPS and $Ti_3C_2T_x$ MXene film.

Highly Flexible and Sensitive Temperature Sensor based on $Ti_3C_2T_x$ (MXene) for Electronic Skin

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Abstract:

Electronic skin (e-skin) has been attracting great research interest and effort due to its potential applications in wearable health monitoring, smart prosthetics, humanoid robots and so on. Temperature is an important parameter for e-skin to perceive surroundings and people [1-2]. However, less research is executed in the field of temperature sensing and current temperature sensors still face many challenges in practical applications, such as high sensing performance, facile preparation, and differentiating from other stimuli. Herein, we propose a facile fabricating strategy for a $Ti_3C_2T_x$ based temperature sensor. As the sensing units, $Ti_3C_2T_x$ nanoparticles and $Ti_3C_2T_x$ lamellas could be obtained simultaneously through controlling the process conditions. The temperature sensors exhibit tunable sensing performance and a desirable incorporation of high sensitivity (up to 986 $^oC^{-1}$) and a wide working range (140 ^oC). Due to the high sensitivity, the sensor can also be used as e-skin for proximity detection and illumination detection from ultraviolet to infrared light. For application demonstrations, a 4×4 array of the sensors was fabricated for the temperature mapping, indicating great potentials in the applications for monitoring of object approaching and temperature variation.

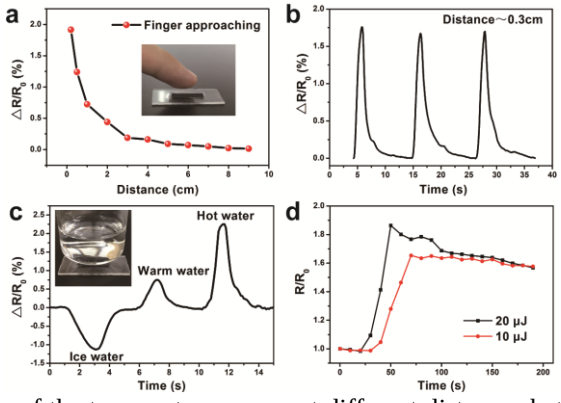

Figure 1 (a) Resistance variation of the temperature sensor at different distances between the finger and the $Ti_3C_2T_x$ film; the inset shows the scene of a finger approaching the sensor. (b) The repeatability of the proximity temperature sensor for 0.3 cm with three circles. (c) Resistance variation of the temperature sensor under the approaching of vials containing ice, warm and hot water; the inset shows the scene of a vial approaching the sensor. (d) Resistance variation of the temperature sensor under infrared laser with different power.

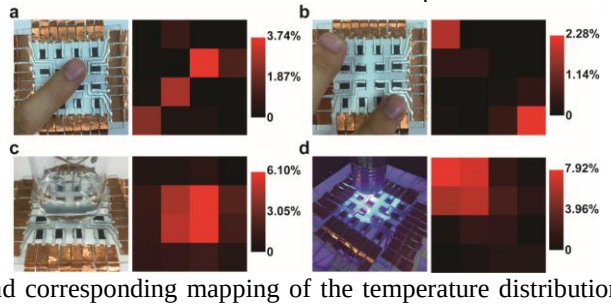

Figure 2 The photographs and corresponding mapping of the temperature distribution via the measurement of the resistance variation by approaching the pixels with a finger (a), two fingers (b), a vial containing warm water (c), and an ultraviolet lamp (d).

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Electrochemical performance of $Ti_3C_2T_x$ (MXene) and its nanocomposite in aqueous media: Towards enhanced sensing applications

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Abstract:

Recently, MXene, 2D metal carbides, have been used in different environmental and biological sensing applications such as detection of glucose, hydrogen peroxide, bromate, phenol and heavy metal ions. Pristine MXenes have demonstrated a strong potential in these applications, thanks to their ordered structure, high surface area, metallic and electronic conductivity, etc. Among other research groups, we have developed an ultrasensitive and selective electrochemical sensor based on nafion-$Ti_3C_2T_x$ for the detection of bromate in drinking water with a detection limit of 41 nM. However, it was demonstrated that the pristine $Ti_3C_2T_x$ itself is not stable at the anodic potential window which limit its applications in the anodic potential window. In this talk we will highlight our recent efforts to prepare highly stable MXene composted electrodes with the hope to promote MXenes in the electrochemical sensing applications. A nanocomposite of platinum or palladium nanoparticles (PtNPs or PdNPs) and $Ti_3C_2T_x$ have been made to overcome the instability of $Ti_3C_2T_x$ and evaluated its sensing performance. The nanocomposite was prepared by self-reduction of platinum (IV) or palladium (II) on the surface of delaminated $Ti_3C_2T_x$ nanosheets to form Pt or Pd@$Ti_3C_2T_x$ in which MXene acted simultaneously as a conductive matrix and a reducing agent. The sensor is constructed from Pt or Pd@$Ti_3C_2T_x$ film casted on glassy carbon electrode and the deposition of PtNPs or PdNPs onto $Ti_3C_2T_x$ nanosheets has improved the stability as well as the electrocatalytic activity. It was found that Pt@$Ti_3C_2T_x$ nanocomposite provided very good response towards the electrochemical determination of bisphenol A (an environmental pollutant) with a detection limit of 32 nM and Pd@$Ti_3C_2T_x$ nanocomposite is capable of giving good response towards the electrochemical determination of L-Cysteine (a biomolecule) with a detection limit of 140 nM.

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Dual functional $CoFe_2O_4$ nanoparticles decoration on Ti_3C_2 MXene nanosheets with enhanced microwave absorption

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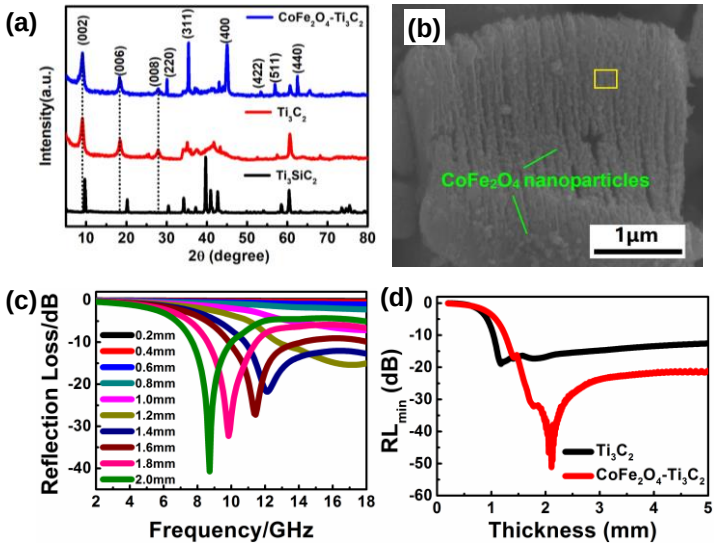
Abstract:

Incorporation of magnetic loss component is more favorable for high-performance microwave absorbing materials. In this paper, *in-situ* hydrothermal derived $CoFe_2O_4$ nanoparticles was firstly introduced as dual functional decoration on Ti_3C_2 MXene nanosheets with enhanced microwave absorbing performance. The as-prepared $CoFe_2O_4$ nanoparticles were attached firmly to the surface or inserted into the interlayer of the Ti_3C_2 MXene. The variation trend between dielectric loss and magnetic loss tangent are exactly the opposite after $CoFe_2O_4$ decoration on Ti_3C_2 nanosheets, suggesting the enhanced magnetic loss plays a more conspicuous role in promoting microwave absorbing performance. Weakened electronic migration at interface and preferable impedance matching coating are considered to be mainly responsible for improved absorbing peaks as well as bandwidth of $CoFe_2O_4$ decorated Ti_3C_2 nanosheets. The optimal reflection loss of -53 dB for $CoFe_2O_4$-Ti_3C_2 composite nanosheets loaded materials with thickness of 2.1 mm could be achieved. These findings are believed to pave the way of further promote microwave absorbing performance of Ti_3C_2 MXene derived architectures from magnetic multi-functionalized decoration of view.



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Tunable Magnetic Response in 2D Materials via Reversible Intercalation of Paramagnetic Ions

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Abstract:

The unique properties of two-dimensional (2D) materials spur fundamental studies and advanced technologies. As one of the important properties, magnetism is highly desired to be incorporated into various 2D materials for active magnetic response, yet it remains challenging to develop a generalized and controllable method to magnetize a wide-range of 2D materials reversibly. In this work, a reversible magnetization method is demonstrated for introducing the active magnetic response to various 2D material multilayers, ranging from graphene oxide (GO) to montmorillonite (MMT), titanium carbide (MXene), molybdenum disulfide (MoS_2), and metal-organic framework (MOF), *via* the de-/intercalation of holmium ions (Ho^{3+}). The magnetic response can be tuned up to 8- to 10-fold increases of the magnetic susceptibilities in all 2D materials by simply controlling the soaking time in the Ho ion solution. Moreover, the magnetic response can be quickly reversed by undergoing a rinsing process in dilute acids together with the recovery of intrinsic physicochemical properties of 2D materials. As a result, the improved magnetic response allows us to manipulate the magnetized 2D materials, enabling the development of a magnet-assisted transfer process for large-area 2D material films as well as the fabrication of magnetically responsive 2D material actuators.

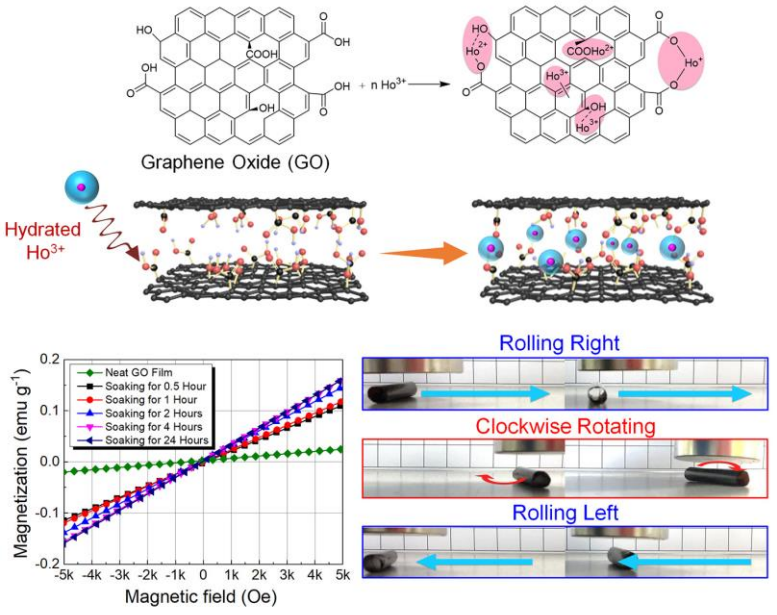

Figure 1 A reversible magnetization method is demonstrated for introducing the active magnetic response to various 2D material multilayers (here, GO was illustrated for an example) via the de-/intercalation of holmium ions (Ho^{3+}). The improved magnetic response allows to manipulate the magnetized 2D materials, enabling the development of a magnet-assisted transfer process for large-area 2D material films as well as the fabrication of magnetically responsive 2D material actuator.

$Ti_3C_2T_x$/PEDOT:PSS Hybrid Materials for Room-Temperature Methanol Sensor

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Abstract:

It is essential to develop a methanol gas sensor with high selectivity and low working temperature for human health and environmental monitoring.[1] In this work, we investigated the gas sensing properties of the hybrid materials consisting of $Ti_3C_2T_x$ and PEDOT:PSS at room temperature. Compared to the pure $Ti_3C_2T_x$ and pure PEDOT:PSS, $Ti_3C_2T_x$/PEDOT:PSS hybrids exhibited enhanced sensing behaviors on acetone, ethanol and methanol. The sensor based on the hybrid with the mass ratio of 4:1 between PEDOT:PSS and $Ti_3C_2T_x$ showed the highest response among all the eight sensors toward acetone, ethanol and methanol gases at room temperature and the highest selectivity to methanol due to the synergistic effect of PEDOT:PSS and $Ti_3C_2T_x$.[2,3] This highest selective sensor based on $Ti_3C_2T_x$ and PEDOT:PSS for detecting methanol can open up new opportunities for exploring more MXenes-based gas sensors with controlled composition and morphologies towards higher performance.

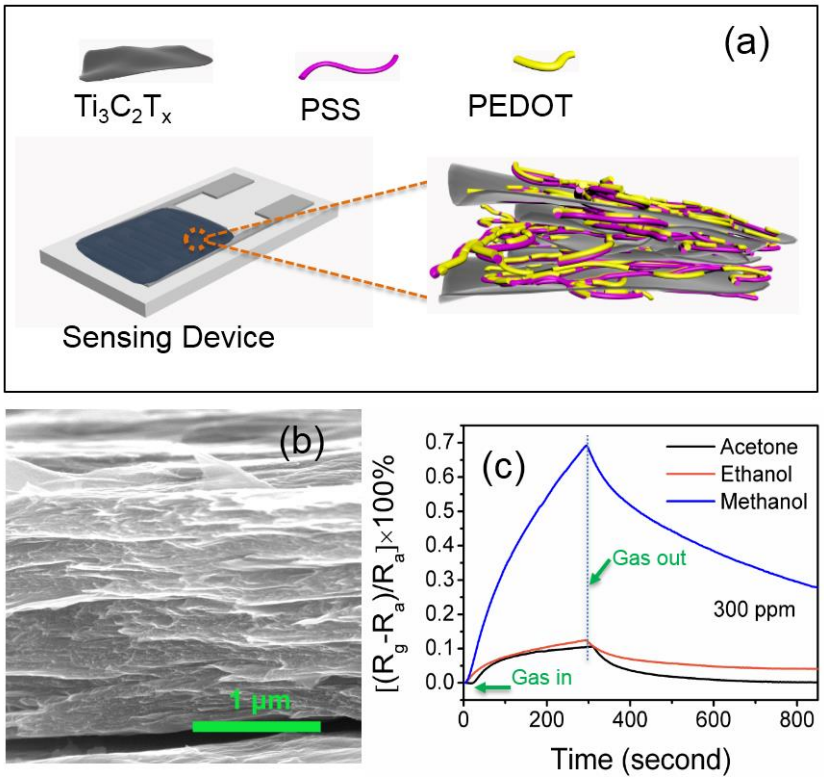

Figure 1 (a) The cross-sectional SEM image of $Ti_3C_2T_x$/PEDOT:PSS hybrid with the mass ratio of 4:1 between PEDOT:PSS and $Ti_3C_2T_x$. (b) Schematic diagram of fabricated gas sensor. (c) The response and recovery curves of the sensor (4:1) toward 300 ppm acetone, ethanol and methanol at room temperature.

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Enhancement of Electromagnetic Absorption Bandwidth of MXene Based Composites Through Structural Design

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Abstract:

Great interests are recently directed to making MXene into flexible devices and functionally reinforced composites due to its metal-like properties and surface-rich functional groups. In addition, the graphene-like 2D materials with a multilayer feature of MXene has high dielectric constant and loss in polymer matrix at low percolation limit promising an ultra-light microwave absorption effectiveness. Yet, the potential of MXene, its orientational structure and composites are to be explored with more computer simulation. In this work, we studied the enhancement of electromagnetic wave absorption bandwidth of paraffin-MXene ($Ti_3C_2T_x$)/Fe_3O_4 coated MXene composites. Computational electromagnetic characterization was carried out in the broad frequency range (2-18 GHz) using a CST-Microwave Studio tool. The simulated result indicates that the single layer MXene composites exhibits excellent reflection loss (RL), -30 dB, however, bandwidth is very narrow even if increasing the thickness to 8 mm, which was well matched with experimental data. In order to enhance the bandwidth of MXene composites, for the first time, we have designed macroscopic pyramidical structure resulting in an excellent RL bandwidth at certain configuration, which is due to the higher interfacial impedance matching. This shows the importance of the structural design of MXene containing polymer nanocomposites for real time applications such as military communication.

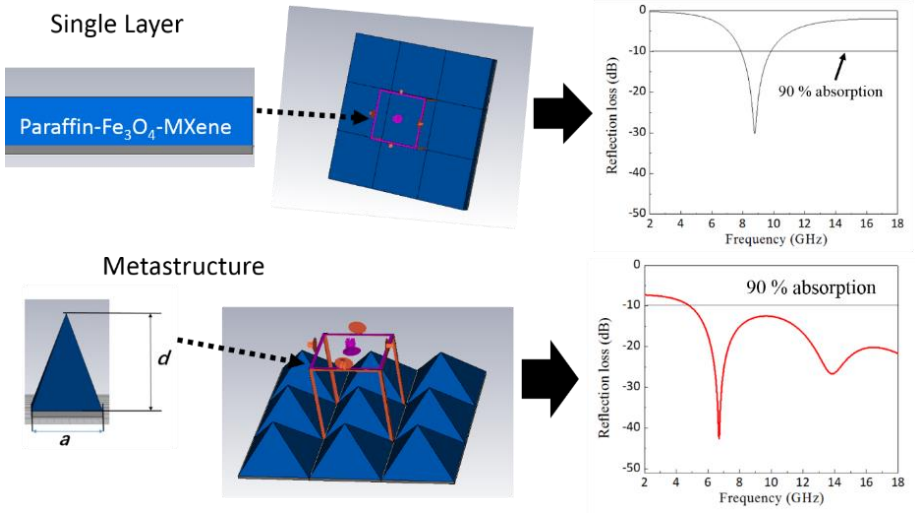

Figure 1 Schematic and performance of designed meta-structure of paraffin-Fe_3O_4-MXene composite with single uniform bulk layer.

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Mechanical Behaviors of $Ti_3C_2T_x$ Papers

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Abstract:

In this work, we report the characterization of mechanical behavior of $Ti_3C_2T_x$ (MXene) papers. Free-standing and flexible $Ti_3C_2T_x$ papers were fabricated by vacuum-assisted filtration of given volume of $Ti_3C_2T_x$ solution via filtration membrane (Celgard 3501, 0.0064um, coated PP). The concentration of $Ti_3C_2T_x$ was about 4 mg/ml, and the thickness of the $Ti_3C_2T_x$ paper varied from 5 μm to 40 μm. X-ray diffraction (XRD) patterns was obtained by benchtop XRD system (Bruker D2 Phaser) using Cu Ka radiation and a scan step of 0.1° with 0.5 s per step. A field-emission scanning electron microscope (FESEM Joel 7610, Japan) was used to obtain high-magnification of cross-section area of $Ti_3C_2T_x$ paper. A typical image of MXene paper is shown in Fig. 1. The thickness and size distribution of $Ti_3C_2T_x$ flakes was obtained by the statistical analysis of more than 200 $Ti_3C_2T_x$ flake samples, using an atomic force microscope. Thermogravimetric analysis (TGA) of a strip of $Ti_3C_2T_x$ paper (about 5 mg) was performed by TGA 550 (TA instrument, USA). Mechanical tests of $Ti_3C_2T_x$ paper was performed on dynamic mechanical analyzer Q800 (TA instruments, USA). For quasi-static tensile, cyclic tensile, and creep test of $Ti_3C_2T_x$ strips, strain-controlled, force-controlled, and creep mode were used, respectively, with preload of 0.01N. A typical stress-strain curve is shown in Fig.2. The results of mechanical characterization of MXene papers will be discussed in the presentation.

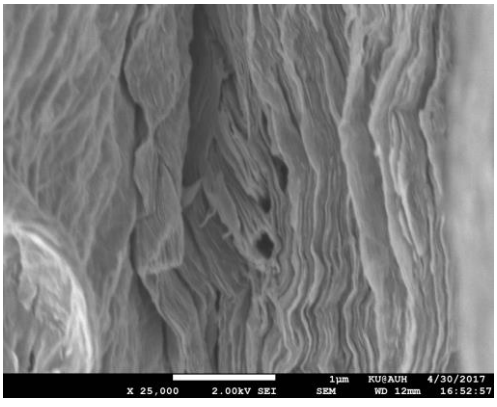

Fig. 1 Cross section of a MXene paper.

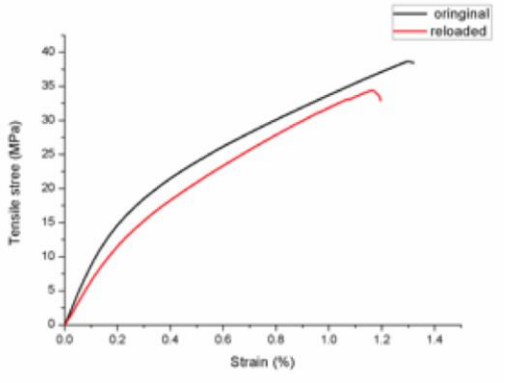

Fig. 2 A typical stress-strain curve of MXene paper under tensile load.

Carbon-coated MXene nanosheets with tremella-like structure as a high performance anode for lithium/sodium ion batteries

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Abstract:

MXenes show great potentials in energy storage due to their metallic conductivity, excellent hydrophilicity, good mechanical flexibility, and superior pseudocapacitive property. However, the MXenes have a strong tendency to restack, leading to the loss of surface active sites. Here, using the most commonly $Ti_3C_2T_x$ MXene, we develop a novel strategy to construct a 3D tremella-like MXene@C by coating a carbon layer on MXene nanosheets through the self-polymerization of dopamine succeeded by carbonization. The carbon layer, which acts as a multi-functional additive, not only construct a 3D tremella-like structure to prevent the MXene nanosheets from restacking and facilitates efficient ionic transport and electron transfer, but also enhance the structural stability during charge/discharge process. In addition, the carbon layer effectively protects the MXene nanosheets from oxidation under high temperature. When working as anode material for both lithium ion batteries (LIBs) and sodium ion batteries (SIBs), the resulting tremella-like MXene@C exhibits ultrahigh specific capacity, superior rate performance, and excellent long-term cycling stability, signifying its potentials as an anode material for both LIBs and SIBs. Moreover, such carbon-coated strategy could be further extended as a general route to fabricate various MXene-based tremella-like structures for diverse applications, such as energy storage, catalysis, sensors, electromagnetic interference shielding, *etc*.

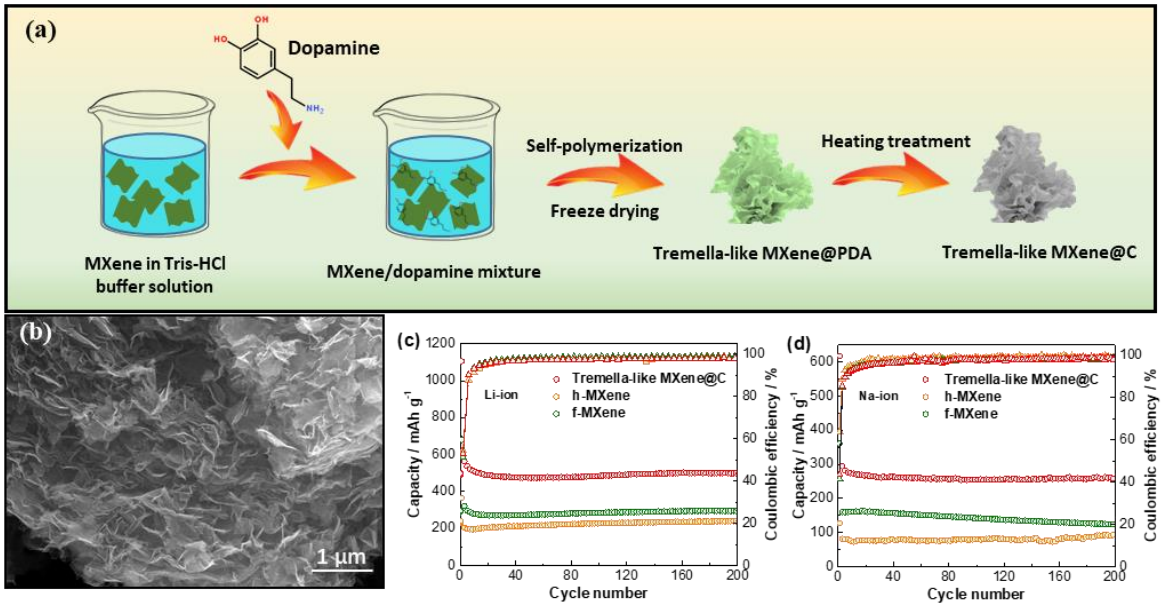

Figure 1 (a) Schematic diagram of the preparation route of tremella-like MXene@C; (b) SEM image of the tremella-like MXene@C; (c) Cycling performance of the tremella-like MXene@C at 0.2C for LIBs; (d) Cycling performance of the tremella-like MXene@C at 50 mA g^{-1} for SIBs.

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Nanoscale Parallel Circuitry Based on Interpenetrating Conductive Assembly for Flexible and High-Power Zinc Ion Battery

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Abstract:

High-rate capability has become an important feature for energy storage devices, but it is often accompanied with a significant reduction in energy density. Therefore, developing an energy storage technology that combines high-rate capability with high energy density is a great challenge for next-generation electronic devices. Here, we construct parallel circuitry at the nanoscale to lower the resistance for ion and electron transport that largely determines the rate performance. The parallel circuitry is constructed through intertwining continuous carbon nanotubes with an interpenetrating conductive assembly based on hierarchically layered MXene ($Ti_3C_2T_x$) functionalized by $KMnO_4$ (MnO_x@$Ti_3C_2T_x$). The assembly shows ultrafast rate capability, e.g. maintaining 50% capacity when the current density increases from 0.1 A/g to 10 A/g. Investigations of the kinetics and charge storage mechanisms confirm the efficiency of the designed parallel circuitry in improving rate capability by providing rapid pathways for ions and electrons, as well as dividing the current flow evenly into individual MnO_x@$Ti_3C_2T_x$ flakes in the assembly. The flexible MnO_x@$Ti_3C_2T_x$ based electrode endows zinc ion batteries with outstanding mechanical robustness and good power delivering performance. The paradigm presented here paves a new way for designing electrodes with high-rate capability towards next-generation energy storage technologies.

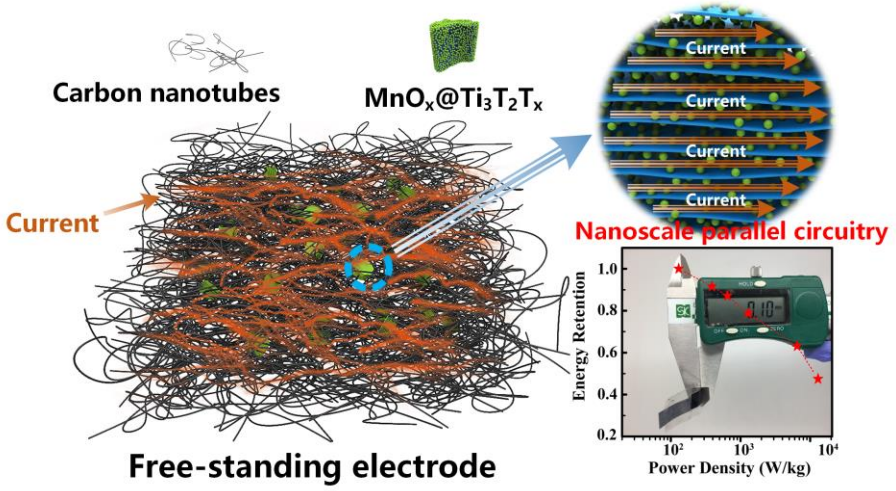

Figure 1 Schematic illustration of the flexible MnO_x@$Ti_3C_2T_x$ based zinc ion battery and its performances.

Fe_3O_4@Ti_3C_2 MXene hybrid with ultrahigh volumetric capacity as anode material for lithium-ion battery

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Abstract:

The volumetric capacity of lithium-ion batteries is becoming an increasingly important parameter restricting their practical applications in limited space, such as portable electronic products and electric vehicles. Therefore, novel electrode materials with high volumetric capacities are urgently desirable. Aiming to pursue such kind of electrode material, a new Fe_3O_4@Ti_3C_2 MXene hybrid is fabricated through a simple ultrasonication of Ti_3C_2 MXene and Fe_3O_4 nanoparticles. Multi-layered Ti_3C_2 MXene in the prepared hybrids acts as a superior host to load Fe_3O_4 nanoparticles due to its opened two dimensional structure, favorable electrical conductivity and low Li^+ diffusion barrier. X-ray diffraction and scanning electron microscopy analysis show that the Ti_3C_2 MXene could be homogeneously covered by Fe_3O_4 nanoparticles at a mass ratio of 5:2. As an anode material, the Fe_3O_4@Ti_3C_2-2:5 hybrid exhibits high reversible capacities of 747.4 mAh g^{-1} at 1 C after 1000 cycles and 278.3 mAh g^{-1} at 5 C after 800 cycles, which indicates its long cycle lifetime and excellent stability. More importantly, the hybrid material possesses an outstanding volumetric capacity up to 2038 mAh cm^{-3} at 1 C due to the high compact density of the electrode of the prapared hybrid. This study provides further insight into the application of the transition metal oxides@MXene hybrids as high volumetric performance anode electrodes for lithium-ion batteries.

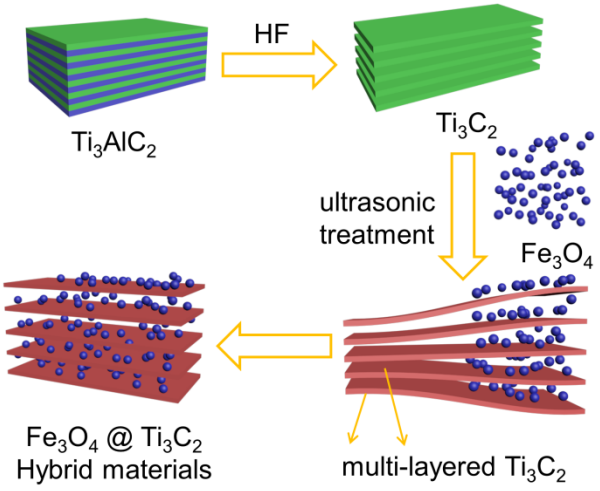

Figure 1. Schematic diagram of intercalation layer

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Designing reasonable bifunctional catalysts based on MXenes toward ORR and OER by theoretical prediction

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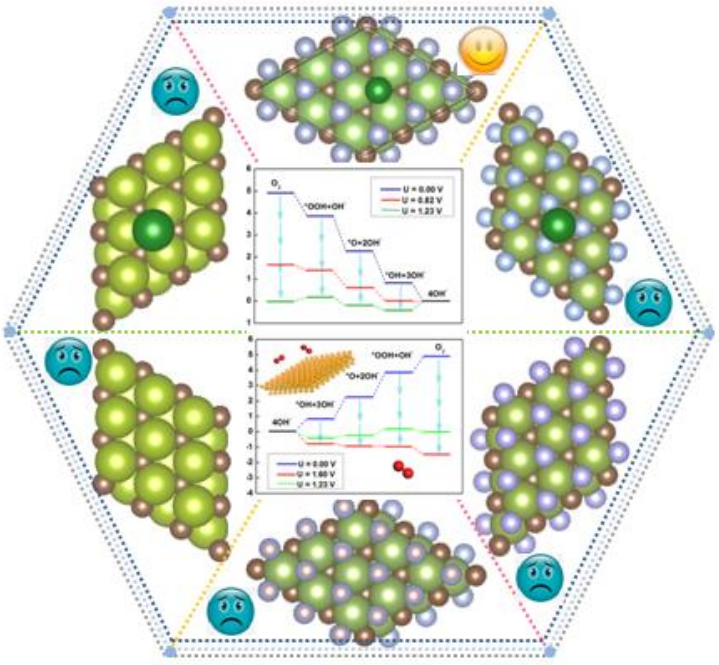
Abstract:

The fast kinetics of the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) were crucial for the further energy conversion technologies. Recently, mxenes, as a promising family of 2D materials, had been widely used in many catalytic reactions with high-efficient and low-cost, but rarely applied as bifunctional catalysts toward ORR and OER. Herein, we firstly realized the relationship between the poor behavior of several mxenes and the electronic structures. Then we took Nb_2CT_X (T=O, F, OH; X=0, 2) as a research template, and presented series of strategies by marring single Pd or Pt metal atoms with MXenes to improving catalytic performances. Afterwards, the most active configurations were picked out and donated as Nb_2CO_2-O_{V1}-Pt and Nb_2CF_2-F_{V1}-Pt with proper d band and binding strength with intermediates. Both of them were efficient bifunctional catalyst to ORR and OER, especially for the case of Nb_2CF_2-F_{V1}-Pt. It was even better than the criterion catalysts (Pt for ORR, and IrO_2 for OER), with theoretical overpotential as low as 0.41V for ORR and 0.39V for OER. Furthermore, we discussed the principal factor that determined the activities and presented a reasonable path of designing effective and inexpensive bifunctional catalysts based on MXenes.



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Functionalization of MXenes as highly active and selective catalysts

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Abstract:

MXenes, a new family of two-dimensional materials, have attracted increasing attention because of their metallic conductivity, hydrophilicity and good mechanical properties.[1] As a result, they have been widely used in diverse fields, including Li-ion batteries, supercapacitors, fuel cells, hydrogen evolution, gas sensors, and so on.[1-12] In addition, MXenes have recently emerged as promising candidates in catalysis. For instance, Wang and co-workers prepared $Mo_2TiC_2T_x$ supported Pt single atoms and used them for hydrogen evolution reaction, which exhibited a mass activity of 40 times higher than that of commercial Pt/C catalyst.[13] Wu et al. reported that MXenes supported Pt nanoparticles can be used for propane dehydrogenation, which shows a propane conversion and propene selectivity of 16% and 95%, respectively, at 550 ^oC.[14] Although great progress in catalysis has been made, MXene composite catalysts for PSH have not been investigated yet, which might be another new and promising application.

Here, we synthesize cobalt-tipped carbon nanotube/Ti_3C_2 nanosheet composites (Co-CNT/Ti_3C_2) for oxygen reduction reaction (ORR) and propyne semi-hydrogenation. It is shown that the optimized Co-CNT/Ti_3C_2 manifest comparable ORR activity (half-wave potential of 0.82 V and diffusion-limiting current density of 5.55 mA cm^{-2}) with commercial Pt/C (half-wave potential of 0.82 V and diffusion-limiting current density of 5.30 mA cm^{-2}) but much better stability.[15] Furthermore, the Ti_3C_2 nanosheet supported Co-based catalyst exhibits a propene selectivity of 96% at the propyne conversion of 99% at 150 ^oC, which have surpassed the reported values in the literature.

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Inkjet-printed MXene broadband ultrafast photonic devices

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Abstract:

MXene, as a novel 2D crystal material, possessing tunable bandgap, low optical attenuation and broadband nonlinear optical responses that may promote the fabrications of advanced electro-photonics devices has gathered remarkable attention recently. However, current investigations of 2D crystals for photonics devices suffer from the limitations of reproducibility, scalability and compatibility. Inkjet printing is one of the powerful additive manufacturers that facilitate well-controlled, low-cost, scalable and small-footprint electro-photonics devices on myriad substrates. Herein, we directly inkjet printed MXene nanosheets in laser resonators with both fiber and free-space geometrics, and achieved extensive spectral band ultrafast laser operations from near- to the mid-infrared regime with pulse duration going to 100 femtoseconds. The demonstrations of versatile inkjet-printed devices based on MXene, while forthputting its distinct electro-optical properties, may allow the realizations of advanced MXene enable photonics devices shortly.

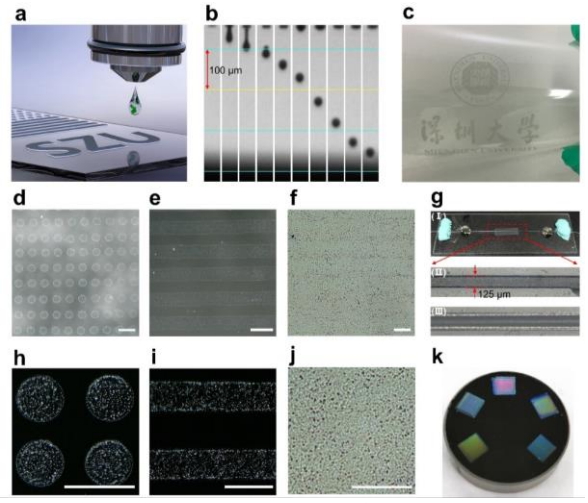

Figure 1. Inkjet-printed MXene photonic devices. a Inkjet printing schematic diagram. **b** Printing droplet sequences observed from the printer stroboscopic camera.**c** Inkjet printed logo of Shenzhen University on a transparent and flexible PET film. **d-f** and **h-j** The printed dots, stripes and plane on glass substrate, scale bar: 100 μm. **g** (Ⅰ) The side-polished fiber saturable absorber. (Ⅱ) Printed (12 layers) and (Ⅲ) unprinted side-polished fiber checked by an optical microscope. **k** Inkjet printed MXene saturable absorber mirror (SAM) with different printing layers. The clockwise printed layers: 10L, 20L, 16L, 8L, 4L.

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Transition metal monolayer decorated Mo_2C MXene for enhancing fuel cell's performance

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Abstract:

Pt-based catalysts are still the promising catalysts for fuel cells, but their large-scale usage suffers from high cost, low abundance, poor stability, poor oxygen reduction reaction (ORR) reactivity on the cathode and CO poisoning on the anode. By using density functional theory, we select a representative MXene, Mo_2C, to screen the best supported metal monolayer on Mo_2C (M_{ML}/Mo_2C, M = Cu, Pd, Pt, Ag and Au) as catalysts towards ORR, aiming to find a promising catalyst to replace Pt/C catalysts used in the proton exchange membrane fuel cells (PEMFCs). According to our stability and adsorption properties, we speculate that Au_{ML}/Mo_2C is a promising ORR candidate with good stability, enhanced durability, comparable or even better ORR activity than the commercial Pt/C catalysts. Besides, to improve the CO tolerance of the anode Pt/C catalysts, we find that Ag_{ML}/Mo_2C may be used as a good catalyst for CO removal in H_2 feeds connected to the anode of fuel cells. It can be used not only as a filter membrane for separating H_2 and CO, but also as an efficient catalyst with high selectivity and activity for preferential oxidation of CO in the H_2 feeds. We hope our present studies could advance the development of fuel cells and inspire more applications about MXene catalysts.

O-terminated Mo_2C MXene for constructing single atom catalysts and single cluster catalysts via vacancy engineering

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Abstract:

MXene is a kind of new 2D materials, which possesses brilliant properties in the field of energy, battery, supercapacitor, catalysis and so on. Up to now, most of the experiments focus on Ti_3C_2 MXene. In contrast, the study of other MXene is limited. Here, we choose a representative Mo_2CO_2 to investigate its properties using density functional theory [1]. We take a Pd atom and CO as a dopant and a probe molecule, respectively, to investigate the catalytic properties of Mo_2CO_2. We find the defective Mo_2CO_2 can be used a good substrate material to anchor single Pd atom forming stable single atom catalysts (SACs) with good catalytic activity for CO oxidation. Besides, we take Cu_3 cluster on Mo_2CO_2 as a representative to test single cluster catalysts (SCCs) [2]. The synergistic effect between Cu_3 cluster and Mo_2CO_2 makes Cu_3/Mo_2CO_2 an efficient SCC with unique properties: good stability, resist to oxidation and CO poisoning, high CO oxidation activity and so on. The high activity is attributed to the doped Cu_3 cluster functioning as an electron reservoir, which could control the electron release and collection and mediate the reaction. To find more stable and efficient SACs for low-temperature CO oxidation, we propose three criteria to screen metals decorated SACs instead of only considering reaction energy [3]. We hope these criteria can be used to screen SACs fastly on MXene materials or beyond.

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In-situ transformed alloy nanoparticles on MXene surface from self-assembled metal hydroxides precursors

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Abstract:

With the increasing attention on the design and synthesis of MXene-based nanohybrids, recently a novel assembly-solid state transformation strategy was developed. The variability of metal hydroxides in this protocol endows it a facile route towards metal sulfides and trichalcogenidophosphates functionalized MXene-based nanohybrids.[1,2] However, there is still necessary to verify the possibilities of this method towards other modified compounds.

In consideration of the active metal species on MXene surface, an *in-situ* thermal reduction was applied on the Ni/Co bimetal hydroxide-modified $Ti_3C_2T_x$ MXene. As shown in Figure 1a and 1b, the Ni/Co bimetal hydroxides could be successfully transformed into alloying species (denoted as $Ni_{1-x}Co_x$@TM, x = 0, 0.1, 0.2 and 0.3), which presents a zero-dimensional (0D) nanoparticles-2D nanosheets hybrids structure. The electrocatalytic hydrogen evolution (HER) activities of the products were also evaluated in an alkaline solution (1 M KOH). As compared with the bare $Ti_3C_2T_x$ MXene, the alloy modified samples all presents a dramatical increase of the HER activity. Especially, the $Ni_{0.8}Co_{0.2}$@TM nanohybrid shows an overpotential of 255 mV to reach the current density of 1000 mA F^{-1}, which about 400 mV lower than the pristine $Ti_3C_2T_x$ MXene (Figure 1c). The results indicate that the alloy-modified MXene could be a promising non-noble metal electrocatalyst for water-alkali electrolysis.

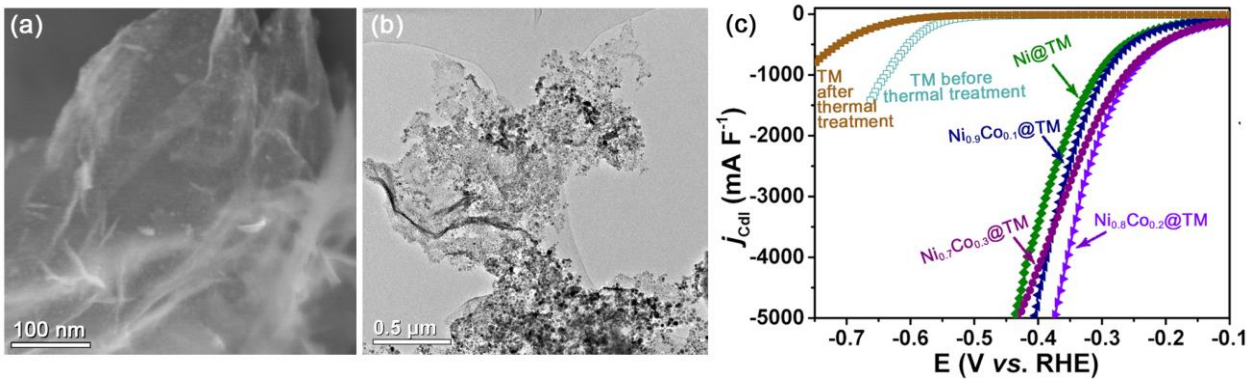

Figure 1. The (a) SEM and (b) TEM images of the $Ni_{0.8}Co_{0.2}$@TM nanohybrids. (c) The normalized LSV curves of the bare $Ti_3C_2T_x$ MXne and the series $Ni_{1-x}Co_x$@TM nanohybrids in 1 M KOH with a scan rate of 5 mV s^{-1}.

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Binary Strengthening and Toughening of MXene/Cellulose Nanofibers Composite Paper with Nacre-Inspired Structure and Superior Electromagnetic Interference Shielding Properties

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Abstract:

With the growing popularity of electrical communication equipment, high-performance electromagnetic interference (EMI) shielding materials are widely used to deal with radiation pollution. However, the heavy-thickness and poor mechanical property of the EMI shielding materials usually limit their applications. In this study, ultrathin and highly flexible $Ti_3C_2T_x$ (d-$Ti_3C_2T_x$, MXene)/cellulose nanofibers (CNFs) composite paper with nacre-like lamellar structure is fabricated *via* a vacuum-filtration induced self-assembly process. By the interaction between one-dimensional (1D) CNFs and two-dimensional (2D) MXene, the binary strengthening and toughening of the nacre-like composites paper is successfully achieved, leading to superior tensile strength (up to 135.4 MPa) and fracture strain (up to 16.7%), as well as ultrahigh folding endurance (up to 14260 times). Moreover, the composite paper exhibits great electrical conductivity (up to 739.4 S m^{-1}) and excellent specific EMI shielding efficiency (up to 2467 dB cm^2g^{-1}) at an ultrathin thickness (minimum thickness, 47 um). The nacre-inspired route in this study offers a promising approach to design strong integrated and flexible MXene/CNFs composite, which can be applied in wearable devices, weapon equipment and robot joints.

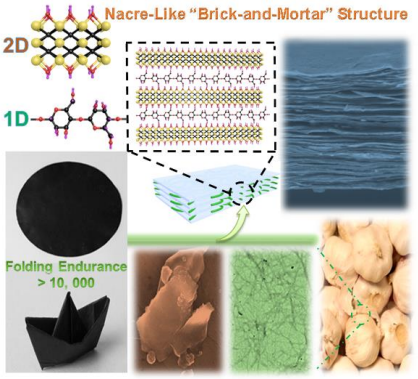

Figure 1. A novel binary nacre-like MXene/cellulose nanofibers composite paper with superior strength and toughness possesses great electrical conductivity and excellent specific EMI shielding efficiency has been fabricated via a vacuum-filtration induced self-assembly process.

References:

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Combinatorial screening of transition metals embedded V_2CT_2 (T=O, F) monolayer (MXene): Promising single-atom catalysts for low temperature CO oxidation

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Abstract:

Using first-principles calculation, the potential of two dimension MXenes materials V_2CT_2 (T=O, F) with functional group vacancy as the substrates of single-atom catalyst (SAC) for transition metal (TM) (Sc-Zn； Pd, Pt; Ag, Au; and Cd, Hg) has been studied. The adsorption sites and calculated energies of TM-Ov/V_2CO_2 and TM-V_2CF_2 indicate that the Zn embedded V_2CO_2 with O vacancy (Zn-Ov/V_2CO_2) and Ni embedded V_2CF_2 with F vacancy (Ni-Fv/V_2CF_2) are the very promising SACs, because it can be strongly trapped in the cavity of the oxygen vacancy and exist in the isolated form. CO oxidation was chosen as a probe reaction to test the catalytic activity of the predicted SACs. By exploring the Langmuir – Hinshelwood (LH) and the Eley-Rideal (ER) mechanism, it is found that the first step of CO oxidation ($CO+O_2 \rightarrow OCOO$) catalyzed by Zn-Ov/V_2CO_2 is the LH mechanism, with energy barrier of 0.20 eV; then the produced OCOO will easily decompose to CO_2 and O ($OCOO \rightarrow CO_2+O$) with an energy barrier of 0.11 eV; The third step ($O+CO \rightarrow CO_2$) proceeds via ER mechanisms, with energy barrier as low as 0.06 eV. For Ni-Fv/V_2CF_2, CO oxidation via LH mechanisms is divided into two steps ($CO+O_2 \rightarrow CO_2+O$, and $O+CO \rightarrow CO_2$), and the energies barriers are merely 0.13 and 0.07 eV, respectively. Therefore, Zn-Ov/V_2CO_2 and Ni-Fv/V_2CF_2 are the very promising SACs for low-temperature CO oxidation reaction. The study presented here suggests that the V_2CT_2 (T=O, F) with T defects are the promising platforms to synthesize SACs.

CO oxidation on Nb_2CO_2 Monolayer with a single Pd atom

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Abstract:

The presence of CO in proton exchange membrane fuel cells (PEMFCs) not only results in the poisoning of anode materials, but also harmful to the environment. MXenes, a new type of two-dimensional materials, have been widely concerned and studied. Some of them have been speculated to have excellent catalytic activity for catalytic reactions [1]. Nb_2CO_2 was one of them [2]. In this paper, we investigate the properties of a kind of single atom catalysts (SACs) formed by single Pd atoms deposited on Nb_2CO_2 containing single oxygen vacancies using the DMol3 code embedded in Materials Studio. It was found that the single Pd atom could be stably anchored at the oxygen vacancy. Three oxidation mechanisms of carbon monoxide on the O_V–Nb_2CO_2 with Pd additives were explored. It was found that the oxidation of carbon monoxide can be completed via a tri-molecular Eley–Rideal (TER) mechanism, which has an activation barrier of 0.42 eV. This result may provide a basis for the selection of anode materials with high CO-tolerance for PEMFCs.

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Activation mechanism of silver toward CO oxidation by tungsten carbide support: A density functional theory study

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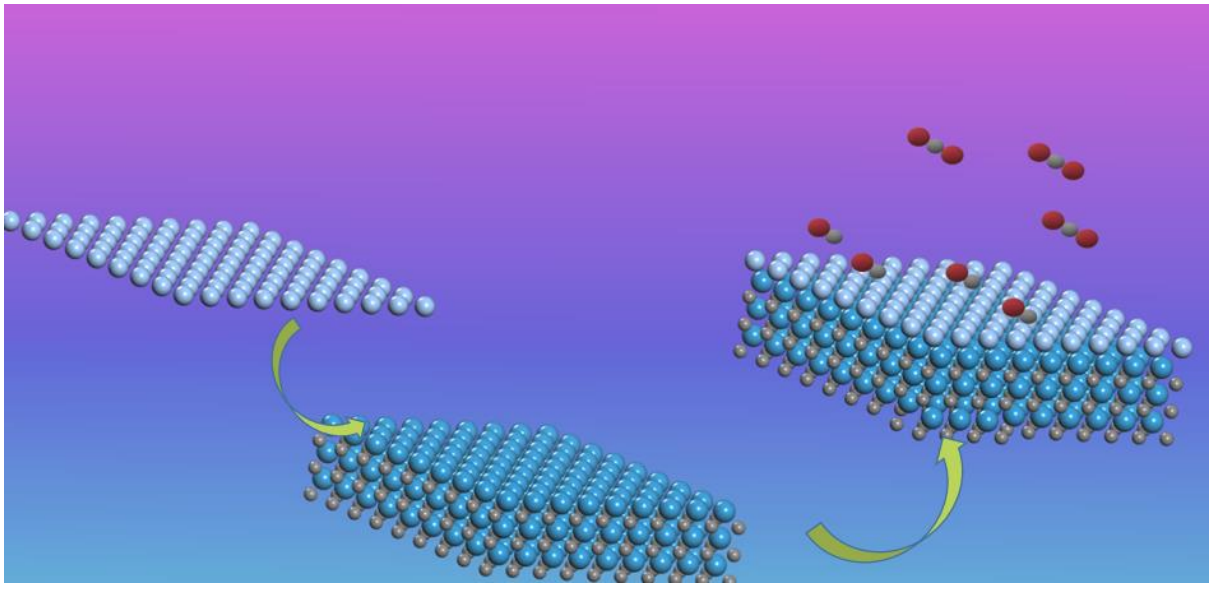
Abstract:

The development of efficient catalysts for low temperature CO oxidation is quit important to the application of fuel cells. In this work, we report that the Ag monolayer on WC (0001) surface (Ag_{ML}/WC) could effectively catalyze CO oxidation through the L-H mechanism ($CO + O_2 \rightarrow OOCO \rightarrow CO_2 + O$). The most sluggish reaction step is suggested to be $CO + O \rightarrow CO_2$ with a barrier of 0.48 eV, which is 1.21 eV lower than the barrier of O_2 dissociation. The electronic structures and d-band centers analyses demonstrated that the promoted activity may originate from the synergistic effect between Ag monolayer and WC. The present study is conducive to design new efficient and cost-effective catalysts without using of the noble platinum, which can effectively promote carbon monoxide oxidation.



Small Pt-based metal nanoparticles decorated v-Ti_2CO_2 as efficient bifunctional catalyst for OER and ORR

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Abstract：

The rational design of ideal catalysts for the oxygen reduction reaction (ORR) is of great significance for solving the electrocatalytic potential problems in proton exchange membrane fuel cells. The Pt_n (n=1, 3, 4) and Pt_3Au alloy nanoparticles supported on v-Ti_2CO_2 are simulated using density functional theory to investigate the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) performance of the catalysts in alkaline media [1,2]. The geometric and electronic properties of different surfaces are studied. The free energy diagrams of the adsorbates and the reverse volcano plots are analyzed. Based on the aforementioned results, it is found that the Pt_3Au alloy nanoparticles decorated v-Ti_2CO_2 catalysts possess the better OER and ORR activity, which are suitable to be used as the bifunctional catalysts. The underlying mechanisms for the improved overpotential result from the moderate hybridization between O 2p orbital and the 5d orbitals of Au and Pt. Our study provides a facile route for designing bifunctional MXene-based electrocatalysts by alloying a transition metal with Pt, which may stimulate realization of suitable alternative catalysts for ORR.

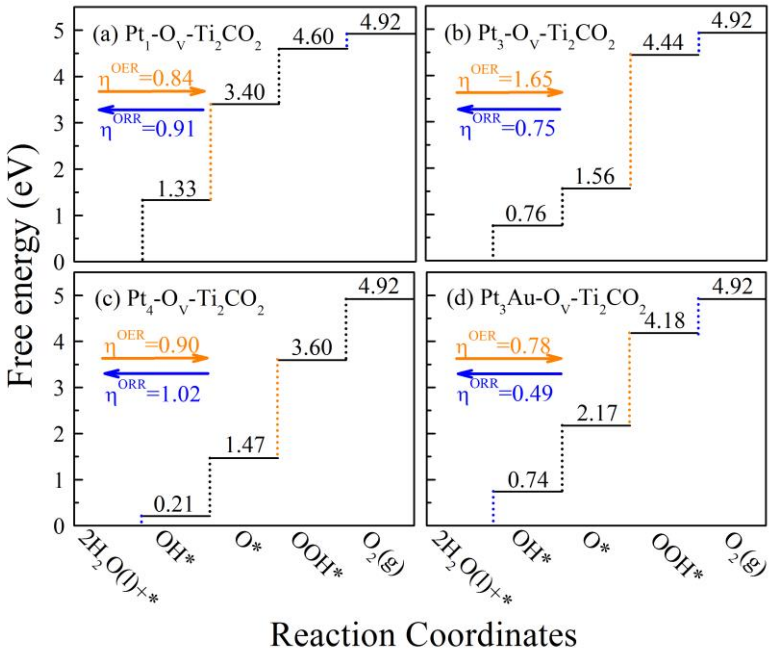

Figure 1. The free energy diagrams of OER and ORR on Pt_n (n=1, 3, 4) and Pt_3Au decorated v-Ti_2CO_2 at the U=0 V. The blue and the orange dot lines are the rate limiting step for ORR and OER, respectively.

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TiC supported platinum monolayer as high-performance catalyst for CO oxidation and water-gas shift reaction: DFT study

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Abstract:

The reaction mechanism towards CO oxidation and water-gas shift reaction of Pt monolayer supported on TiC(001) is revealed by using empirical dispersion-corrected density functional theory calculations. A number of possible reaction pathways for CO oxidation, considering the cases that the adsorbed O_2 dissociates first or directly react with CO. It is found that the dissociation of adsorbed O_2 molecule as the initial step is more favorable with lower activation barriers compared with the direct reaction mode. Hence the dissociation of adsorbed O_2 molecule plays a very key role in the CO oxidation reaction. Our analyses also reveal that the reaction is most likely predominant via an initial ER mechanism and a subsequent LH mechanism. [1] It is found that the Pt_{ML}/TiC(001) exhibits an obviously lower density of Pt-5d states nearby the Fermi level compared with that for Pt(111) and the monolayer Pt atoms undergo electronic perturbation when in contact with the TiC(001) support that can strongly improve the WGS activity of supported Pt atoms. Our calculations clearly demonstrate that the dominant reaction path follows a carboxyl mechanism involving a key COOH intermediate, rather than the common redox mechanism. [2] The present studies indicate that the TiC supported Pt monolayer can serve as a good catalyst towards CO oxidation and water-gas shift reaction.

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Eosin Y-Sensitized Partially Oxidized Ti_3C_2 MXene for Photocatalytic Hydrogen Evolution

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Abstract:

Ti_3C_2, one of the most extensively studied 2D MXenes, is rarely reported for its potential application in dye-sensitized photocatalysis. Platinum is commonly used as co-catalyst in photocatalytic hydrogen evolution but it increases the cost and hence restricts the commercialization of this technology. Eosin Y (EY) is widely studied in dye-sensitized system as it is not only low-cost and easily commercially available, but also exhibits excellent visible light absorption ability. Herein, we oxidized Ti_3C_2 MXene in water at 60 °C for different time, to form TiO_2/Ti_3C_2 on amorphous carbon (AC) composites. The oxidized MXene was used as photocatalyst in dye-sensitized system for hydrogen evolution to replace noble metal co-catalyst such as Pt. The highest hydrogen production rate of 33.4 μmol · h^{-1} · g^{-1} was achieved by TiO_2/Ti_3C_2@AC-48h composite with the sensitization of 1 mM EY, which is 110 times higher than that of oxidized Ti_3C_2 without EY. This work shows the potential of 2D MXenes use in dye-sensitized photocatalysis for hydrogen evolution.

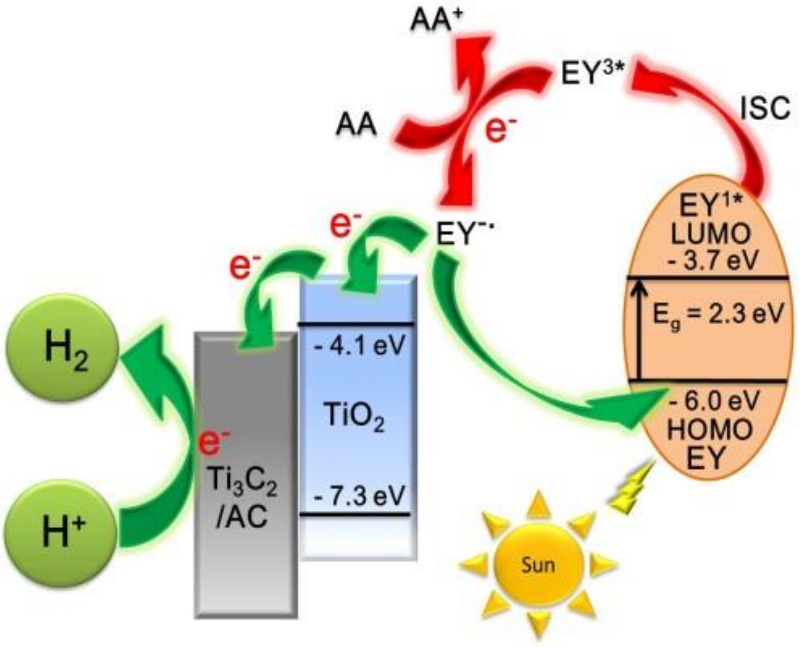

Figure 1. The schematic diagram of hydrogen production for EY-sensitized TiO_2/Ti_3C_2@AC composite under visible light irradiation.

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SnO_2-Ti_3C_2 MXene electron transport layers for perovskite solar cells

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Abstract:

MXenes, a class of two-dimensional (2D) transition metal carbides and nitrides, have a wide range of potential applications due to their unique electronic, optical, plasmonic, and other properties. Herein, we explore the use of Ti_3C_2 MXene in organic-inorganic lead halide perovskite solar cells (PSCs) due to its metallic conductivity. SnO_2-Ti_3C_2 MXene nanocomposites with different contents of Ti_3C_2 (0, 0.5, 1.0, 2.0, 2.5 wt.‰) were used as electron transport layers (ETLs) in low-temperature processed planar-structured PSCs. Mixing SnO_2 with 1.0 wt.‰ Ti_3C_2 effectively increases the power conversion efficiency (PCE) from 17.23% to 18.34%, whereas the device prepared with pristine Ti_3C_2 as the ETL achieves a PCE of 5.28%. Photoluminescence and electrochemical impedance spectroscopy results reveal that the metallic Ti_3C_2 MXene nanosheets provide superior charge transfer paths, enhancing electron extraction, electron mobility, and decreasing the electron transfer resistance at the ETL/perovskite interface, and thus leading to higher photocurrents. This work proposes a new field of application for MXenes and a promising method to increasing efficiency of solar cells.

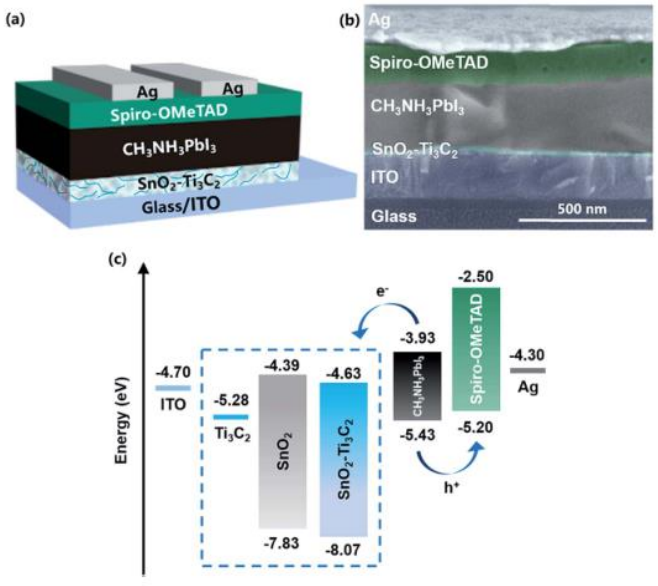

Fig. 1 (a) Device architecture of ITO/ETL/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Ag based on representative SnO_2–Ti_3C_2 as the ETL, (b) cross-sectional SEM image of the PSC device, and (c) schematic energy-level diagram of each layer.

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Magnetic and electronic properties of the Cr-based MXene (Cr_2C)

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Abstract:

The effects of different functional groups on the magnetic interaction and electronic properties of transition metal carbide Cr_2C were studied by first-principles calculations. We predict that the transition metal carbide Cr_2C is a potential controllable two-dimensional magnetic material. The introduction of surface functional groups as chemical dopants in the synthesis process has great influences on the electronic properties and magnetic interaction of the Cr_2C materials. The results of electronic structure calculations (as shown in Fig1.) indicate that different functional groups have a great influence on the electronic structure of Cr_2CX_2 (X = O, F, OH), including the transition from metallic state to insulating state. The Heisenberg equation is used to calculate the magnetic interaction between Cr ions with different functional groups. The results show that the lowest magnetic interaction among the three functional groups is the O functional group, but the effect is larger than that without the functional group. Next, in order to reduce the magnetic interaction after adding functional groups, we studied the effects of N doping on the electromagnetic interaction and electronic properties of Cr_2C. The results show that the N-doped Cr_2C materials are always metallic with the different functional groups. The magnitude of magnetic interaction is found to be reduced due to the substitution doping of N.

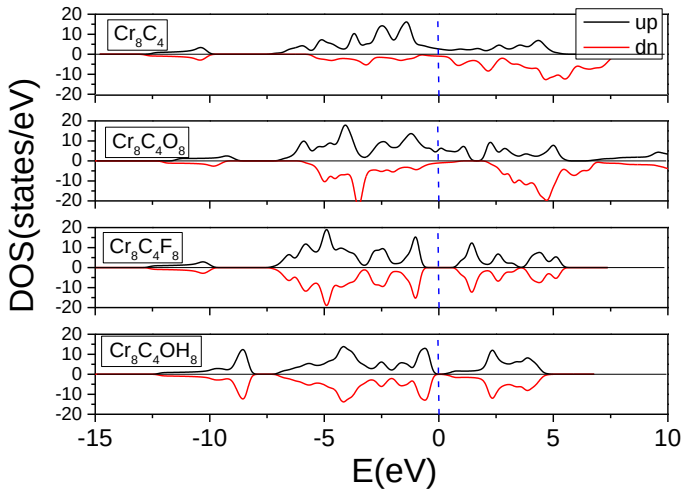

Figure 1. Total Density of State of Cr_2CX_2 (X = O, F, OH) with Different Functional Groups.

In Situ Growth of MnO Naonorods on MXene-based Scaffold for Supercapacitive Biosensing

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Abstract:

Novel MnO@carbon nanocomposite shows not only high capacities for electrochemical energy storage, but also high sensitivity for molecular and cellular biosensing based on its open and fast transport of molecules or electrons through the carbon-based scaffold matrix towards underlying the detector substrate. [1] As a new 2D material, MXene provides unprecedented physiochemical properties by combining excellent metallic conductivity and high hydrophilicity. Moreover, the high aspect ratio of delaminated MXene rendering it promising electrochemical and biofunctional nanoscale building block in multifunctional polymer nanocomposite-based scaffold, and gearing up for many exciting applications in healthcare technology and electronic devices [2,3]. In our study, novel MXene-based scaffold has been constructed by triggering the redox reaction for growing MnO nanoroads *in situ* on the surface of Ti_3C_2 nanosheets. The MnO@MXene nanocomposites developed by our group has demonstrated highly reversible electrochemical capacity and long-term stability as the next generation supercapacitive biosensing electrode (Figure 1). In addition, the potential of the use MnO@MXene composites for emerging biomedical application such as anti-tumor therapeutics will also be discussed.

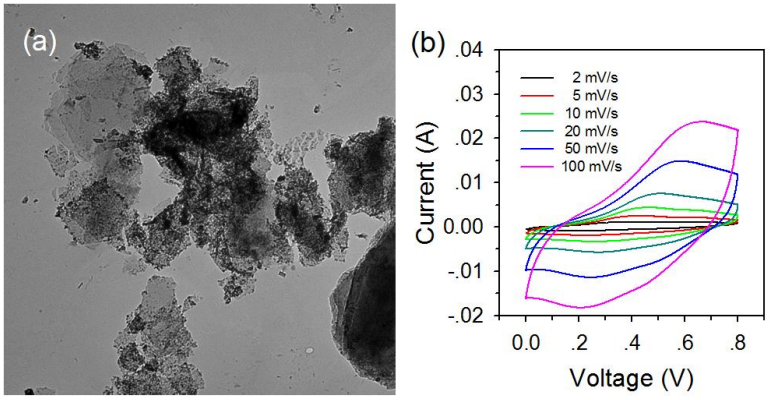

Figure 1. (a) TEM images of the MXene-MnO (2:1 mass ratio) composite; and (b) CV curves of the composite in different scan rate in 1.0 M Na_2SO_4 solution.

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Using Intercalation of Cationic Surfactant to Open Magnesium Storage Capability of Two-Dimensional MXene

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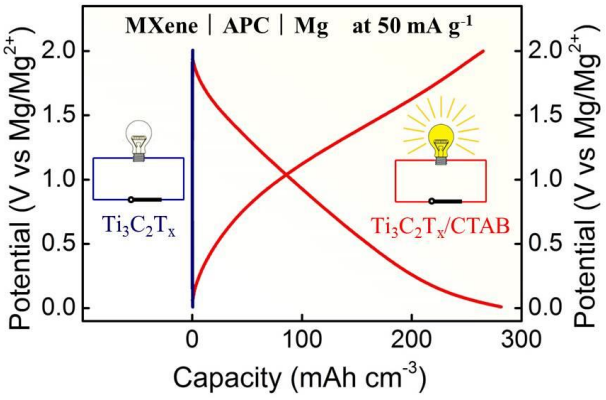
Abstract:

Ti_3C_2 MXene, a new kind of two-dimensional transition metal carbides, has attracted extensive attention in supercapacitors and lithium-ion and post lithium-ion batteries because of its outstanding excellent electrical conductivity as well as high volumetric capacity. Nevertheless, a previous study showed that multivalent Mg^{2+} ions cannot reversibly insert into MXene, resulting in a negligible capacity. Here, we demonstrate a simple strategy to achieve high magnesium storage capability for Ti_3C_2 MXene by preintercalating a cationic surfactant, cetyltrimethylammonium bromide (CTAB). Density functional theory simulations verify that intercalated CTA^+ cations reduce the diffusion barrier of Mg^{2+} on the MXene surface, resulting in the significant improvement of the reversible insertion/deinsertion of Mg^{2+} ions between MXene layers. Consequently, the MXene electrode exhibits a desirable volumetric specific capacity of 300 mAh cm^{-3} at 50 mA g^{-1} as well as outstanding rate performance. [1] Our study realized the application of MXene material in Mg batteries, and the performances presented here make such paper-like MXene a promising candidate for magnesium batteries with high volumetric specific capacity.



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Synthesis of V_2C MXene etching with lithium fluoride and hydrochloric acid

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Abstract:

MXenes, as new promising two dimensional materials, have drawn extensive attention in energy storage, electro/photo catalysis, gas- and biosensors, photothermal therapy, and other fields [1-3]. V_2C is an important member of MXenes and the theoretical calculation indicates V_2C MXene has better performances as energy storage materials [4,5]. Up to now, the main approach to synthesis V_2C MXene is etching V_2AlC precursor with HF solution [6-8]. Besides the serious pollution and corrosion of HF, another imperfection is the impurity of as-synthesized V_2C MXene, which inevitably contains V_2AlC precursor. Herein, V_2C MXene with higher purity were successfully synthesized by etching V_2AlC with the mixture of lithium fluoride (LiF) and hydrochloric acid (HCl). After etching for 96 h or more, the diffraction peaks of V_2AlC precursor disappeared and new peaks ascribed to V_2C MXene occurred (shown in Fig.1 a). The sample etched for 120 h exhibited typical accordion-like morphology and uniform multilayered structure (shown in Fig.1 c and d). The obtained V_2C MXene presented unique supercapacitive performances. The specific capacitances, tested at 0.5 A g^{-1}, 1 A g^{-1}, 2 A g^{-1}, 3 A g^{-1}, 5 A g^{-1} and 10 A g^{-1}, could achieve 195 F g^{-1}, 158 F g^{-1}, 130 F g^{-1}, 114 F g^{-1}, 95 F g^{-1} and 70 F g^{-1}, respectively. In addition, the mixture solutions of sodium fluoride (NaF) with HCl and potassium fluoride (KF) with HCl can also be used to successfully synthesize multilayer V_2C MXene with higher purity. (This work was supported by the National Natural Science Foundation of China (No. 51472186 and No. 51402221).

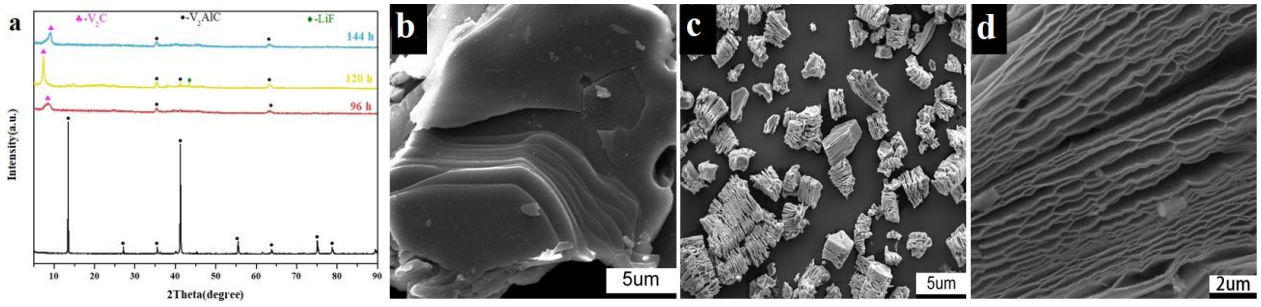

Fig.1 (a) XRD patterns of V_2AlC and V_2C MXene etched with LiF and HCl solution for different time; and SEM images of (b) V_2AlC and (c, d) V_2C MXene etched for 120 h.

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High efficiency photocatalytic hydrogen production over ternary Cu/TiO_2@$Ti_3C_2T_x$ enabled by MXenes

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Abstract:

Exposing the highly active facets has been regarded as a powerful approach to high-performance photocatalysts. More importantly, effectively harvesting light to generate long-lived charge carriers to suppress the recombination of electrons and holes is crucial for photocatalytic water-splitting.

Herein, a heterostructure comprised of {001} facets of TiO_2 nanosheets and MXene was synthesized by a facile hydrothermal partial oxidation of Ti_3C_2. The in-situ growth of TiO_2 nanosheets on Ti_3C_2 allows for the interface with minimized defects. The highly active {001} facets of TiO_2 afford high-efficiency photogeneration of electron-hole pairs, meanwhile the carrier separation is substantially promoted. [1]

We experimentally prove that the $Ti_3C_2T_x$ MXene from the wet HF etching method behaves as a low work function material (ϕ = 3.4 eV).[2] Thanks to this unique electronic property, the photogenerated electrons on TiO_2 hybridized with $Ti_3C_2T_x$ accumulate and tunnel to Cu_2O to reduce it to elemental Cu as a reduction cocatalyst. The resulting Cu/TiO_2@$Ti_3C_2T_x$ photocatalyst efficiently split water to produce hydrogen at 860 μmol g^{-1} h^{-1}. The similar design of HER photocatalyst has been also demonstrated in a novel Ag/Nb_2O_5 nanorod@Nb_2C hybrid. The results presented here demonstrate the promise of MXene materials in photocatalytic solar energy utilization. The insight into the electronic property of MXene sheds light on the new approach to the rational design of high-efficiency photocatalysts composed of MXenes.

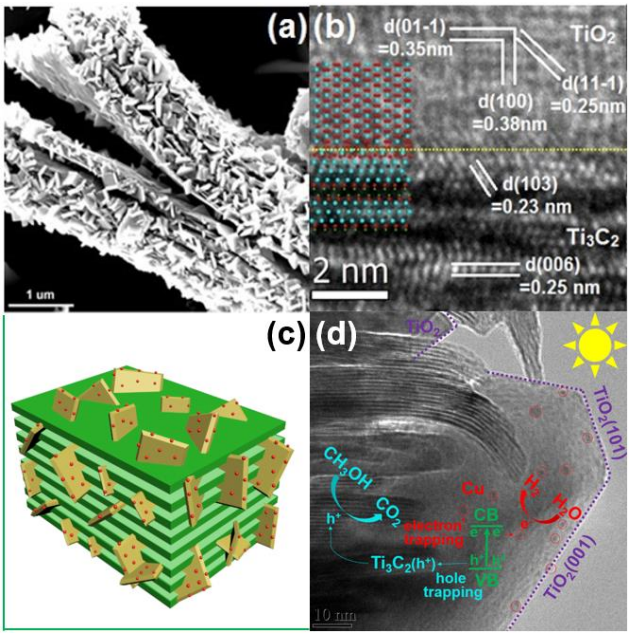

Figure 1 (a) and (b) are SEM and TEM images of Ti_3C_2/anatase (001) TiO_2, respectively. (c) Schematic illustration of the Cu/(001)TiO_2/Ti_3C_2. (d) TEM image and photocatalytic mechanism of Cu/(001)TiO_2/Ti_3C_2.

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Engineering lattice space of $Ti_3C_2T_x$ MXene for enhancing its performance in storing Li^+ and K^+

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Abstract:

Improving the performance of MXenes in storing Li^+ and K^+ has been a focus topic in the energy storage field. Now, a series of quaternary ammonium ions with gradually varied size were used as intercalations to precisely control the layer spacing of $Ti_3C_2T_x$ MXene. The characteristics of storage Li^+ and K^+ were systematically studied and the matching mechanism between interlayer spacing and the size of electrolyte ions were also studied. With the increase of interlayer spacing, the ion diffusion kinetics was improved as well as imbedding ratio of Li^+/K^+ was enhanced. After NH_4^+ intercalated, the interlayer spacing of MXene is enlarged to be 1.18 nm. The capacity in storing Li^+ is 152 mAh g^{-1}, which is 21% higher than the pristine $Ti_3C_2T_x$ (120 mAh g^{-1}). During storage K^+, more K^+ are absorbed in the layers after intercalation, for $(C_2H_5)_4NBr@Ti_3C_2$, the capacitive contribution accounts for 79% at 1 mV s^{-1}. The specific capacity of $(C_2H_5)_4NBr@Ti_3C_2$ is 81 mAh g^{-1} at 0.1 A g^{-1}, which is 35% higher than Ti_3C_2 (60 mAh g^{-1}).

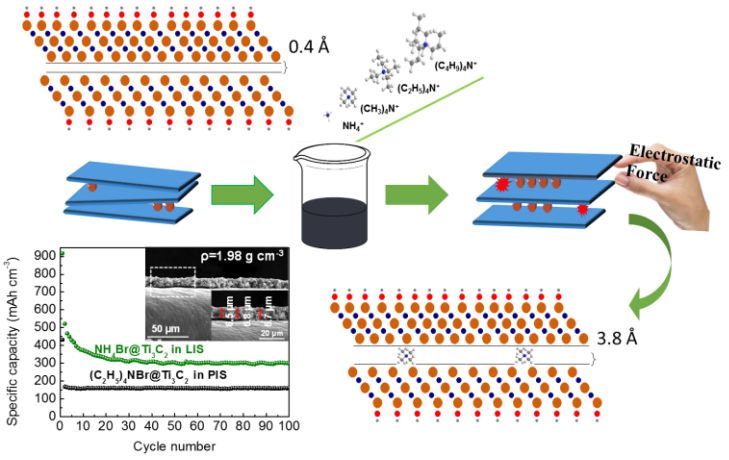

Figure 1. Schematic diagram of intercalation layer

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mp-MXene /TiO_{2-x} NDs with Titanium-based Photo-Fenton Dual reaction centers for Dramatic Enhancement of the Catalytic Efficiency in Advanced Oxidation Processes

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Abstract:

Recent discovery of TiO_2 working as a potential Fenton reaction catalyst by self-doping of low-valence Ti species makes it a promising candidate for photo-Fenton "dual-reaction-center" catalyst alternative to iron-based Fenton regents.[1] In current work, using multi-layered $Ti_3C_2T_x$ [2] as an active Ti source, a porous MXene-TiO_{2-x} composite was developed and served as an efficient photo-Fenton catalyst. Under light irradiation, the catalyst degrades more than 96% of RhB (30mg/L) in 10 min, which is ~14 times faster than commercial P25 with the same [Ti] and H_2O_2 dosage. The excellent performance could arise from the high-concentration $\bullet O_2^-$ generated by a synergetic effect of pseudo-Fenton reaction and photocatalysis according to the analysis results of XPS, EPR and the control experiments.

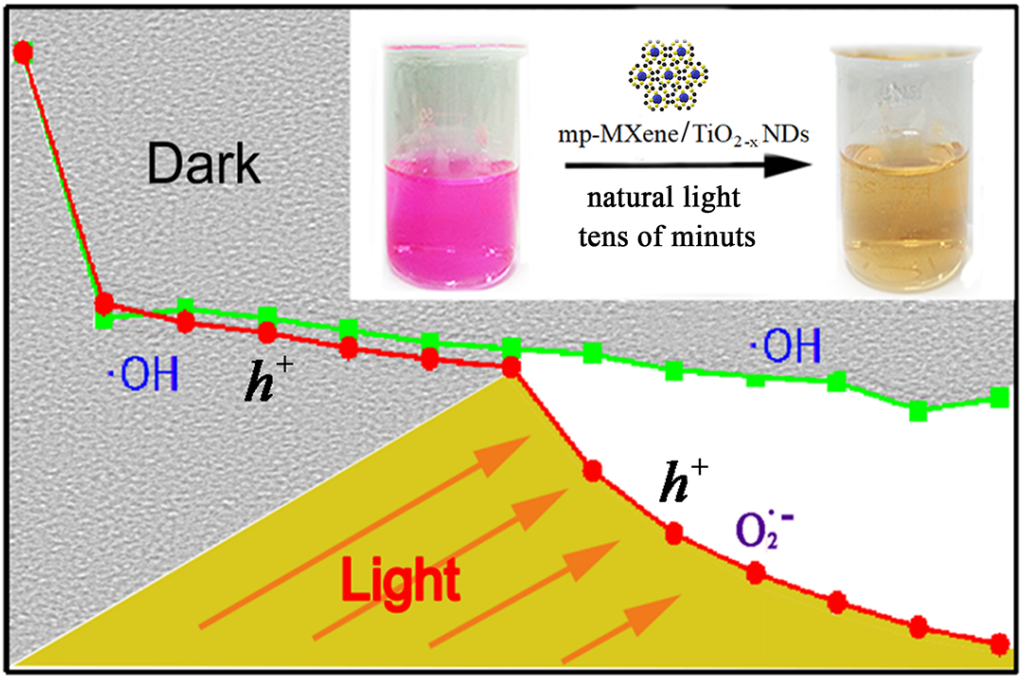

Figure 1 Pseudo-Fenton reaction works synergistically with photocatalysis to greatly accelerate the oxidative degradation rate.

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TiO_xN_y nanoparticles/C composites derived from MXene as anode material for potassium-ion batteries

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Abstract:

Excessive energy consumption has inspired a dramatic development of lithium-ion batteries (LIBs). However, the rare and costly lithium resource have limited its application. To solve this tough situation, attention has been focused on sodium-ion batteries (SIBs), potassium-ion batteries (PIBs) or other metal-ion batteries due to richer resources and low cost[1,2]. Over the years MXene ($Ti_3C_2T_x$) has showed promising properties as anode material for energy storage system. However, a fundamental problem related to $Ti_3C_2T_x$, low theoretical capacity, limits its further development and application. The TiO_2/Ti_3C_2, $NaTi_{1.5}O_{8.3}$ and $K_2Ti_4O_9$ were prepared by oxidation transformation of $Ti_3C_2T_x$, which proved to be a good way for expanding the application of $Ti_3C_2T_x$ and prompted us to develop more derivatives from $Ti_3C_2T_x$[3,4]. Here, titanium oxynitride nanoparticles/carbon composites (TiO_xN_y/C, x+y=1) are successfully prepared from $Ti_3C_2T_x$ MXene and first explored as anode material for potassium-ion batteries. The TiO_xN_y/C nanoparticles are embedded in carbon composites and fabricated a carbon-encapsulated structure, which could prevent the agglomeration of nanoparticles during the cycling process. Due to the carbon-encapsulated structure has great potential in developing high-performance and stable-structure electrodes, the TiO_xN_y/C exhibits an impressive rate performance and ultra-long cycling performance. This work provides a new method for preparing MXene-derived and a promising anode material for potassium-ion batteries.

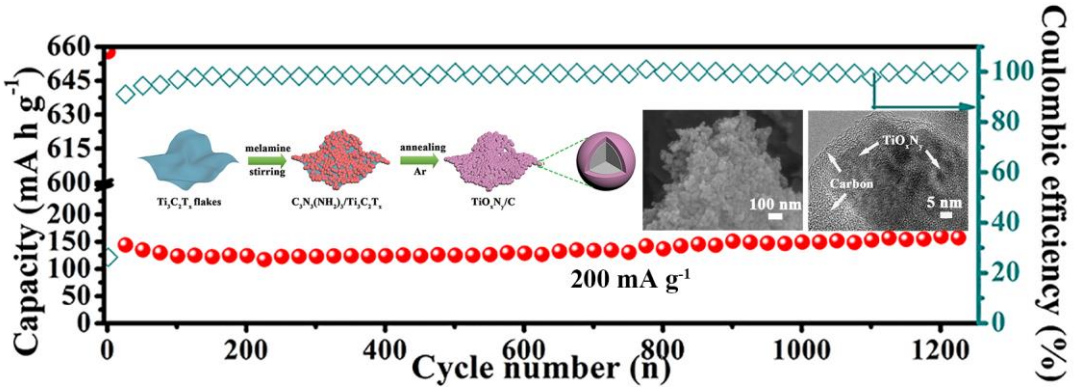

Figure 1 Schematic illustration of the synthesis process and characterization of TiO_xN_y/C.

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Highly fluorescent green emission Ti_3C_2 MXene quantum dots for bio-imaging and copper ion detection

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Abstract:

In this work, N,P-MQDs were successfully synthesized from Ti_3AlC_2 through a facile top-down route by two-step stripping method, including hydrofluoric acid etching and strong acid reflux, followed by a one-step hydrothermal method. The as-prepared N,P-MQDs exhibit green fluorescence with a relative high quantum yield (18.9%), good photostability and relative pH resistance. Endowed with these favorable properties, the as synthesized N,P-MQDs are proved to be good fluorescent tracer material in biological imaging. Moreover, a sensitive and label-free sensing platform was developed for fluorescent measurement of Cu^{2+}, exhibiting a broad application prospect in the field of both biology and environment.

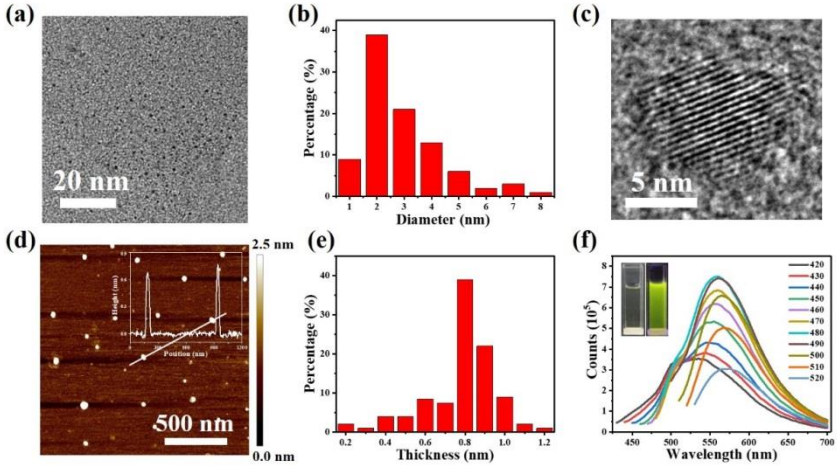

Figure 1. (a) TEM image, (b) Diameter size distribution, (c) HRTEM image, (d) AFM image of the as-synthesized N,P-MQDs. Inset (top-right): height profiles of corresponding line in the AFM image. (e)Thickness distribution of N,P-MQDs. (f) Fluorescence emission spectra of the prepared N,P-MQDs (120 ℃) at different excitation wavelengths. Inset (top-left): photographs under UV light (365 nm).

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Freestanding Highly Conductive $Ti_3C_2T_x$ MXene for Electrochemical Energy Storage

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Abstract:

2D transition metal carbides (MXenes) are promising candidates for electrochemical energy storage due to their unique physical and chemical properties, such as outstanding electrical conductivity, versatile chemistry and high mechanical stability.[1] We have investigated the electrochemical performance of the representative $Ti_3C_2T_x$ MXene in both supercapacitors and batteries. The flexible micro-supercapacitors based on freestanding MXene films show high volumetric capacitance and energy density up to 183 F cm^{-3} and 12.4 mWh cm^{-3}, which is higher than most carbon materials. [2] In addition, utilizing an easy-processing spray coating of $Ti_3C_2T_x$ MXene ink, the paper-based micro-supercapacitor with areal capacitance of 23.4 mF cm^{-2} can be massively fabricated. [3] However, MXene-based supercapacitors show a serious self-discharge behavior, which seriously affected its energy storage properties. To further understand the self-discharge mechanism of $Ti_3C_2T_x$ MXene, we have studied the self-discharge behavior of MXene in both aqueous and ionic electrolytes. On the other hand, through tailoring appropriate surface functionalization and the intrinsic electrical properties, the heteroatom-controlled $Ti_3C_2T_x$ MXene films based lithium-ion batteries show reversible capacities of 221 mAh g^{-1} at a current density of 0.1 C. [4]

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Fabrication, characterization and mechanical properties of MAX phases triggered in-situ TiC and γ′-Ni_3(Al,Ti) synergistically reinforced nickel matrix composite

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Abstract:

A novel type of Ni-based composites was successfully fabricated from pure Ni andTi_2AlC powder mixtures by hot-press sintering technology. The microstructural analysis indicates that the initial reinforcement Ti_2AlC particles transformed into TiC phase, while the additional Al-Ti atoms decomposed from Ti_2AlC diffused into the Ni matrix. The de-intercalated Al-Ti atoms would subsequently react with Ni to give rise to the formation of γ′-Ni3(Al,Ti) precipitates. Detailed interfacial analysis was carried out using high-resolution transmission electron microscopy (HRTEM). Semi-coherent carbide/nickel interface was determined and the orientation relationship between TiC and Ni phases appears to be [001] TiC//[011] FCC Ni and (020) TiC//(111)Ni. Completely coherent relationship between γ′ and γ-Ni was identified. The size and morphology of heterogeneous TiC-γ′ which have critically influenced mechanical properties can be tailored by thermal treatment process. The tailored microstructural features were thus obtained under different fabrication procedures combined with subsequent heat treatments, which also provides the insights about the factors influencing the critical strength in TiC-γ′/Ni composites. The TiC-γ′/Ni composites fabricated under 1200 oC with subsequent solution and aging treatments exhibited tensile strength of ~1300 MPa with ~6.2% ductility. The superior combination of strength and ductility can be attributed to the more homogenous distribution and location of ultrafine TiC (100-700 nm) and γ′ (50 nm) nanoparticles in the Ni matrix, which played a synergistic effect on determining the enhanced mechanical behaviors.

SnO_2-Ti_3C_2 MXene electron transport layers for perovskite solar cells

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Abstract:

MXenes, a class of two-dimensional (2D) transition metal carbides and nitrides, have a wide range of potential applications due to their unique electronic, optical, plasmonic, and other properties. Herein, we explore the use of Ti_3C_2 MXene in organic-inorganic lead halide perovskite solar cells (PSCs) due to its metallic conductivity. SnO_2-Ti_3C_2 MXene nanocomposites with different contents of Ti_3C_2 (0, 0.5, 1.0, 2.0, 2.5 wt.‰) were used as electron transport layers (ETLs) in low-temperature processed planar-structured PSCs. Mixing SnO_2 with 1.0 wt.‰ Ti_3C_2 effectively increases the power conversion efficiency (PCE) from 17.23% to 18.34%, whereas the device prepared with pristine Ti_3C_2 as the ETL achieves a PCE of 5.28%. Photoluminescence and electrochemical impedance spectroscopy results reveal that the metallic Ti_3C_2 MXene nanosheets provide superior charge transfer paths, enhancing electron extraction, electron mobility, and decreasing the electron transfer resistance at the ETL/perovskite interface, and thus leading to higher photocurrents. This work proposes a new field of application for MXenes and a promising method to increasing efficiency of solar cells.

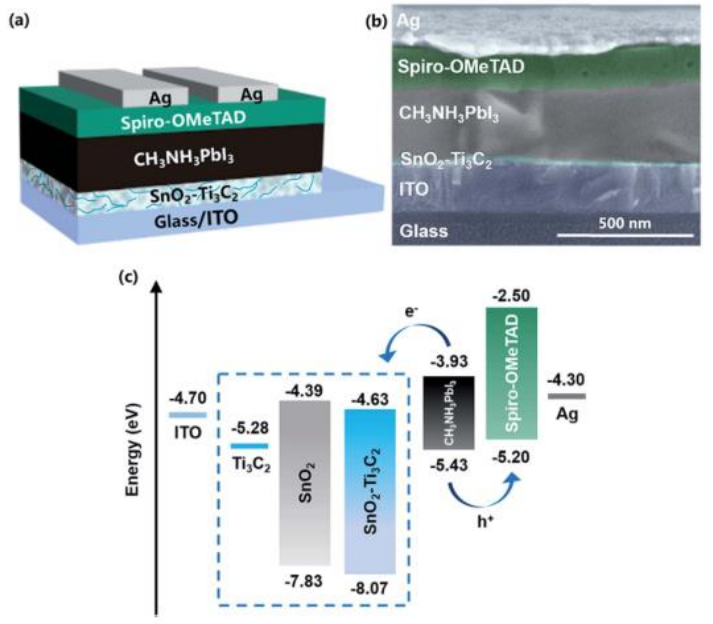

Fig. 1 (a) Device architecture of ITO/ETL/$CH_3NH_3PbI_3$/Spiro-OMeTAD/Ag based on representative SnO_2–Ti_3C_2 as the ETL, (b) cross-sectional SEM image of the PSC device, and (c) schematic energy-level diagram of each layer.

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Macroporous Three-Dimensional MXene Architectures for Highly Efficient Solar Steam Generation

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Abstract:

Efficient utilization of abundant solar energy for steam generation is an attractive, renewable, and environment-friendly technology for seawater desalination and wastewater purification, enabling solutions to address the global long-standing water scarcity issues. However, the low energy efficiency, high cost and complex systems with multiple components of state-of-the-art technologies hindered their practical applications. Herein, we report the first example of three-dimensional (3D) MXene architectures (3DMAs)-based solar steam generators via a facile two-step dip coating process without any annealing or high temperature carbonization. The 3DMAs prepared by a cost-effective, scalable, simple fabrication method, show effective broadband solar absorption (~98%) and excellent solar thermal conversion ability based on 2D to 3D morphological transformation of MXene, making good use of intrinsic theoretical photothermal performance of MXene. The particularly hydrophilic nature of MXene and macroporous structure of melamine foam endow the 3DMAs continuous water supply owing to its strong capillary effect. As a result, the 3DMAs achieve water evaporation rates of 1.41 and 7.49 kg m^{-2} h^{-1} under the solar illumination of 1 sun and 5 sun with a superb solar steam efficiency up to 88.7% and 94.2%, respectively. This scalable 3DMA can be used to produce clean water from both seawater and wastewater with rejections close to 100% for organic dyes and metal ions. This work creates a platform to develop novel composite materials for solar-driven seawater desalination and wastewater purification via, opening a new window for the utilization of MXene as photothermal agent in practical applications.

Fabrication of tunable hierarchical MXene@AuNPs nanocomposites constructed by self-reduction reactions with enhanced catalytic performances

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Abstract:

MXene, a new type of two-dimensional layered transition metal carbide material differing from graphene, demonstrates intriguing chemical/physical properties and wide applications in recent years. Here, the preparation of the self-assembled MXene-gold nanoparticles (MXene@AuNPs) nanocomposites with tunable sizes is reported. The nanocomposites are obtained via the self-reduction reactions of MXene material in a HAuCl4 solution at room temperature. The sizes of the Au particles can be well-controlled by regulating the self-reduction reaction time. They can greatly influence the catalytic behaviors of the MXene@AuNPs composites. MXene@AuNPs composites with optimized reduction time show high catalytic performances and good cycle stability for model catalytic reactions of nitro-compounds, such as 2-nitrophenol and 4-nitrophenol. This work demonstrates a new approach for the preparation of tunable MXenebased self-assembled composites.

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Modulating the Schottky barriers in MoS_2/MXenes heterostructures via surface functionalization and electric field

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Abstract:

Controlling the Schottky barriers (SB) in semiconductor/metal heterostructures is greatly vital to improve the performance of field effect transistors. Yet the modulation mechanisms have not been well understood. In this work, on the basis of first-principles calculations, we have demonstrated that both surface functionalization and external electric fields (E_{ext}) play significant roles in modulating the contact types (n-type or p-type) and SB heights at the interface by using the contact between MoS_2 and Nb_2C-based MXenes as a case study. The results show that weak van der Waals (vdW) interactions dominate between the interlayer. Importantly, the n-type SB-free contact is available in OH-terminated Nb_2C/MoS_2 heterostructure and continuously controllable p-type SB is found in the MoS_2/Nb_2CO_2 and MoS_2/Nb_2CF_2 heterostructures under proper vertical E_{ext} strength. We unraveled that the modulation of Schottky barrier originates from the tunable metal work function induced by functionalized termination and the variable interface potential step induced by external electric field. Our work provides important clues for contact engineering and improvement of the MoS_2 device performance.

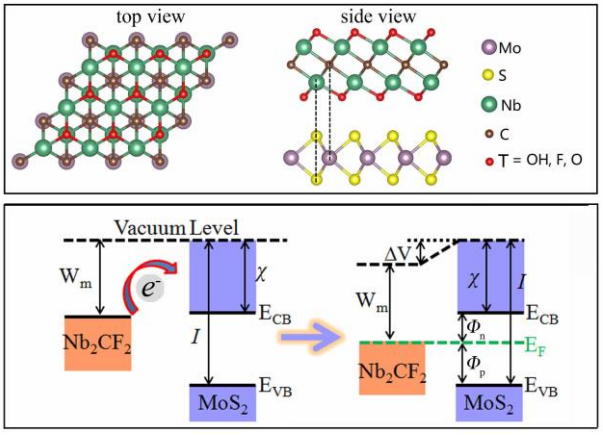

Figure 1. The modulation of Schottky barrier originates from the tunable metal work function and the variable interface potential step.

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Freeze-Dried 3D MXene/MWCNT Aerogel for Impressive Supercapacitor

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Abstract:

Three-dimensional MXene/carbon nanotube (MX-CNTs) aerogels have attracted much consideration due to their unique properties, such as highly porous structure, high specific surface areas, lightweight solid and low density. These properties make them a special choice for various applications including energy storage, catalysis conversion, sensing, selective adsorption and separation, and biomedical engineering. In this study, 3D MX-CNTs aerogel was fabricated using vacuum freeze-drying process. Internal structure feature and morphology analysis were characterized by X-ray diffraction (XRD) and field emission scanning electron microscope (FE-SEM), and electrochemical performances on the supercapacitor were measured by cyclic voltammetry (CV), constant current charge and discharge, alternating-current impedance test on. The main results show that the carbon nanotubes into the MXene-based aerogel can prevent the restack of MXene (Ti_3C_2) nanosheets due to van der Waals forces, and lead to three-dimensional interconnected porous structure with large specific surface area and excellent compression recovery performance. It also demonstrates potential electrode applications in porous and flexible supercapacitor with impressive electrochemical performance.

References:

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[2] X. Q. Xie, K. J. Kretschmer, B. Anasori, B. Sun, G.X. Wang, Y. Gogotsi. ACS NANO Materials. 2018, 1, 505-511

An ultrafast conducting polymer@MXene positive electrode with high volumetric capacitance for advanced asymmetric supercapacitors

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Abstract:

Pseudosupercapacitors that synergize the merits of batteries and double-layer capacitors are one of the most promising candidates for high-energy and high-power energy storage applications. 2D transition metal carbides (MXenes), an emerging family of pseudocapacitive materials with ultrahigh rate capability and volumetric capacitance, have attracted extensive research interest in recent years. However, MXenes can only be used as negative electrodes as they are easily oxidized at low positive anodic potential. To construct a high-performance MXene-based asymmetric device, a positive electrode with compatible performance is highly desired. Herein, we report an ultrafast polyaniline@MXene cathode prepared by casting a homogenous polyaniline layer on 3D porous $Ti_3C_2T_x$ MXene. This rational design pushed the stable anodic working potential window of MXene to 0.55 V vs. Ag/AgCl in aqueous electrolyte and enabled the resultant flexible polyaniline@MXene positive electrode a high volumetric capacitance of 1632 F cm^{-3} at 10 mV s^{-1} and an ultrahigh rate capability with 827 F cm^{-3} at 5000 mV s^{-1}, which surpassed almost all reported positive electrodes. An asymmetric device was further fabricated with MXene as anode and polyaniline@MXene as cathode, which showed high energy density of 50.6 Wh L^{-1} at 1.7 kW L^{-1} and 24.4 Wh L^{-1} at an ultrahigh power density of 127 kW L^{-1}.

Macroporous Three-Dimensional MXene Architectures for Highly Efficient Solar Steam Generation

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Abstract:

Efficient utilization of abundant solar energy for steam generation is an attractive, renewable, and environment-friendly technology for seawater desalination and wastewater purification, enabling solutions to address the global long-standing water scarcity issues. However, the low energy efficiency, high cost and complex systems with multiple components of state-of-the-art technologies hindered their practical applications. Herein, we report the first example of three-dimensional (3D) MXene architectures (3DMAs)-based solar steam generators via a facile two-step dip coating process without any annealing or high temperature carbonization. The 3DMAs prepared by a cost-effective, scalable, simple fabrication method, show effective broadband solar absorption (~98%) and excellent solar thermal conversion ability based on 2D to 3D morphological transformation of MXene, making good use of intrinsic theoretical photothermal performance of MXene. The particularly hydrophilic nature of MXene and macroporous structure of melamine foam endow the 3DMAs continuous water supply owing to its strong capillary effect. As a result, the 3DMAs achieve water evaporation rates of 1.41 and 7.49 kg m^{-2} h^{-1} under the solar illumination of 1 sun and 5 sun with a superb solar steam efficiency up to 88.7% and 94.2%, respectively. This scalable 3DMA can be used to produce clean water from both seawater and wastewater with rejections close to 100% for organic dyes and metal ions. This work creates a platform to develop novel composite materials for solar-driven seawater desalination and wastewater purification via, opening a new window for the utilization of MXene as photothermal agent in practical applications.

MXene-Based All-Solid-State Electrochemical Actuators

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Abstract:

Natural muscles which have powerful output capabilities can perform complex movements such as stretching, bending and twisting. People have been trying to imitate the movement of natural muscles and developing artificial muscles which are comparable to natural muscles. Compared with other materials (such as metals and ceramic materials), polymer artificial muscle materials have the advantages of low density, small volume, large deformation, and easy processing. Specially, due to the fast response speed and low driving voltage, the ionic electro-actuator has received extensive interest. Moreover, the electrode material has a critical impact on the actuation performance for ionic electro-actuators. In particular, the electrochemical properties of the electrode material have an extremely significant effect on the actuation performance. However, the traditional metal electrode materials are easily broken during the deformation.[1] After discovering the new two-dimensional material MXenes in 2011, many studies have reported that MXene has excellent electrochemical properties.[2] Therefore, the MXene is selected as the electrode material of actuators to study its actuation performance.

Preparation of electrode layers: The MXene was synthesized by the minimally intensive layer delamination (MILD) method as previously reported.[3] Then MXene films were obtained by vacuum filtration.

Preparation of the electrolyte layer: Polyvinyl alcohol (PVA) was added to the sulfuric acid solution (H_2SO_4) and dissolved at high temperature under continuously stirring to obtain a uniform transparent solution. Then the electrolyte layer was prepared by a solution casting method of H_2SO_4-PVA solution.

Assembly of the sandwiched actuators: The H_2SO_4-PVA film was peeled off from the mold and laminated by two as-prepared electrode films. Then the sandwiched films were assembled by a hot-pressing machine. Furthermore, the assembled films were aged at room temperature and cut into strips with a size of 5×20 mm^2 for the actuation performance tests.

Figure 1 is the actuation performance tests of the actuator. A typical electrochemical actuator consists of a sandwich structure which is composed of one ion-conductive electrolyte membrane laminated by two electron-conductive electrode membranes. When an alternating voltage is applied, the actuator can bend back and forth due to the electrode expansion and contraction induced by ion motion. The actuation performance tests of actuators are under a 0.3 V, 0.05 Hz square wave voltage. Under this square voltage, the peak-to-peak displacement of the MXene electrode based actuators is 0.68 mm.

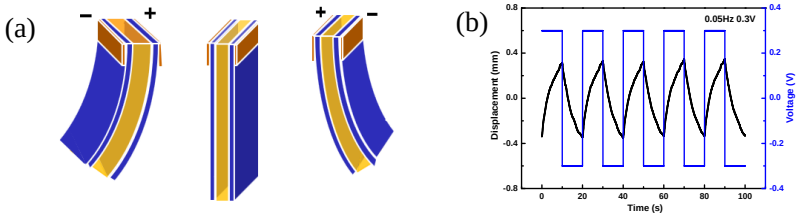

Figure 1. The actuation performance tests of the actuator: (a) the schematic diagram of actuators, (b) cyclic bending curves of actuators under a 0.3 V, 0.05 Hz square wave voltage.

References:

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Element Replacement Approach by Reaction with Lewis Acidic Molten Salts to Synthesize Nanolaminated MAX Phases and MXenes

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Abstract:

Nanolaminated materials are important because of their exceptional properties and wide range of applications. Here, we demonstrate a general approach to synthesize a series of Zn-based MAX phases and Cl-terminated MXenes originating from the replacement reaction between the MAX phase and the late transition metal halides. The approach is a top-down route that enables the late transitional element atom (Zn in the present case) to occupy the A site in the pre-existing MAX phase structure. Using this replacement reaction between Zn element from molten $ZnCl_2$ and Al element in MAX phase precursors (Ti_3AlC_2, Ti_2AlC, Ti_2AlN, and V_2AlC), novel MAX phases Ti_3ZnC_2, Ti_2ZnC, Ti_2ZnN, and V_2ZnC were synthesized. When employing excess $ZnCl_2$, Cl terminated MXenes (such as $Ti_3C_2Cl_2$ and Ti_2CCl_2) were derived by a subsequent exfoliation of Ti_3ZnC_2 and Ti_2ZnC due to the strong Lewis acidity of molten $ZnCl_2$. These results indicate that A-site element replacement in traditional MAX phases by late transition metal halides opens the door to explore MAX phases that are not thermodynamically stable at high temperature and would be difficult to synthesize through the commonly employed powder metallurgy approach. In addition, this is the first time that exclusively Cl-terminated MXenes were obtained, and the etching effect of Lewis acid in molten salts provides a green and viable route to prepare MXenes through an HF-free chemical approach.

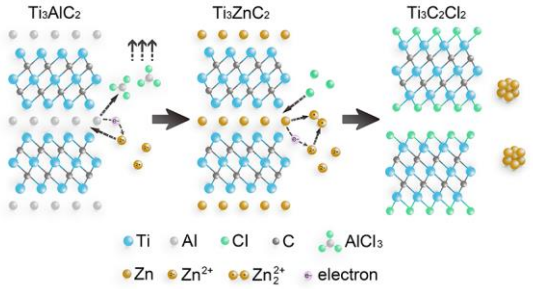

Figure 1. A schematic showing the phase evolution from Ti_3AlC_2 to Ti_3ZnC_2 to $Ti_3C_2Cl_2$.

References:

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Single-layer V_2C MXene Nanosheets for Thermoelectrocatalytic Hydrogen Evolution

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Abstract:

Electrocatalytic water splitting is considered as a promising technology to produce clean and renewable hydrogen fuel; however, the sluggish reaction kinetics impede the overall energy conversion efficiency, making it fail to meet the requirement for practical applications[1,2]. MXene is a two-dimensional material that possesses both electrocatalytic activity and photothermal conversion property[3-5], which inspires us to integrate thermal energy with electrocatalysis to enhance the performance. In this work, a solar-driven "thermoelectrocatalytic" water splitting is demonstrated, where thermionic energy harvested from solar irradiance conversion is introduced into the electrocatalytic system. The exfoliated single-layer V_2C MXene nanosheets with the light absorption in the range of 400-1200 nm are chosen as the electrocatalyst. We find that the temperature of V_2C@nickel foam electrode immersed in water increases by 10.5 ^oC under simulated sunlight illumination for 30 min, resulting in a significant decrease of HER overpotential from 231 to 181 mV. Furthermore, the relationship between the light-to-heat conversion and electrocatalytic behavior is established. The development of thermoelectrocatalytic water splitting technology for efficient hydrogen generation will bring about new insights into prospective thermoelectric, thermophotovoltaic and catalytic fields.

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Hydrous RuO_2 decorated MXene Coordinating with Silver Nanowire Inks Enabling Fully-Printed Micro-Supercapacitors with Extraordinary Volumetric Performance

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Abstract:

The fabrication of fully-printable, flexible micro-supercapacitors (MSCs) with micron-scale electrode resolution simultaneously possessing high energy and power density remains a significant technological hurdle to date. In part to overcome this grand challenge, the 2D material MXene has garnered significant attention for its application, amongst others, as a printable electrode material for high performing electrochemical energy storage devices. Herein, a facile and in-situ process is proposed to homogeneously anchor hydrous ruthenium oxide ($RuO_2 \cdot xH_2O$) nanoparticles on $Ti_3C_2T_x$ MXene nanosheets. The resulting RuO_2@MXene nanosheets can associate with silver nanowires (AgNWs) to ultimately serve as a printable electrode with micron-scale resolution for high performing, fully-printed MSCs. Due to the amalgamation of properties and the synergistic effects stemming from the individual constituents, the flexible MSCs demonstrated high printing resolution, high electrochemical performance with regard to volumetric capacitance, and energy and power density, excellent cycling stability, and durable and robust mechanical properties.

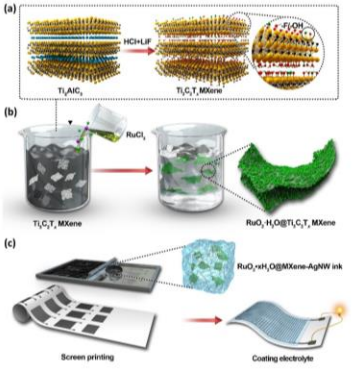

Figure 1. Schematic illustration of the fabrication process.

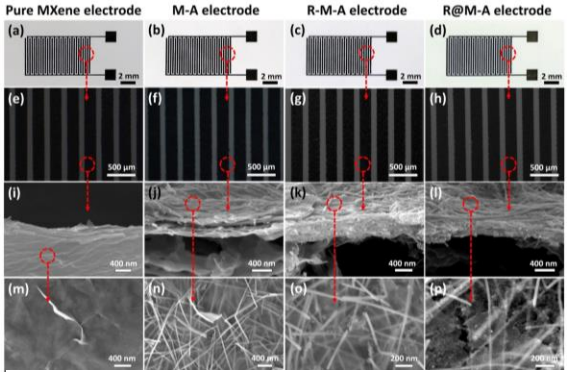

Figure 2. Optical images and optical microscopy images of screen-printed MSCs.

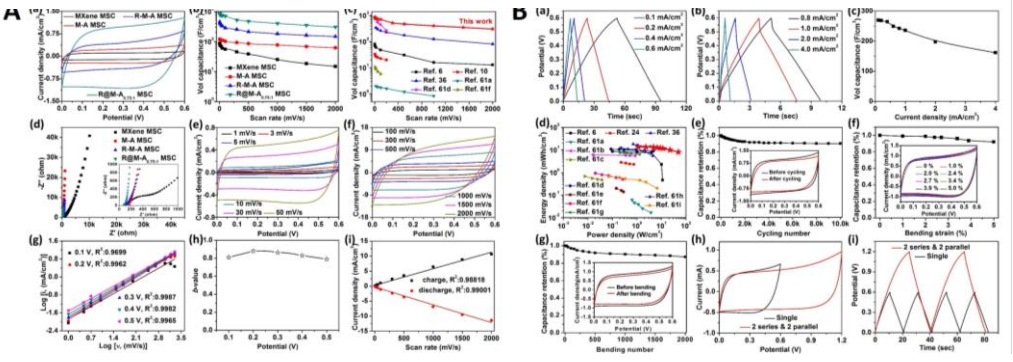

Figure 3. Electrochemical performance of the screen-printed MSCs.

References:

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MXene@MoS_2 composites for high-perfornce lithium-ion capacitors

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Abstract:

Since MXenes is a type of novel two-dimensional material with excellent metallic conductivity, hydrophilic surfaces and mechanical stability, it has a wide range of applications in supercapacitors (SC), lithium-ion batteries (LIB), and lithium-ion capacitors (LIC). To further improve electrochemical properties of the energy storage devices, some of strategies such as intercalating, compositing, doping, assembling can be employed. Lithium-ion capacitor (LIC), which combine the advantages of LIB and SC into one device, do not sacrifice much energy density while maintaining the high-power density. However, the unbalanced ion kinetics between the faradaic anode and the capacitive cathode in LICs usually lead to a poor rate capability and low cycling stability. Herein, we synthesized the single-layer $Ti_3C_2T_x/MoS_2$ composite anode by a facile one-step hydrothermal method. The MoS_2 improves the ionic accessibility of $Ti_3C_2T_x$ layers through increasing the interlayer space and enhance its specific capacity. When tested as anode material for a coin cell at a voltage range of 0.01-3V (vs Li/Li^+), it exhibited a high initial capacity of 1111 mAh/g and 708 mAh/g capacity retention after rate capability test. The electrode presents a high rate performance as well as a reversible capacity of 144 mAh/g at 2 A/g. These results show that the $Ti_3C_2T_x/MoS_2$ composite can be a promising candidate for using in high-performance lithium-ion capacitor.

References:

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Fabrication of femtosecond laser induced subwavelength nanogratings on the MXene ($Ti_3C_2T_x$) film

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Abstract:

Laser induced periodic surface structures (LIPSSs) holds great promise as multi-functionalized surface element for increasing demand of miniaturized electronic devices. Herein, this study firstly experimentally demonstrates the fabrication of subwavelength nanogratings for the MXene film with the different polarization direction and pulses number of incident laser in air condition. The results reveal the formation of laser parameters dependent subwavelength nanogratings (Λ=100-200nm) on the surface of the MXene sheet. Firstly, the direction of surface subwavelength nanaogratings is influenced by the incident laser polarization, via changing the laser polarization, the direction of surface nanograting also appears relevant different. In addition, with the increase of incident pulses number, the depth of subwavelength nanogratings starts to deepen, when the incident pulses number come to 500 under the fluence of 100mJ cm^{-2}, it is apparent that much ablation zone covers on the irradiated surface. Owing to the MXene sheet consists of a large number of micro-sheets (~1-2μm), micro-nano heterostructure also can be found under femtosecond laser irradiation with 100mJ cm^{-2} and 20 pulses number. This research provides a new thought for the optoelectronic devices application of MXene ($Ti_3C_2T_x$).

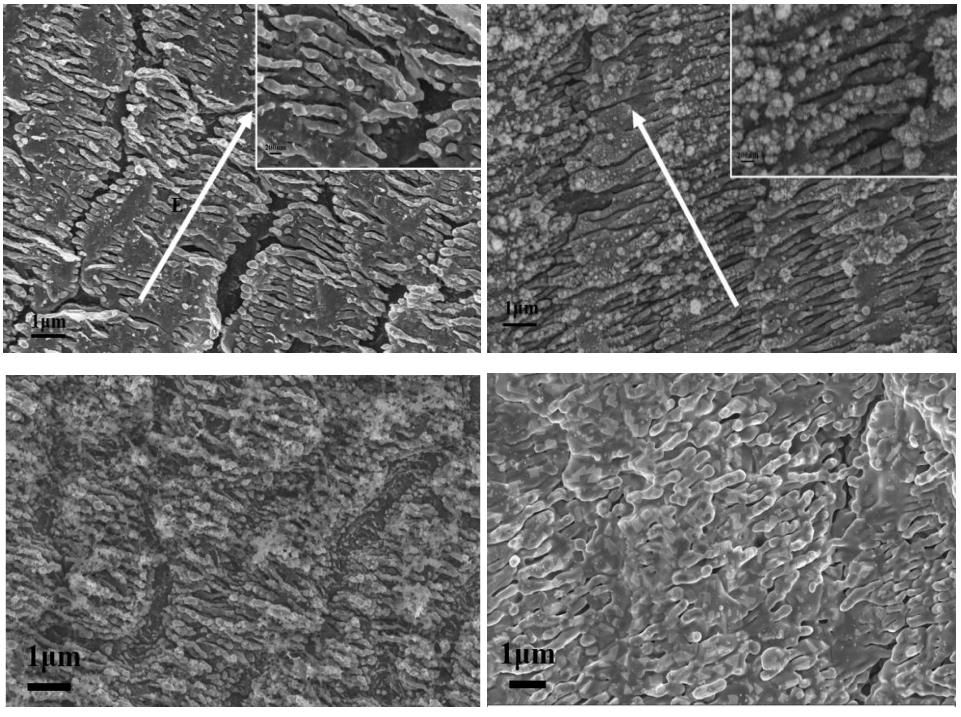

Figure 1. (a) and (b) surface morphology of laser induced subwavelength nanogratings under the laser irradiation with the polarization direction of 60 degrees and 120 degrees. (c) and (d) surface microstructures of laser irradiation with 5 pulses and 500pulses.

References:

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Rationally designing S/$Ti_3C_2T_x$ as cathode material with an interlayer for high-rate and long-cycle lithium-sulfur batteries

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Abstract:

Lithium-sulfur batteries suffer from poor cycling stability and inferior rate capability, mainly caused by the low conductivity and lithium polysulfides dissolution. To tackle these problems, this work demonstrates that $Ti_3C_2T_x$ "clay", synthesized by selectively extracting the Al layers from the Ti_3AlC_2 phases with a mixture of HCl and LiF, is an effective host material for sulfur cathodes. To further enhance the rate performance and cycling stability of S/$Ti_3C_2T_x$ composites, a single-walled carbon nanotube thin film was prepared by a simply vacuum filtration method and inserted between the cathode and the separator as an interlayer for Li-S batteries. The S/$Ti_3C_2T_x$ composite with an interlayer could deliver a high initial discharge capacity of 1458 mAh g^{-1} at a current density of 0.1 A g^{-1} and an ultralow capacity decay of 0.04% per cycle at 0.8 A g^{-1} for over 1500 cycles was achieved. And more importantly, a reversible capacity of 608 mAh g^{-1} was obtained at a high current density of 8.2 A g^{-1} (≈5C), demonstrating a superior rate capability. These results suggest that the S/$Ti_3C_2T_x$ composite is a promising sulfur cathode material and the introduction of the interlayer will pave the way for future development and design of the high-rate with long-cycle Li-S batteries.

Bioinspired Ultrasensitive and Stretchable MXene-based Strain Sensor via Nacre-Mimetic Microscale "Brick-and-Mortar" Architecture

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Abstract:

The development of wearable strain sensors with simultaneous large stretchability (strain >55%) and high sensitivity (gauge factor >100) remains a grand challenge to this day. Herein, we demonstrate that strain sensors based on this nacre-mimetic microscale "brick-and-mortar" architecture can simultaneously achieve ultrahigh sensitivity and large stretchability, while performing well in linearity, reliability, long-term durability, and monotonicity.

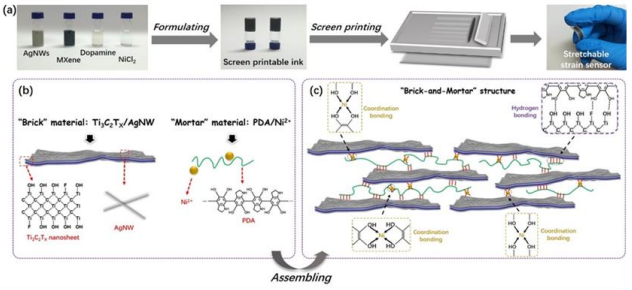

Figure 1. (a) Schematic of the fabrication process for the bioinspired sensor. (b) Schematic illustration of the structures for the "brick" materials ($Ti_3C_2T_x$ and AgNWs) and "mortar" material (PDA/Ni^{2+}). (c) Schematic illustration of the sensor based on the "brick-and-mortar" architecture. Interfacial interactions between $Ti_3C_2T_x$-AgNW and PDA/Ni^{2+} including hydrogen and coordination bonding.

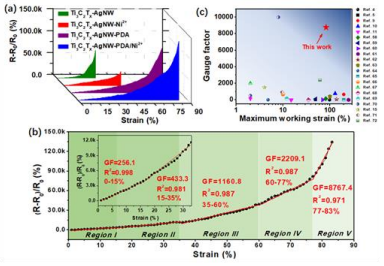

Figure 2. (a) The GF and linear behavior of different sensors. (b) Detailed gauge factor and linear behavior of the strain sensor. (c) Gauge factor as a function of maximum working range of the present $Ti_3C_2T_x$-AgNW-PDA/Ni^{2+} sensor, and various recently reported strain sensors.

The MXene-based strain sensors were fabricated by directly screen-printing the nanocomposite gel onto stretchable polyurethane substrate. The bioinspired sensor demonstrated a gauge factor >200 over a range of working strains up to 83%, and achieved a high gauge factor exceeding 8700 in the strain region of 76-83%.

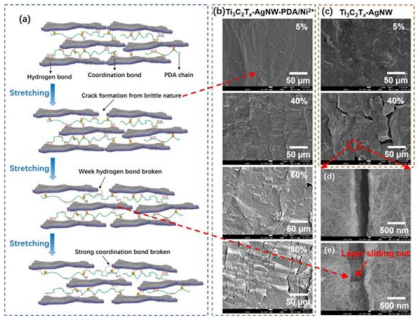

Figure 3. (a) Schematic illustration of the sensing mechanism of the $Ti_3C_2T_x$-AgNW-PDA/Ni^{2+}strain sensor. (b) Surface SEM images of the (b) $Ti_3C_2T_x$-AgNW-PDA/Ni^{2+} and (c) $Ti_3C_2T_x$-AgNW strain sensors under specific applied strains. Magnified SEM images showing the cracks generated in the (d) $Ti_3C_2T_x$-AgNW and (e) $Ti_3C_2T_x$-AgNW-PDA/Ni^{2+} strain sensors under 40% strain.

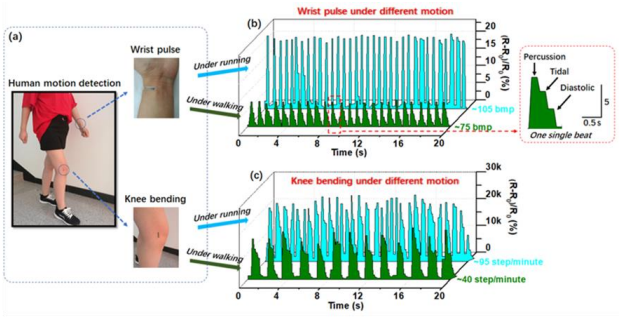

Figure 4. Monitoring human body under different motion states using the sensors. (a) Photographs of wearable strain sensors attached to a human wrist for pulse monitoring, and to a knee-joint for knee bending detection. (b) Relative resistance variation of a wrist pulse while a subject is walking and running. (c) Relative resistance changes of knee bending while walking and running.

This successful combination of high sensitivity and large stretchability is attributed to the microscale hierarchical architecture and the synergistic toughing effects from interfacial interactions of hydrogen and coordination bonding, layer slippage, and molecular chain stretching. Moreover, this bioinspired strain sensor is employed to monitor human activities under different motion states to demonstrate its feasibility for wearable, full-spectrum, human health and motion monitoring systems.

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Scalable MXene based micro-supercapacitor for on-chip energy storage

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Abstract:

The rapid progress of portable electronic devices urgently requires power sources to develop toward miniaturization, high performance and high integration density. [1] Micro-supercapacitors are ideal power sources for applications such as portable personal electronics, microsensors, and nanorobots. [2] Furthermore, $Ti_3C_2T_x$ MXene is consider as the most potential candidate for energy storage due to its high electrical conductivity and electrochemical performance. [3] Herein, a silicon-based on-chip micro-supercapacitor based on $Ti_3C_2T_x$ MXene is first reported. The $Ti_3C_2T_x$ electrodes are prepared through spin coating and laser cutting, which can be easily to manufacture on a large scale. While the thickness of $Ti_3C_2T_x$ MXene increased to about 264 nm, the device exhibits high areal and volumetric capacitance of 471 μF cm^{-2} and 17.8 F cm^{-3}, respectively. And the micro-supercapacitor can deliver an energy density of 0.89 mWh cm^{-3} at a power density of 12 mW cm^{-3}, with a high specific capacitance retention rate of 94.6% even after 8000 cycles.

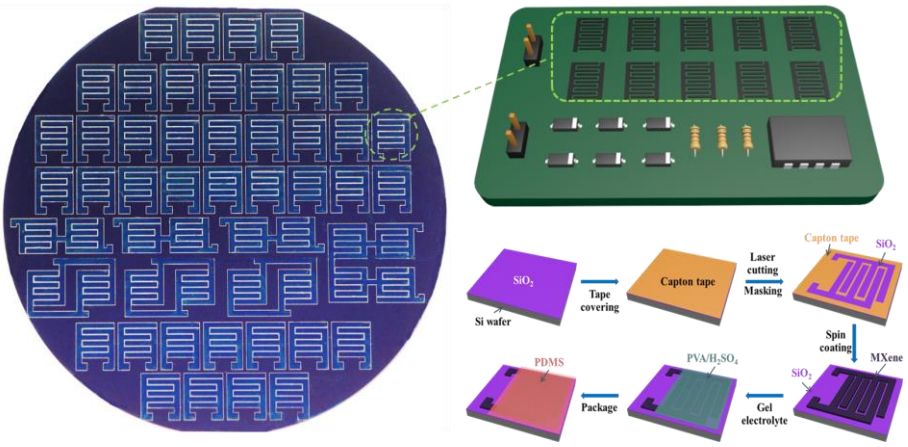

Figure 1. Preparation of scalable MXene based micro-supercapacitors

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The capacitance performance of Ti_3CN MXene is optimized by adjusting the duration of etching

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Abstract:

The quaternary nitrogen-containing MXenes is attracting more and more attention with the dramatic increases of application and research about ternary carbon-containing MXenes (e.g. Ti_3C_2 MXenes). However, research on Ti_3CN as a supercapacitor material is rarely reported due to the corresponding heterostructure resulted from nitrogen atom doping, and the corresponding heterostructure gift unique electronic, magnetic and optical properties. Herein, we report that adjusting the duration of etching can regulate the relative amount of Ti, C and N elements as well as increase the number of vacancy defects appropriately. Finally, we obtained the Ti_3CN (MXene) films with excellent electrical conductivity, 0.8 Ω, mass capacitance of 377 F/g (the current density is 0.5 A/g) under the synergistic coupling effect of surface termination groups (such as O2–、OH–、F–), and we effectively controlled thickness of films ranging from 6-8 μm performed as excellently flexible MSCs owing to their self-functionalized surfaces. Amazingly, the variation of capacitance and resistance is consistent with the relative nitrogen content in Ti_3CN (MXene) films, and the appropriate vacancy defects is beneficial to improve the capacitance, because more resultant channels are used for ion shuttling.

Three-dimensional porous MXene/polyaniline composite prepared by one-step co-electrodeposition method for high-performance capacitance

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Abstract:

Two-dimensional (2D) MXenes have attracted intense researching interesting for electrochemical energy storage because of their excellent electronic properties [1-3]. In this work, we described a facile and effective method to fabricate three-dimensional (3D) porous MXene/polyaniline (MXene/PANI) composite film electrodes through one-step co-electrodeposition method. In this process, the 2D $Ti_3C_2T_x$-MXene nanosheets acted as core polymerization due to the functional groups (such as –F, –OH, or –O) on their surface, and the aniline monomer radical cations would gradually polymerize on surface and layer space of the 2D MXene nanosheets to form three-dimensional (3D) porous MXene/PANI composite films (Figure 1). Benefiting from the superior electrical conductivity 2D MXene nanosheets and 3D porous structure composite facilitates electron transfer and ionic diffusion, the MXene/PANI composite film electrodes exhibited outstanding electrochemical performance with a high gravimetric capacitance of 417 $F \cdot g^{-1}$ at scan rate of 10 $mV \cdot s^{-1}$ in three-electrode system. When the scan rate increased 200 $mV \cdot s^{-1}$, the MXene/PANI composite film electrodes also demonstrated high specific capacitance (216.8 $F \cdot g^{-1}$). Moreover, after 2000 times of cycling tests at a scan rate of 20 $mV \cdot s^{-1}$, the MXene/PANI composite film electrodes showed excellent reliability and good cycling stability (approximately 83.4 % retention after 2000 cycles, at 1 $A \cdot g^{-1}$).

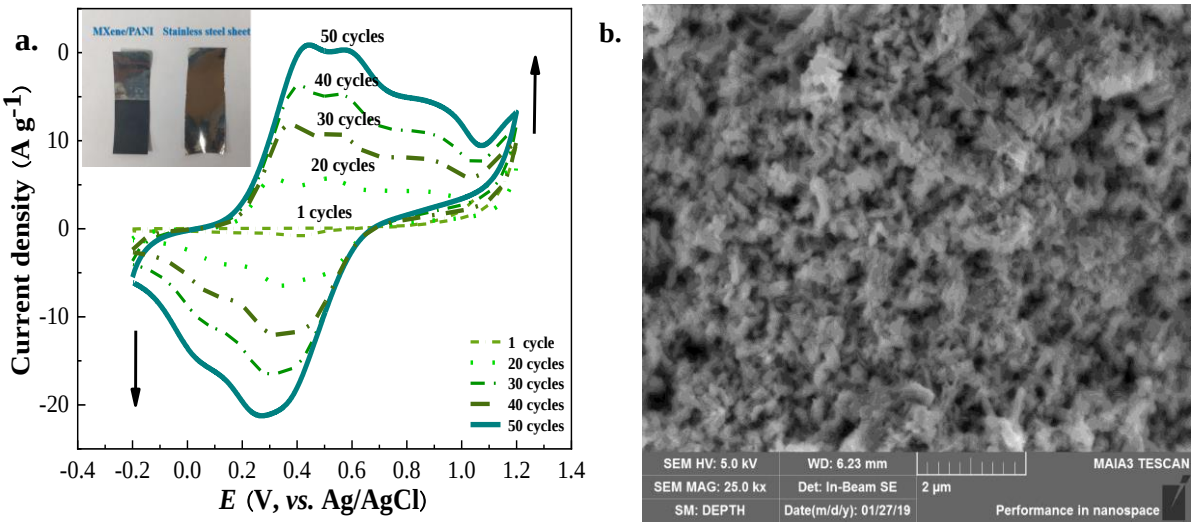

Figure 1. a. Cyclic voltammograms of depositing of the 3D MXene/PANI composite film electrodes, at scan rate of 50 $mV \cdot s^{-1}$, the voltage range is 0.2 V ~ 1.2 V; **b.** SEM image of 3D MXene/PANI composite film.

References:

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Lightweight, High Strength ANF/MXene Composite Film with Superior Electromagnetic Interference Shielding Performance

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Abstract:

For the essential role of controlling or mitigating electromagnetic wave in electronic systems for a variety of civil and military applications, extensive efforts have been historically devoted to developing high-performance electromagnetic interference (EMI) shielding materials.[1,2] However, the large thickness and poor mechanical properties of the traditional EMI shielding materials have limited the practical applications. Herein, we have chosen the emerging 2D material MXene with high conductivity and aramid nanofibers (ANF) with high mechanical strength to prepare lightweight and high strength ANF/MXene composite film.

MXene solution was dispersed in deionized water, and the ANF solution was mixed with water and stirred to homogenous dispersion. Then the MXene suspension was mixed with ANF solution, the mixed solution was filtrated by a PTFE membrane, as shown in **Figure 1**. Furthermore, the obtained ANF/MXene composite films was immersing in water for 24 h to remove the KOH.

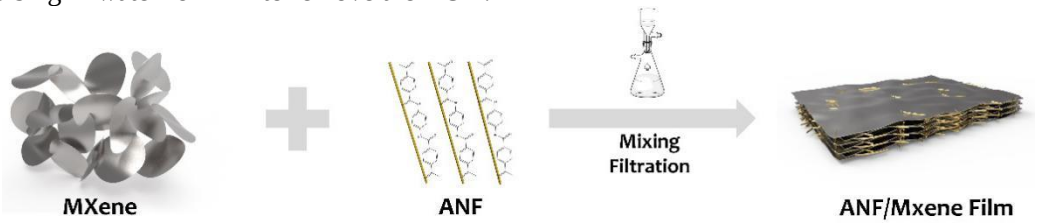

Figure 1. Illustration of the preparation process of the ANF/MXene composite film through filtration.

As shown in **Figure 2**a, this composite film with a thickness of several micrometres displayed a shielding effectiveness as high as 35 dB, and the EMI effectiveness would increase with the MXene contents. In addition, the ANF/MXene composite film exhibits a mechanical strength above 200 MPa, as shown in Figure 2b. Figure 2c shows the probably microwave shielding mechanism of the composite film.

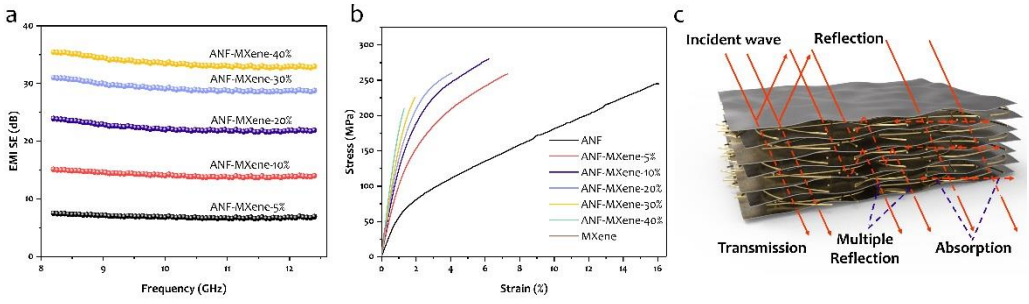

Figure 2. (a) EMI SE of ANF/MXene composite film with different MXene contents. (b) Tensile stress-strain curve of ANF/MXene composite film with different MXene contents. (c) Schematic illustration for the explanation of the EMI shielding of ANF/MXene composite film.

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Investigation of oxidation behavior of two-dimensional Ti_3C_2 MXene according to storage condition

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Abstract:

Two-dimensional (2D) transitional metal carbides (MXenes) show outstanding performances in many applications, such as electrodes, energy storage, and electrocatalysts. However, $Ti_3C_2T_x$ MXene flakes deteriorate rapidly under ambient conditions.[2] Here, we discuss the factors affecting the rate of oxidation of $Ti_3C_2T_x$ MXene flakes, and present guidelines for their storage to suppress a conversion of the titanium carbide to titanium dioxide. The oxidation stability of the $Ti_3C_2T_x$ flakes is dramatically improved in a system where the water molecules and the temperature were well-controlled, maintaining the intrinsic properties of the as-prepared material. It turned out that aqueous solutions of $Ti_3C_2T_x$ MXene can be chemically stable for several weeks. It was also found that if the $Ti_3C_2T_x$ flakes are dispersed in organic solvent, the degradation process can be significantly delayed. Besides, the oxidation stability of the MXene flakes is dramatically improved even in the presence of oxygen-containing air.

References:

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A First Principles Study of O_2 Dissociation on Pd modified ZrC(001) Surface

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Abstract:

Pt/C catalyst is widely used to promote the reaction rate of oxygen reduction reaction (ORR), while encounters the scarcity and high cost of Pt and poor stability problems in the electrochemical environment. The supported catalysts with the Pd on ZrC(001) surface were proposed using the *ab initio* density functional theory (DFT) calculations. The adsorption and dissociation of O_2 on the Pd_n/ZrC(001) surface with different Pd coverages of 1/4, 1/2, 3/4 and 1ML were investigated. With the analysis of the geometric and electronic structure of Pd_n/ZrC(001), we found that there existed strong interactions between the adsorbed metal atoms and the substrate that were beneficial to enhance the stability and activity. Among the Pd_n/ZrC(001) systems, the dissociation barrier of O_2 on Pd_{ML}/ZrC(001) is the smallest than that on the surfaces of Pd_1/ZrC(001), Pd_2/ZrC(001), Pd_3/ZrC(001) and Pt(111). In addition, the dissociation barrier of O_2 on Pd_{ML}/ZrC(001) is smaller than that on Pd_{ML}/TiC(001) due to the stronger interaction between novel metals and underlying ZrC(001). According to the results, ZrC(001) could serve as an ideal catalytic substrate and Pd_{ML}/ZrC(001) exhibits good catalytic properties which could be expected to be an effective catalyst for ORR.

Excellent third-order nonlinear optical properties of MXene $Ti_3C_2T_x$

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Abstract:

Based on MXene's tunable narrow bandgap structure, it has great potential in the field of optoelectronics. We explored the third-order nonlinear optical properties of $Ti_3C_2T_x$ through Z-scan technique with the experimental setup shown in Figure 1, where the excitation light source is a 780 nm wavelength femtosecond laser. We synthesized $Ti_3C_2T_x$ (T = F, O, or OH) through an etching method[1] and the NMP-$Ti_3C_2T_x$ dispersion was spun onto the glass. In the experiment, the nonlinear saturation absorption characteristics were observed by open aperture Z-scan measurement, which provides support for the generation of ultrafast pulses as saturable absorbers [2, 3]. The closed aperture Z-scan measurement showed that the $Ti_3C_2T_x$ has Kerr effect, which makes it possible to act as modulators in optical communication[4]. Here, we also studied the phenomenon of spatial self-phase modulation (SSPM) of the NMP-$Ti_3C_2T_x$ dispersions, as shown in Figure 2. The experimental results suggest that this coherent light scattering is due to the broadband, ultrafast, and large third-order optical nonlinearity of MXene, and may be applied in the novel nonlinear optoelectronic devices[5, 6].

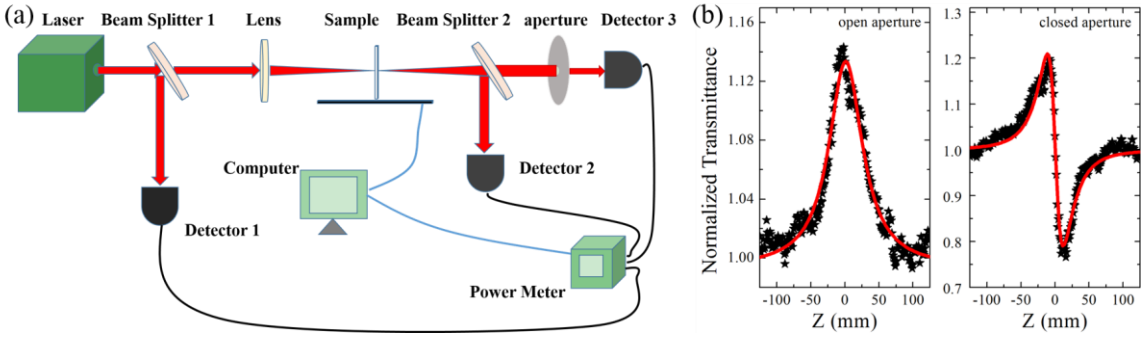

Figure 1. (a) The experimental diagram of Z-scan; (b) The open and closed aperture Z-scan measurements of $Ti_3C_2T_x$ film sample at intensity of 2.6 MW/cm^2.

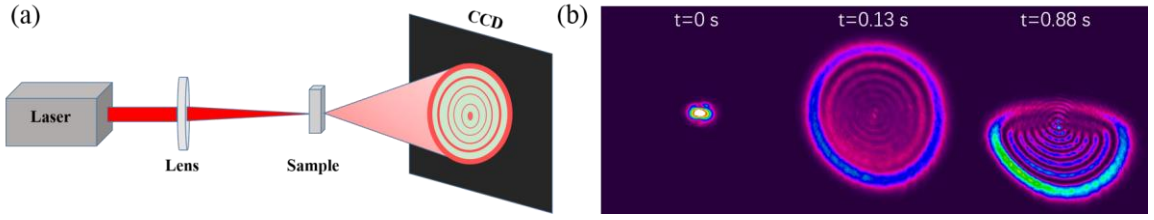

Figure 2. (a) Schematic diagram of the experimental setup; (b) The SSPM measurements of NMP-$Ti_3C_2T_x$ dispersions sample at intensity of 79.6 MW/cm^2.

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Fe_3O_4@Ti_3C_2 MXene hybrid with ultrahigh volumetric capacity as anode material for lithium-ion battery

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Abstract:

The volumetric capacity of lithium-ion batteries is becoming an increasingly important parameter restricting their practical applications in limited space, such as portable electronic products and electric vehicles. Therefore, novel electrode materials with high volumetric capacities are urgently desirable. Aiming to pursue such kind of electrode material, a new Fe_3O_4@Ti_3C_2 MXene hybrid is fabricated through a simple ultrasonication of Ti_3C_2 MXene and Fe_3O_4 nanoparticles. The Fe_3O_4@Ti_3C_2-2:5 hybrid exhibits high reversible capacity of 747.4 mAh g^{-1} at 1 C after 1000 cycles, which indicates its long cycle lifetime and excellent stability. More importantly, the hybrid material possesses an outstanding volumetric capacity up to 2038 mAh cm^{-3} at 1 C due to the high compact density of the electrode of the prepared hybrid. It is convinced that this new Fe_3O_4@Ti_3C_2 hybrid would be promising anode electrode material with high volumetric capacity. The method used here is facile and general, and could be used to prepare other TMOs@MXene hybrids applied in energy storage.

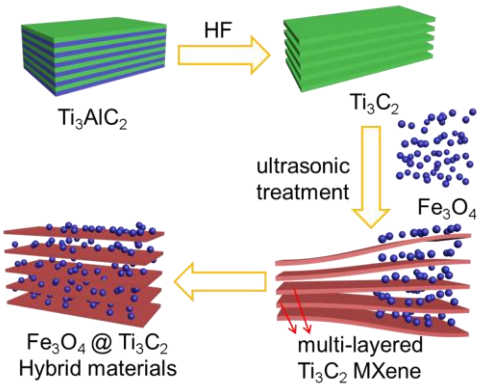

Figure 1. Schematic showing the preparation process of Fe_3O_4@Ti_3C_2 hybrids.

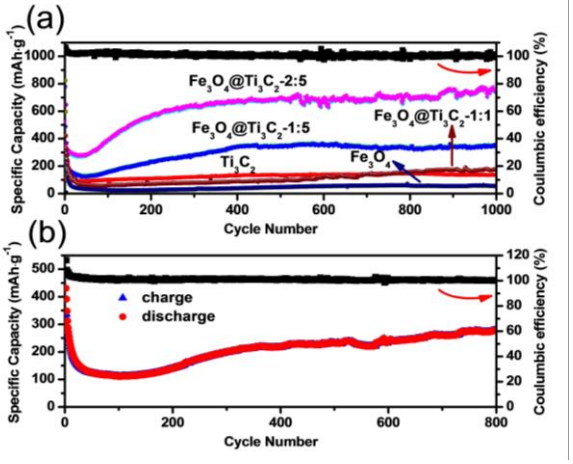

Figure 2. (a) Long cycling performance of Ti_3C_2, Fe_3O_4, Fe_3O_4@Ti_3C_2-1:5, Fe_3O_4@Ti_3C_2-2:5 and Fe_3O_4@Ti_3C_2-1:1 electrodes at 1C; (b) Long cycling performance of Fe_3O_4@Ti_3C_2-2:5 at 5C.

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Preparation and electrochemical performance of two-dimension layered transition metal oxide/carbon composites for asymmetric supercapacitor

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Abstract:

Since the discovery of two-dimensional graphene material by a. k. Geim, the scientific community has started a research boom in two-dimensional materials. Two-dimensional materials such as black phosphate, transition metal hydroxide, transition metal chalcogenide, metal/carbon nitride (MXenes), and other various two-dimensional nanomaterials have got extensive research. Our team mainly explored the preparation methods of two-dimensional nanosheets: Positively charged $Ni(OH)_2$ nanosheets with regular hexagon, $Co(OH)_2$ nanosheets with round shape, random-shaped Co-Ni LDH nanosheets and negatively charged GO sheets were exfoliated in water by liquid-phase exfoliation. Then, two-dimensional layered NiO@RGO, CoO@RGO, $NiCo_2O_4$@RGO nanocomposites were prepared by layer-by-layer assembly of transition metal hydroxide with positively charges nanosheets and GO sheets with opposite charges, followed by annealing treatment. In order to test its electrochemical performance, the composite material was applied in the asymmetric supercurrent. For example, the $NiCo_2O_4$@RGO//AC asymmetric supercapacitor achieves excellent electrochemical performance with a high energy density of 57 W h kg^{-1} at a power density of 375 W kg^{-1}. Furthermore, transition metal phosphide and graphene composite materials were prepared which shows better electrochemical properties in asymmetric supercapacitors compared with oxide.

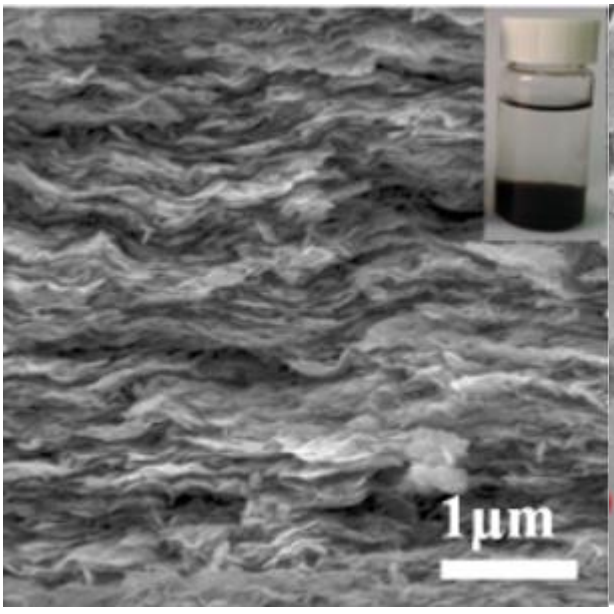

Figure 1. SEM images of NiO@RGO

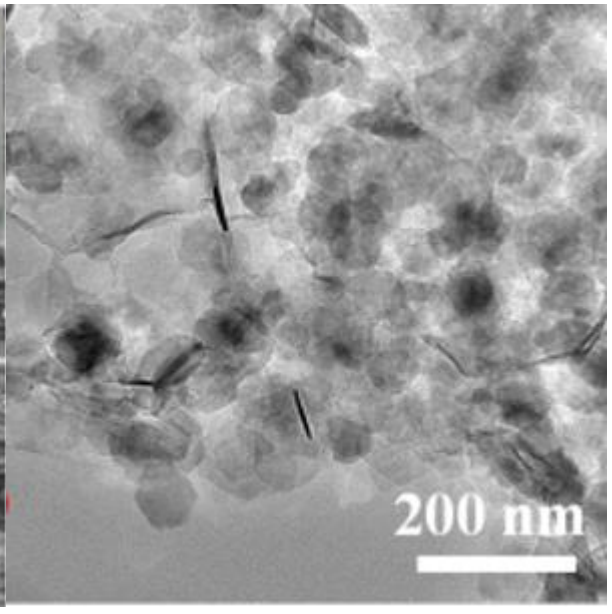

Figure 2. TEM images of NiO@RGO

References:

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Production of MXene flakes with desired sizes and their size-dependent performance

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Abstract:

The properties and corresponding functions of two-dimensional materials strongly depend on their lateral sizes. However, two-dimensional materials are usually produced with a broad size distribution, making it hard to pin down the size-dependent performance of as-made flakes. Additionally, the original particle size set the limitation for the largest flakes that can be produced using the exfoliation or delamination process. MXene, as a new family of two-dimensional materials, has attracted growing attention worldwide, due to its properties, such as excellent high conductivity and hydrophily. We conducted selective etching on large size MAX (Ti_3AlC_2) to produce multi-layered MXene (Ml-MXene). The successful and complete etching needs more acid, higher reaction temperature and longer reaction time, compared with the common conditions for the smaller precursors. The liquid phase exfoliation of the as-made Ml-MXene produced colloidal dispersion of MXene flakes with a broad size distribution. MXene flakes with desired sizes and narrow size distributions were selected using liquid cascade centrifugation (LCC). Multi-step centrifugation in LCC can be designed to produce a series of desired sizes virtually without MXene being wasted. The properties of the size-selected MXene flakes and their assembled films were characterized. The size-dependent performances were studied for ions storage and molecule/ion separation.

Electrochemical intercalation of Sn-containing MAX phase(Nb_2SnC) with Li-ions

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Abstract:

As society rapidly progresses, the need for adequate energy storage increases. Therefore developing energy conversion and storage device with excellent performance and high stability is particularly important to human[1]. In this study, we report the performance of Nb_2SnC ternary transition metal carbide (MAX phase) upon intercalation of Li ions. Because of the presence of Sn layers, which can undergo alloying reaction with Li, this material may be promising for energy storage applications. Contrary to most electrodes, the performance of this material improves along with the cycle number, specifically the capacity increases gradually from 80 mAh g^{-1} to 150 mAh g^{-1} at a current density of 0.5 A g^{-1} during 600 charge/discharge cycles. Post-cycling study suggests that the lithium ions react with outer Sn to form Li_xSn[2-3], which can gradually exfoliate a few layers and single layers, extract Sn from the structure, and break the particles into smaller and more active particles,the volume expansion and cracking of the electrode is usually a drawback in most Sn-based electrode, but this work shows that it can be beneficial for Nb_2SnC, because it drastically increases its electrochemical performance. Since Nb_2SnC is just one of many MAX phases, this work lays the foundation for the exploration of the MAX phases as the anodes of lithium ion or other batteries, as well as help for the expansion and application of the MAX family.

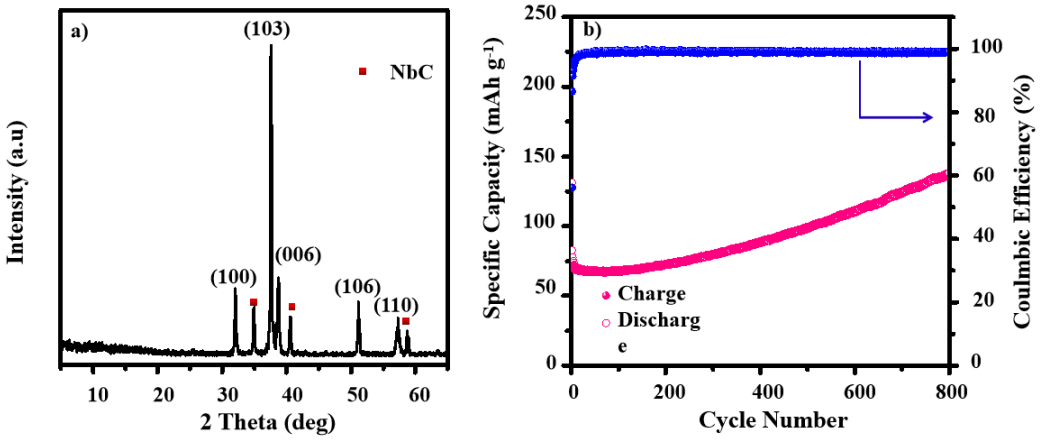

Figure 1: (a) XRD patterns of Nb_2SnC; (b) Cycling performance of Nb_2SnC at 500 mA g^{-1}

References:

[1] Shahzad, F.; Alhabeb, M.; Hatter, C. B.; Anasori, B.; Man, H. S.; Koo, C. M.; Gogotsi, Y.,. Science, 2016, 353 (6304), 1137-1140
[2] Xiaoyu, S.; Xingkang, H.; Yingpeng, W.; Ren, R.; Haihui, P.; Jingbo, C.; Guihua, Z.; Shun, M.; Junhong, C. ACS Applied Materials & Interfaces, 2018, 10, 26170-26177.
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Revealing the pseudo-intercalation charge storage mechanism of MXenes in acidic electrolyte

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Abstract:

Since the discovery of $Ti_3C_2T_x$ in 2011, the family of 2D transition metal carbides, carbonitrides and nitrides (collectively known as MXenes) has quickly attracted the attention of those developing energy storage applications such as electrodes for supercapacitors with acidic aqueous electrolytes. The excellent performance of these MXenes was attributed to a pseudocapacitive energy storage mechanism, based on the non-rectangular shape of cyclic voltammetry curves and changes in the titanium oxidation state detected by *in-situ* X-ray absorption spectroscopy. However, the pseudocapacitive mechanism was not well understood and no dimensional changes due to proton insertion have been reported. In this work, we used *in-situ* X-ray diffraction and density functional theory to investigate the charge storage mechanism of $Ti_3C_2T_x$ in 1M H_2SO_4. Results revealed that an 0.5 Å expansion and shrinkage of the *c*-lattice parameter of $Ti_3C_2T_x$ occurs during cycling in a 0.9 V voltage window, showing that the charge storage mechanism is intercalation pseudocapacitance with implication for MXene use in energy storage and electrochemical actuators.

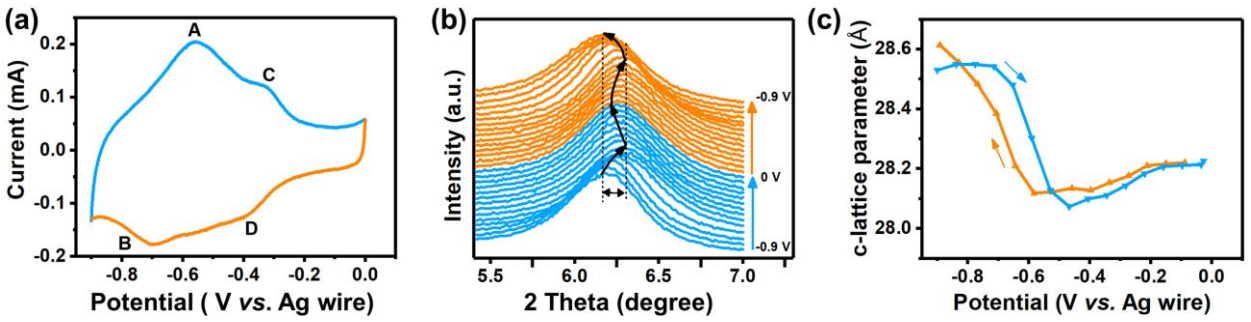

Figure 1. Electrochemical *in-situ* X-Ray Diffraction study of $Ti_3C_2T_x$ in 1 M H_2SO_4: (a) Cyclic voltammogram at 0.2 mV s^{-1}. (b) *In-situ* XRD patterns during electrochemical cycle. (c) Change of the *c*-lattice parameter with potential.

References:

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[2] B. Anasori, M. R. Lukatskaya, Y. Gogotsi, Nat. Rev. Mat. 2017, 2, 16098.

[3] M. R. Lukatskaya, O. Mashtalir, C. E. Ren, Y. Dall'Agnese, P. Rozier, P. L. Taberna, M. Naguib, P. Simon, M. W. Barsoum, Y. Gogotsi, Science 2013, 341, 1502.

Two-dimensional vanadium carbide (V_2C) MXene as electrode for supercapacitors with aqueous electrolytes

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Abstract:

MXenes are transition metal carbide and/or nitride nanosheets, conferring good conductivity with tunable transition metal oxide-like surface termination that can undergo redox reactions. Ti_3C_2, has been investigated as an electrode for supercapacitors in a wide variety of electrolytes. In neutral and basic electrolytes, capacitances between 45 F/g and 135 F/g were obtained and the charge storage mechanism was demonstrated to be pseudo-intercalation by *in-situ* X-ray diffraction [1]. Among the large family of MXenes, V_2C is of particular interest as it is one of the lightest and the vanadium surface layers could potentially enable pseudocapacitive behavior. It was previously demonstrated that V_2C has an ion intercalation mechanism when this material was proposed as an electrode for lithium and sodium ion batteries [2]. In this paper, we prepared a freestanding V_2C film for the first time, investigated its electrochemical behavior as an electrode for supercapacitors in three different aqueous electrolytes (H_2SO_4, KOH, and $MgSO_4$). These electrolytes were selected to gain insight on the effect of the electrolytes, because it was shown that Ti_3C_2 performance greatly depended on the electrolyte used. These three electrolytes were selected because of their clear difference, as one is acidic with the smallest cation H^+, one is neutral with divalent Mg^{2+}, and the last one is basic with a larger K^+ ion. The best performance was obtained in 1M H_2SO_4 with a gravimetric capacitance up to 487 F/g at 2 mV/s.

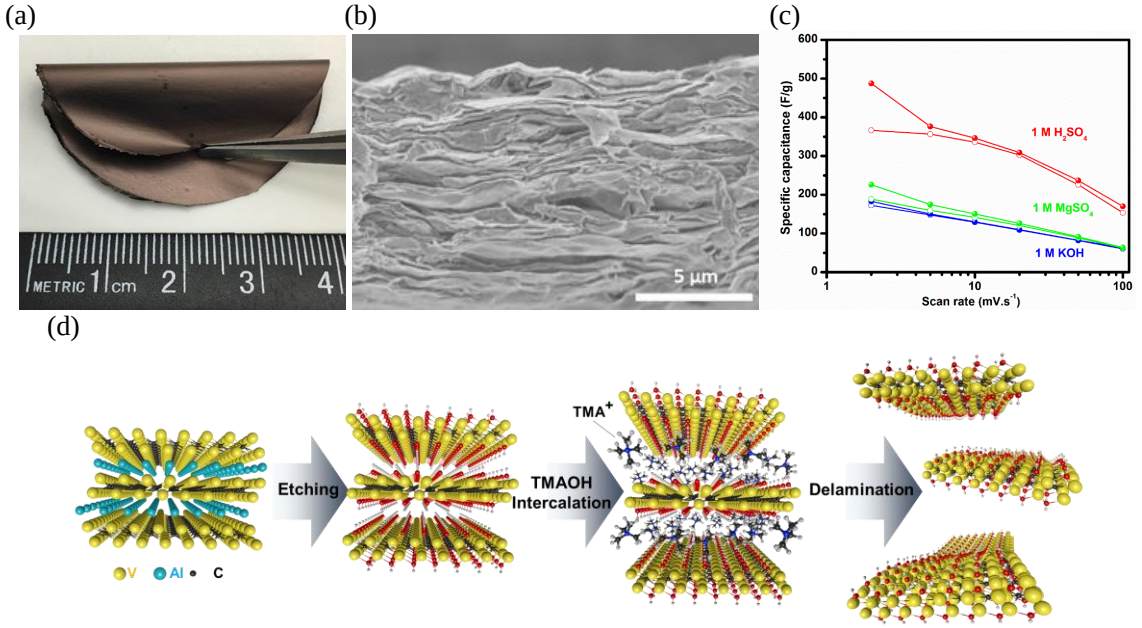

Figure 1. Photographs of V_2CTx flexible film (a); SEM (b); Rate performance in different electrolytes (c); Preparing schematic diagram (d).

References:

[1] M.R. Lukatskaya, O. Mashtalir, C.E. Ren, Y. Dall'Agnese, P. Rozier, P.L. Taberna, M. Naguib, P. Simon, M.W. Barsoum, Y. Gogotsi, Science 341 (6153) (2013) 1502–1505.
[2] Y. Dall'Agnese, P.L. Taberna, Y. Gogotsi, P. Simon, J. Phys. Chem. Lett. 6 (12) (2015) 2305–2309.

Two-dimensional Ti_3C_2 MXene Electrochemical Behavior in Environmentally Friendly Methanesulfonic Acid Electrolyte

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Abstract:

Two-dimensional transition metal carbides and carbonitrides called MXenes have gained much attention as electrode materials in electrochemical energy storage devices. In particular $Ti_3C_2T_x$ achieved outstanding performances in sulfuric acid (H_2SO_4) electrolyte, a common but hazardous chemical. In this work, an environmentally friendlier alternative acidic electrolyte, methanesulfonic acid (MSA CH_3SO_3H) is proposed. The energy storage performances of $Ti_3C_2T_x$ in aqueous and neat MSA ionic liquid electrolytes are investigated. The record specific capacitance is 298 F g^{-1}, obtained at a scan rate of 5 mV s^{-1} in 4 M MSA, which exhibited excellent cycle stability with retention of nearly 100% over 10,000 cycles. Noteworthy, this electrochemical performance is similar to the performance of $Ti_3C_2T_x$ in H_2SO_4, while using a greener electrolyte.*In-situ* X-ray diffraction analysis reveals the intercalation nature of the charge storage mechanism. Specifically, the lattice changes up to 5.16 Å during cycling, which is the largest reversible volume change observed in MXenes in aqueous electrolytes.

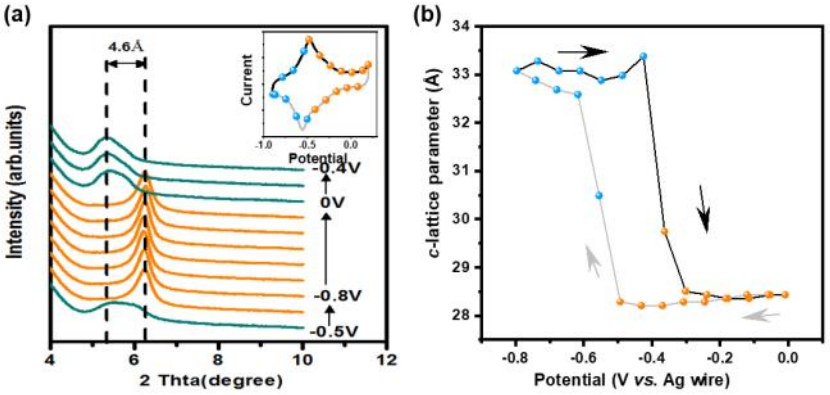

Figure 1. In-situ X-Ray diffraction analysis of $Ti_3C_2T_x$ in 4 M MSA. (a) XRD patterns during cycling and (b) corresponding c-lattice parameter vs. Potential.

References:

[1] Naguib, M., Kurtoglu, M., Presser, V., Lu, J., Niu, J., & Heon, M., et al.Adv Materials 2011. 23(37): 4248-4253.
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Preparation of 3D MXene by ice-templating method for Energy Storage

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Abstract:

Intelligent design of the electrode's architecture is the key to launching the next generation of energy storage devices. High-power energy storage solution would ideally be consisting of active nanomaterials and storing energy through fast redox reactions. A new family of two-dimensional materials called MXene is one of these nanomaterials attracting the attention for batteries and supercapacitors applications. However, MXene electrodes usually consist of restacked MXene nanosheets in which the electrolyte ions do not access easily its electrochemical active sites because the diffusion lengths through horizontal MXene layers are too long and the interlayer gap distance between MXenes layers is too small due to strong Van der Waals interactions, which restrict its power capability. In this work, we use an ice-templating method to finely control the architecture of Ti_3C_2-MXene's electrode, to optimize its ion diffusion and electrochemical reaction kinetics. We demonstrated that ice-templated 3D Ti_3C_2 to the current collector ease cations insertion/de-insertion and obtained a high capacity of 240 mAh/g at 1A/g.

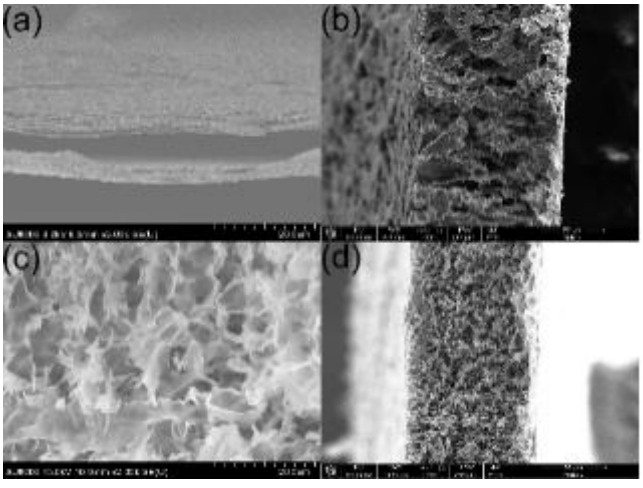

Figure 1. SEM images of (a) Ti_3C_2Tx flexible film material; (b) 3D $Ti_3C_2T_x$ prepared at -196 ºC; (c-d) 3D $Ti_3C_2T_x$ preparaed at -30 ºC.

High-Performance Supercapacitors Based on Biomass derived Carbon Dots/ MXene Films with "2D/0D Sheet-Dot" Architecture

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Abstract:

A flexible and conductive "2D/0D Sheet-Dot" MXene/CDs (carbon dots) film is successfully fabricated by using electrostatic self-assembly between negatively charged $Ti_3C_2T_x$ MXene nanosheets and positively charged CDs modified with cetyltrimethylammonium bromide, in which CDs are synthesized from biomass by a green and economic one-pot hydrothermal process. During the self-assembling process, CDs acted as intercalant are inserted in-between MXene layers, which not only effectively prevents restacking but also significantly increases the interlayer spacing of MXene nanosheets[1]. Serving as a supercapacitor electrode material, the distinctive architecture could provide more electroactive sites to become accessible and guarantee an effective ion pathway for electrolyte ions[2]. The optimized freestanding electrode from pomelo juice indicates high capacitance of 533 F g^{-1} at a scan rate of 2 mV s^{-1} in 1 M H_2SO_4 aqueous electrolyte and excellent rate capability. Moreover, four kinds of biomass-derived CDs are applied to construct binder-free flexible electrodes and the effect of particle size and heteroatoms on the supercapacitor electrochemical performance are discussed. This work exploits a simple route for assembling 2D MXene that is easy to restack into "2D/0D Sheet-Dot" MXene/CDs film which is more stable and expounds a novel concept for the construction of MXene-based high performance supercapacitors.

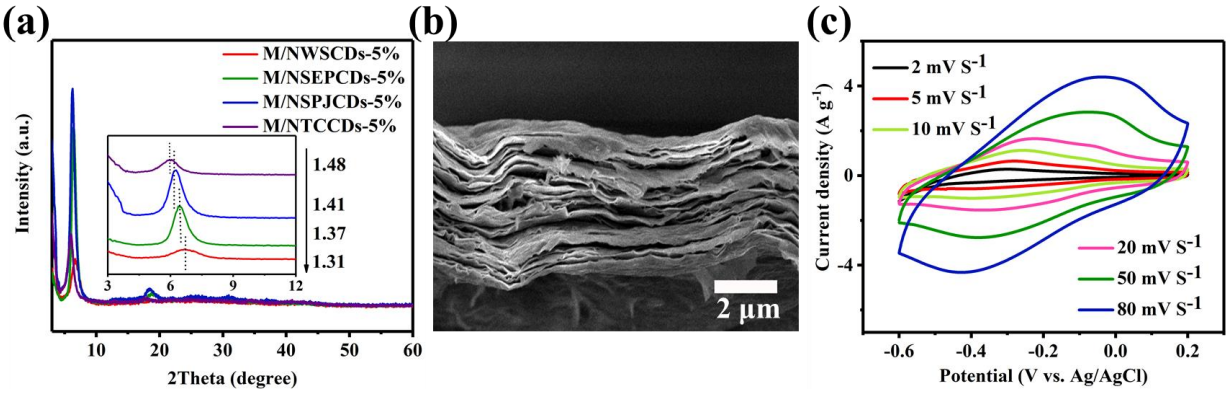

Figure 1. (a) XRD patterns of the four different biomass-derived MXene/CDs hybrids; (b) cross-sectional SEM image of M/NSPJCDs-5%; (c) CV curves of the M/NSPJCDs-5% electrode at different scan rates.

References:

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Preparation of Ti_2CT_x by Molten Salt method

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Abstract:

The two-dimensional transition metal carbide Ti_2CT_x was prepared by molten salt method. a molten fluoride salt (LiF-NaF-KF) is used to etch Al from Ti_2AlC powder precursor at 600 °C for 40 min under an argon atmosphere. The few-layered nanosheets and monolayers of Ti_2CT_x were delaminated, where T is a surface termination. The TEM show that the multilayer Ti_2CT_x is separated into a small layer of Ti_2CT_x after intercalation treatment with tetrabutylammonium hydroxide, and a single layer of extremely thin MXene sheets are stacked together; like the precursor Ti_2AlC, Ti_2CT_x also has a symmetrical hexagonal lattice. The results of infrared spectroscopy showed that Ti_2CT_x prepared by the molten salt systems contained two surface terminations of hydroxyl and oxygen, and no fluorine. The results of cyclic voltammetry show that Ti_2CTx prepared by molten salt method has good electrochemical stability and rate performance; there is no obvious redox peak in CV curve.

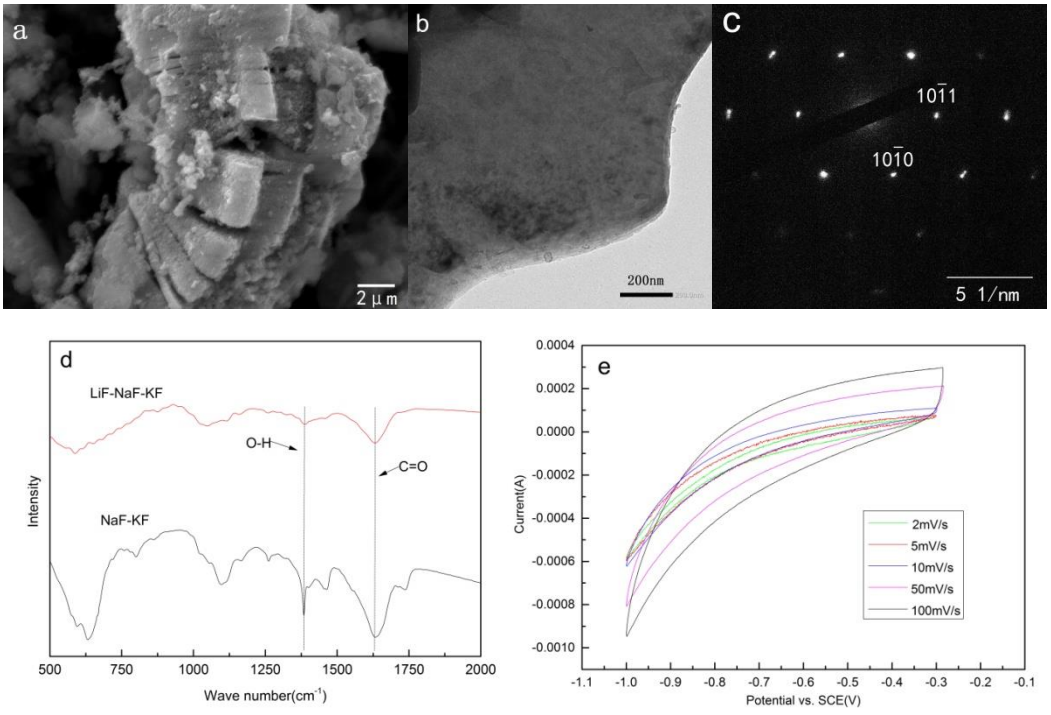

Figure 1 (a) SEM image of molten salt treated Ti_2AlC, (b) TEM micrograph of delaminated flakes (c) the SAED pattern of the Ti_2CT_x flake showing the hexagonal basal plane symmetry of the parent MAX phase, (d) Infrared spectrum of molten salt product, (e) Cyclic voltammetry curve of molten salt product.

In situ XRD of V_2C in aqueous electrolyte for supercapacitor

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Abstract:

V_2C, a good candidate for energy storage attribute to the large interlayer distance accessible for ion intercalation and great conductivity has showed great potential on Lithium battery[1],Sodium battery[2], and supercapacitor[3]. However, the charge storage mechanism has not been understood yet compare to Ti_3C_2, the most investigated MXene material. Here the electrochemical characteristics of delaminated V_2C in aqueous electrolyte (1M H_2SO_4, 1M KOH, 1M NaOH, 1M LiOH, 0.5M Na_2SO_4, 1M $MgSO_4$) are investigated by in situ X-ray diffraction. For all electrolyte, the interlayer spacing of V_2C flakes decreases during cathodic process, which can be ascribed to electrostatic attraction effect between intercalated Hydration Cations and negatively charged V_2C nanosheets. The expansion of interlayer space during anodic process can attribute to the Cations' de-intercalation. We can conclude that V_2C follows intercalation pseudocapacitance for charge storage as same as Ti_3C_2.

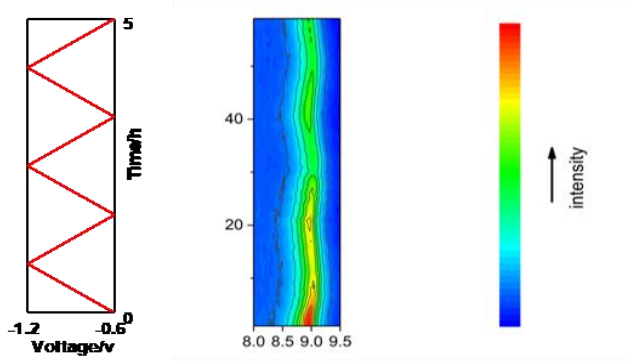

Figure 1. (002) peak position of V_2C with potential in 1M KOH

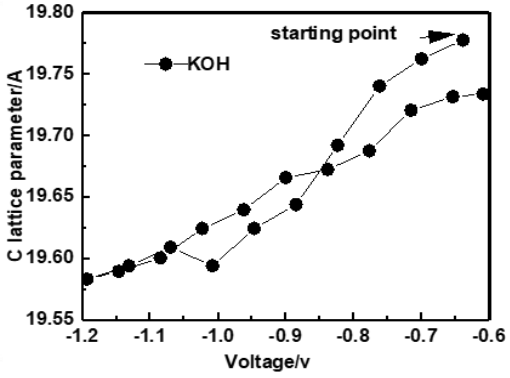

Figure 2. Change of c lattice parameter with potential in 1M KOH

References:

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[2] Dall'Agnese Y, Taberna P L, Gogotsi Y, et al. Journal of Physical Chemistry Letters, 2015, 6(12):2305.
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MXene-based Double Network Hydrogels for Flexible Supercapacitors

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Abstract:

Flexible energy storage devices with large capacity, high stability and good mechanical properties are required for powering wearable electronics. Electrically conductive hydrogels with excellent mechanical flexibility and electrochemical properties are promising candidate for flexible electrode materials, the key challenges is to improve the specific capacitance. We present a novel method to fabricate three-dimensional MXene-based hydrogels. The procedure includes freeze−thaw cycles, in situ polymerization, and plasma treatment, which can be further expanded for large-scale production of other hydrogel systems. The performance of the hydrogel electrode is investigated by using electrochemical measurements and stretch test. Electrodes made of the N-doped Ti_3C_2@Polyacrylamide/Sodium Alginate exhibited promising capacitive characteristics. The specific capacitance is 645 Fg^{-1} under 1 Ag^{-1} charge/discharge current and remain 90 % after 1000 consecutive cycles. The mechanical properties of Ti_3C_2@Polyacrylamide/Sodium Alginate hydrogels were investigated by tensile tests, which demonstrated that Ti_3C_2-based double network hydrogel had a remarkable tensile strength of 900 KPa and a large elongation over 240 %. As-prepared MXene hydrogels are promising electrode materials for flexible supercapacitors.

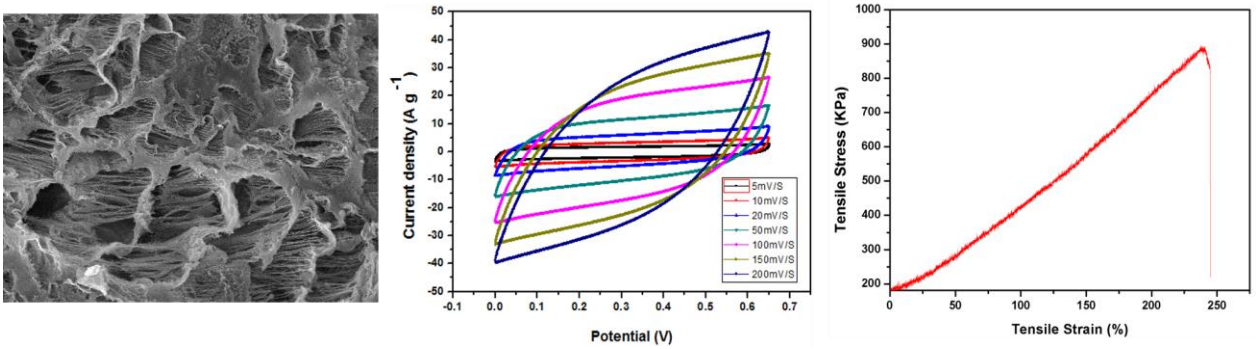

Figure 1. The micro-structure of the MXene-based hydrogel, which shows high electrochemical activity and high mechanical strength

References:

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Effect of etching time on microwave absorption properties of MXene $Ti_3C_2T_x$

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Abstract:

$Ti_3C_2T_X$, a layered two-dimensional transition metal carbide belonging to MXenes, is a potential microwave absorbing material because of its large specific surface area, high electrical conductivity, and multifunctional processing [1]. We synthesized $Ti_3C_2T_X$ MXenes through a HF etching method[2] and systematically investigated how filler loading, coating thickness influence the dielectric properties and microwave absorption ability from 2 GHz to 18 GHz. Moreover, we also discussed the impact of other factors, including flaky morphology, interlayer spacing and etching time, on the microwave absorption, which also play an important role in both absorption intensity and absorption bandwidth [3,4]. The results demonstrate that $Ti_3C_2T_X$-36 possesses best microwave absorption performance with the strongest absorption of -50 dB. The qualified absorption bandwidth (RL<−10 dB) [5,6] is up to 4.3 at the matching thickness of 1.5mm.

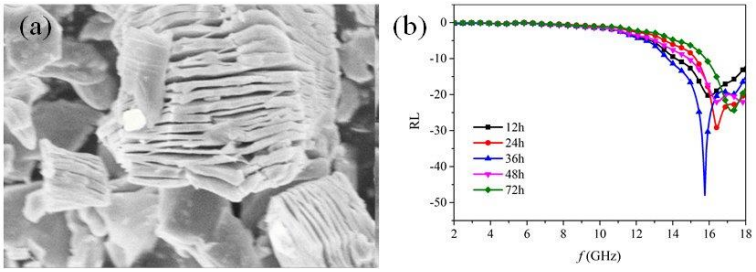

Figure 1. (a) The SEM image of the as-synthesized $Ti_3C_2T_X$-36; (b) The RL curves of $Ti_3C_2T_X$-12, $Ti_3C_2T_X$-24, $Ti_3C_2T_X$-36, $Ti_3C_2T_X$-48, $Ti_3C_2T_X$-72.

References:

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Highly conducting MXene fibers for fiber-shaped supercapacitors

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Abstract:

Fiber-shaped supercapacitors (FSCs) are lightweight and conformal forms of energy storage devices that are being developed for powering portable and wearable electronics. Recently, 2D transition metal carbide $Ti_3C_2T_x$ (T_x stands for surface termination), the most widely studied MXene, has been demonstrated as one of the promising electrode materials for fiber-shaped supercapacitors.[1] Among various fiber fabrication methods, wet-spinning is an industrially viable approach to fiber production and has therefore attracted considerable attention for the fabrication of various FSC electrodes, such as graphene fibers, CNT fibers and conducting polymer fibers. The wet-spun composite fibers for use in FSCs must ensure that the active material and the binder are homogeneously dispersed but neither of the two components must limit the function of the other component particularly at high active material loading, i.e. the high conductivity and electrochemical performance of the active material must be maintained and the binder must provide durability and flexibility. However, the poor interaction between MXene flakes and spinnable templates resulted in low electrical conductivity and compromised energy storage performance.

In our work, MXene fibers with high conductivity and enhanced energy storage properties were prepared using poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) as a highly conductive and flexible binder.[2] We demonstrated the continuous production of PEDOT:PSS/MXene hybrid fibers (over decades meters) with a conductivity of ~1489 S cm-1 and tensile strength can be tailed from ~58 MPa to ~143 MPa, which are about 5-time higher than previously reported MXene composite fibers. When MXene loading increased to 70 wt. %, composite fiber shows enhanced volumetric capacitance of ~614.5 F cm-3 at 5 mV s-1 and excellent performance of 375.2 F cm^{-3} at high scan rate (1000 mV s-1). We also demonstrate elastic wire-shaped supercapacitors using a coiled design to yield 96 % capacitance retention after 200 stretch-release cycles to 100 % strain. This work demonstrates a scalable approach towards the processing of high-performance MXene-based fiber electrodes that could be used in the future for fiber-based energy storage devices and other textile-based wearables. Fiber-shaped supercapacitors (FSCs) are lightweight and conformal forms of energy storage devices that are being developed for powering portable and wearable electronics.

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High-throughput theoretical study of potential stable MAX phases

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Abstract:

Recently, an emerging family of 2D early transition metal carbides and nitrides, named MXenes, has attracted tremendous attentions since the discovery[1, 2] of Ti_3C_2 by Gogotsi's group in 2011. The natural stone with a layered structure and highly electrically conductive make MXenes show promise in electrical energy storage, electrocatalysis and other applications. Meanwhile, MXenes' versatile chemistry also renders their properties tunable for the above mentioned applications. For example, each formula unit of Sc_2C[3] can adsorb up to two Li/Na atoms, which corresponds to a relatively high theoretical capacity of 462 or 362 $mAhg^{-1}$. However, these high performance MXenes have not yet been produced. This is because MXenes are mainly limited by the parent MAX phases. Thus, it's important to design new stable MAX phases containing previously unrealized transition metals. Up to now, the new structures usually come from solid solutions, various surface terminations, and multi-transition-metal layers. Herein, we performed high throughput DFT calculations, with the consideration of all possible prototype MAX phases ($M_{n+1}AX_n$, n = 1, 2, and 3) and other possible ternary compounds. We found a series of new stable MAX phases against elements, binary, and ternary compounds, such as Sc_2BiC, Sc_2SnC. Our results shed lights on designing new MAX phases to further expand the MXenes family and introduce potential exotic properties for underlying applications.

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Bottom-up Synthesis of MXenes

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Abstract:

Inspired by the achievements of graphene, the two-dimensional (2D) materials have attracted intense attention in recent years. Since 2011, MXenes as an emerging 2D materials have attracted many attentions. Experimentally, MXenes can be synthesized from selective etching of traditional MAX phases in the corrosive fluoride-contained solution. The size and quality of MXenes are limited in the preparation process, which affects the practical application of MXenes. Herein, based on theoretical calculations, we propose a bottom-up method to grow MXenes. More transition metal elements may form MXene materials on the hexagonal substrate. More interestingly, we found that MXene structure can contained two different transition metals, which can be stabilized on the hexagonal substrate. These findings may provide a new way to obtain more combinations and large-scale MXenes. Thus, these MXenes are predicted to have potential applications in electrochemical energy storage and functional polymer composites [1-3].

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A facile method to fabricate Ti_3C_2 MXene modified metal oxide composites

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Abstract:

Non-precious metal catalysts, such as nickel oxide, with efficient activity and abundance in the earth are highly required. However, poor conductivity and high cohesion significantly limit the application of NiO nanoparticles in energy storage devices. Herein, we develop a facile ultrasonication method to introduce NiO nanoparticles into multi-layered Ti_3C_2 MXene and form a novel NiO/Ti_3C_2 nanomaterials. The layered Ti_3C_2 MXene is prepared through etching an Al layer from Ti_3AlC_2 with HF at mild temperature. The SEM image of the as-obtained MXene exhibits a unique layered structure. NiO nanoparticles in NiO/Ti_3C_2 composites homogeneously disperse on the surface and interlayer of Ti_3C_2 MXene, thus hindering the aggregation of NiO and enhancing the exposure of catalytic active sites. The uniform distribution and morphology of the NiO nanoparticles are further confirmed by the magnified TEM images. XRD spectra suggests NiO nanoparticles are formed on Ti_3C_2 MXene, which is in accordance with the SEM and TEM images. In this composite, multi-layered Ti_3C_2 MXene enacts a superior host to load NiO nanoparticles result of its open layered structure, good electronic conductivity and excellent chemical stability. The high metallic conductivity of Ti_3C_2 substrate sever as conductive network facilitated electron transfer speed and the chemical stability are beneficial for achieving high stability. Given this, NiO/Ti_3C_2 nanomaterials would possess good electrochemical performance, thus having a promising application prospect in energy storage devices.

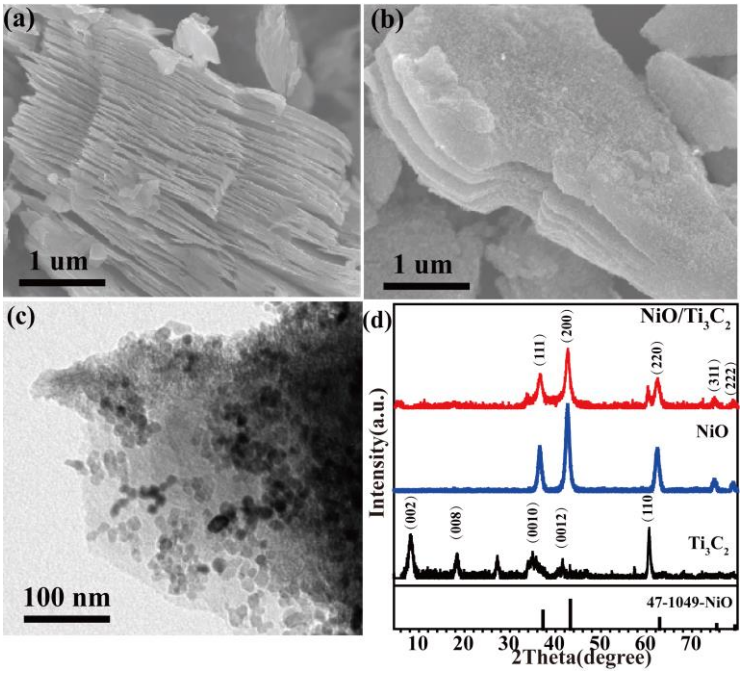

Figure. The SEM images of (a) Ti_3C_2 and (b) NiO/Ti_3C_2; (c) The TEM image of NiO/Ti_3C_2; (d) XRD patterns of Ti_3C_2, NiO and NiO/Ti_3C_2 nanomaterials.

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A scalable research on the synthesis of MXenes-based nanoscrolls

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Abstract:

MXenes is a new type of two-dimensional material. Due to properties of the two-dimensional structure, MXenes can be stacked into many different assemblies. However, the MXenes flakes is also flexible. A series of new nanostructures can be formed through morphological transformation. In this work, we use $Ti_3C_2T_x$ colloid as precursor to explore the preparation of MXenes-based nanoscrolls. The preparation of the $Ti_3C_2T_x$ colloid was as previously reported [1-4]. The $Ti_3C_2T_x$ nanoscrolls were prepared by the regulation of their interface and acidity and the treatment of surface functional groups. Figure 1 describes morphology of different stages in the process of changing from flakes to nanoscrolls. At first the eage of $Ti_3C_2T_x$ flakes bended as shown in Figure 1(a).Then Figure 1(b) shows the big $Ti_3C_2T_x$ flakes broke into smaller $Ti_3C_2T_x$ flakes and bended futher more. At last we can see in the Figure 1(c) that $Ti_3C_2T_x$ flakes bended into nanoscrolls. It has a distinct hollow tubular structure like carbon nanotubes. Due to the special structure of MXenes-based nanoscrolls, it has board application prospects. MXenes-based nanoscrolls can be used to wrap other nanostructures to immobilize or protect them. This work can be applied in many subjectsin the future, such as energy chemistry, catalysis, biomedicine, energy storage, etc.

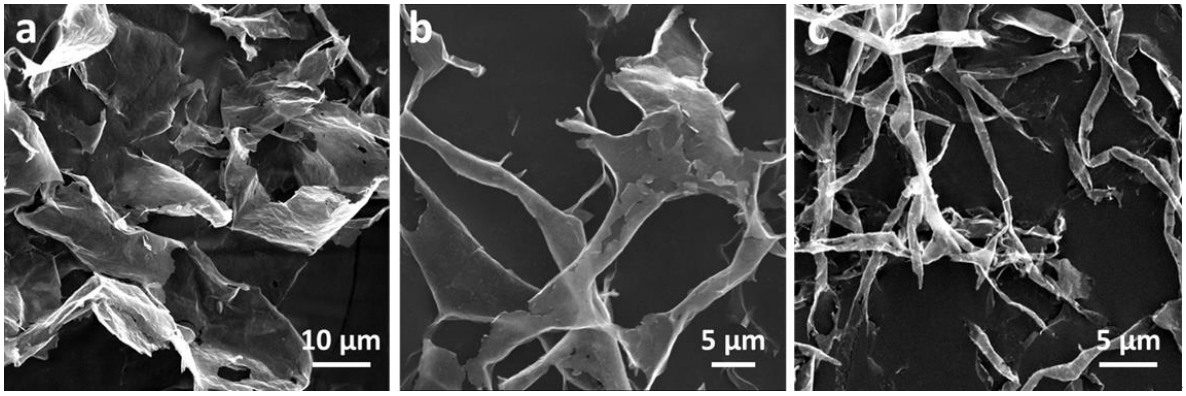

Figure 1. SEM images of (a) $Ti_3C_2T_x$ flakes, (b) $Ti_3C_2T_x$ flakes and nanoscrolls and (c) $Ti_3C_2T_x$ nanoscrolls.

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Functionalization of MXenes as highly active and selective catalysts

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Abstract:

MXenes, a new family of two-dimensional materials, have attracted increasing attention because of their metallic conductivity, hydrophilicity and good mechanical properties.[1] As a result, they have been widely used in diverse fields, including Li-ion batteries, supercapacitors, fuel cells, hydrogen evolution, gas sensors, and so on.[1-5] In addition, MXenes have recently emerged as promising candidates in catalysis. For instance, Wang and co-workers prepared $Mo_2TiC_2T_x$ supported Pt single atoms and used them for hydrogen evolution reaction, which exhibited a mass activity of 40 times higher than that of commercial Pt/C catalyst.[6] Wu et al. reported that MXenes supported Pt nanoparticles can be used for propane dehydrogenation, which shows a propane conversion and propene selectivity of 16% and 95%, respectively, at 550 ^oC.[7] Although great progress in catalysis has been made, MXene composite catalysts for PSH have not been investigated yet, which might be another new and promising application.

Here, we synthesize cobalt-tipped carbon nanotube/Ti_3C_2 nanosheet composites (Co-CNT/Ti_3C_2) for oxygen reduction reaction (ORR) and propyne semi-hydrogenation. It is shown that the optimized Co-CNT/Ti_3C_2 manifest comparable ORR activity (half-wave potential of 0.82 V and diffusion-limiting current density of 5.55 mA cm^{-2}) with commercial Pt/C (half-wave potential of 0.82 V and diffusion-limiting current density of 5.30 mA cm^{-2}) but much better stability.[8] Furthermore, the Ti_3C_2 nanosheet supported Co-based catalyst exhibits a propene selectivity of 96% at the propyne conversion of 99% at 150 ^oC, which have surpassed the reported values in the literature.

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MXene/Nanoporous SnSb composite as anode for Li-ion battery

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Abstract:

As one of the most promising anode materials, alloy-type anode is drawing worldwide attentions for next-generation Li-ion batteries (LIBs) due to its high theoretical capacity.[1] However, it suffers from a drastic volume expansion during the lithiation and delithiation process that results in the pulverization of alloy matrix, continuous formation of the solid-electrolyte interface (SEI) and therefore leading to performance fading.[2] Fabrication of 3D nanoporous alloys by dealloying method shows great prospects which could accommodate the volume change and promote the electrolyte penetration.[3-4] However, the long-term cycle performance and ionic conductivity should be further improved.

Herein, MXene, a novel 2D layered transition metal carbides with high conductivity (4600 $S \cdot cm^{-1}$) and excellent mechanical property is introduced and composed with nanoporous SbSn alloy (NP-SnSb) to form a 2D/3D-trans-dimension nanocomposite material (Figure1a). The result indicates that the composite shows a "spring-like" structure. The combination of MXene and nanoporous alloy synergistically enhance the Li-storage stability. Compared with pure NP-SnSb, the trans-dimension combination of two components obviously improve the cycle stability. The capacity retention is 62% after 50 cycles when NP-SnSb is only 18% (Figure 1b).

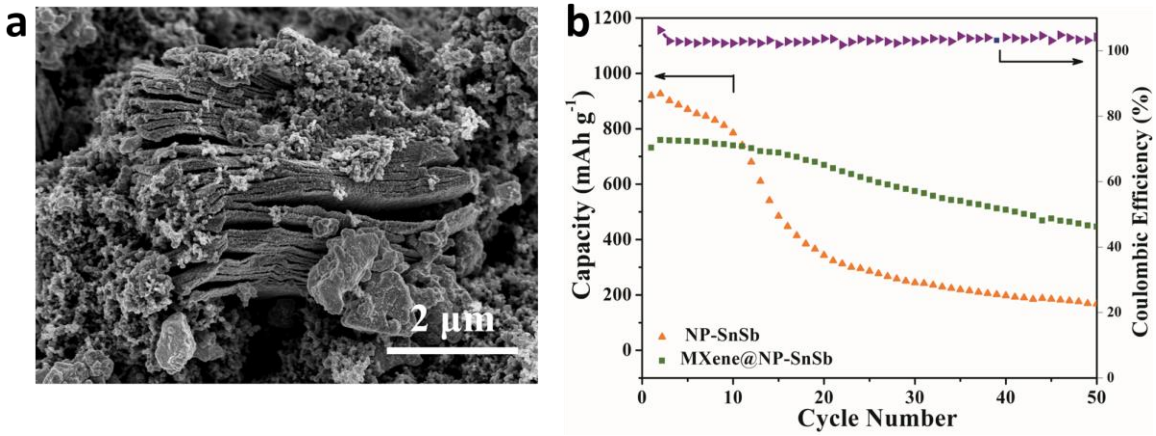

Figure 1. (a) SEM image of MXene@NP-SnSb and (b) cycle performance of prepared anodes.

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Optimization the surface Oxygen terminations of MXene toward improved Li-ion storage performance at low-temperature

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Abstract:

Lithium-ion batteries (LIBs) is gaining great success in the field of portable energy storage device, electric vehicles as well as smart grid. [1] However, the performance fading at low temperature (LT) and the possible safety concerns prohibit their widely applications in cold climate and other low temperature environment. [2,3] The main reasons accounting for the poor LT battery performance includes: the sluggish kinetics of Li^+ desolvation and Li^+ insertion/de-insertion. Herein, we report a new strategy to enhance the Li-ion storage performance in MXene by optimizing the surface oxygen terminations through controlling the gas atmospheres during sintering. The as-prepared $Ti_3C_2T_x(O)$ displays well-defined 2D layered structural characteristics as the pristine MXene. Investigated as anode in LIBs, it delivers a capacity of 404 $mAhg^{-1}$ even after 500 cycles at room temperature. Moreove, it displays a capacity of 208 $mAhg^{-1}$ even at low temperature of -20°C, compared to graphite anode. For the pure MXene, its capacity is 123.8 $mAhg^{-1}$ at -20°C. The capacity of $Ti_3C_2T_x(O)$ is about three times of commercial graphite anode after cycle 120 cycles at -20°C. These results indicate that surface oxygen optimization strategy could effective improve the low temperature Li-storage capacity and stability of batteries.

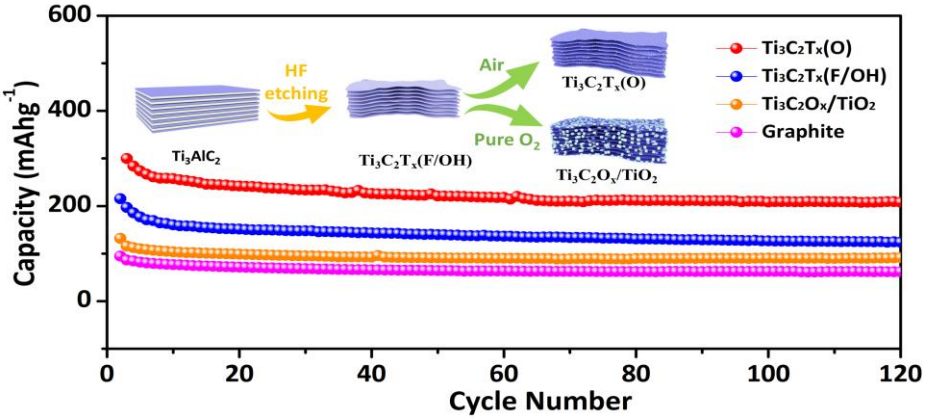

Figure 1. Schematic illustration of the fabrication process and the electrochemical performance of different materials at current density 100 mA g^{-1} for 120 cycles at -20 ℃.

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Ti_3C_2 nanoribbon skeleton main body and MOF/GO as Li-S batteries with ultra high capacity research

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Abstract:

Li-S batteries have attracted wide attention from researchers due to their high specific capacity and high energy density, and have become one of the research hotspots of new lithium batteries. However, the bottleneck restricting the industrialization of lithium-sulfur batteries cannot be ignored. First, the sulfur element itself has low conductivity. The volume expansion ratio is large, which will lead to the problem of active material utilization, low rate capacity and high overpotential [1]. In recent years, MXene materials have large interlayer spacing, high conductivity and good ion transport. The transport characteristics show excellent electrochemical performance: such as suitable deintercalation of lithium potential, high first-cycle Coulomb efficiency, long cycle life and high rate performance, and have great application potential in the energy field [2]. At the same time, the MOF-based separator acts as an ion sieve in a lithium-sulfur battery, which selectively sifts Li + ions while effectively suppressing the shuttle effect of polysulfides [3]. In this paper, the Ti_3C_2 MXene nanobelt frame is used as the intermediate layer of the S/polysilicon main body and the micro-nano MOF-GO polypropylene (PP) separator, which can improve the battery rate performance and suppress the shuttle effect of polysulfide, and preparation of Li-S battery with excellent performance.

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Two-dimensional titanium carbide MXenes doped nano-$CuFeS_2$ as anode material for lithium-sulfur battery

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Abstract:

Compared with traditional lithium-sulfur battery materials, transition metal sulfides have the advantages of high energy density and wide source. $CuFeS_2$ materials have good optical, electrical and magnetic properties and are widely used in solar energy, catalysts and lithium batteries [1-3]. When $CuFeS_2$ is used as a lithium ion battery material, it has low conductivity at room temperature and cannot meet the requirements of practical use. It is necessary to cooperate with other good conductors to improve its electrochemical performance. As an emerging material, MXenes exhibits excellent electrochemical properties due to its large interlayer spacing, graphene-like layered structure [4] and high electrical conductivity [5], which has caused it to become more and more in the field of energy storage. The more attention you have. In this paper, MXenes is used as a good conductor, and the self-made nano-$CuFeS_2$ is uniformly dispersed between the sheets to improve the electrochemical performance of the $CuFeS_2$ material.

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Novel titanium nitride halide TiNX (X = F, Cl, Br) monolayers: potential materials for highly efficient excitonic solar cells

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Abstract:

The growth in the area of two-dimensional (2D) crystals offers renewed opportunities for efficient, ultrathin excitonic solar cells (XSCs) beyond those three-dimensional traditional materials. Here, based on first principles, we propose a family of achievable 2D tetragonal-structured titanium nitride halides (TiNX, X = F, Cl, Br) as donor and acceptor materials for XSCs in virtue of their desirable optoelectronic properties, such as a direct bandgap with moderate size, superior optical absorption, ultrahigh photoresponsivity together with very small effective masses and exciton binding energy. More importantly, we find that they can be easily superimposed onto each other to form effective solar cell systems with the type-II heterojunction alignment. We predict that the maximum energy conversion of the designed TiNF/TiNBr, TiNCl/TiNBr and TiNF/TiNCl bilayer solar cells can reach as high as ~18%, 19% and 22%, respectively, which are far superior to those of typical conjugated polymer or fabricated 2D solar cell systems. Our work suggests these potential bilayer systems are appealing 2D solar cell materials with high efficiency.

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Functionalized MXenes as ideal electrodes for Janus MoSSe

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Abstract:

On the basis of first-principles calculations, we examined the possibility of functionalized transition metal carbides and nitrides (f-MXenes) as ideal electrode materials for two-dimensional (2D) Janus MoSSe through interfacial electronic properties and Schottky barriers within MoSSe/f-MXene van der Waals (vdW) heterostructures. We found that the interactions between MoSSe and f-MXenes are weak, and thus the intrinsic electronic features of MoSSe could be reserved. Based on band structure calculations, the minus n-type (vanishing) Schottky barrier heights could be assigned to MoSSe/$Ti_2C(OH)_2$ and MoSSe/$Mo_2C(OH)_2$, and the p-type Schottky barrier height assigned to Sc_2NO_2 turns out to be negligible. When taking the charge redistribution at the interfaces into account, our band structure results are consistent with the modified Schottky–Mott equation. Our work provides a reference for selecting ideal electrode materials and channel materials for electronic applications.

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Sc_2C as a Promising Anode Material with High Mobility and Capacity: A First-Principles Study

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Abstract:

Two-dimensional (2D) Sc_2C, an example of a MXene, has been attracting extensive attention due to its distinctive properties and great potential in applications such as energy storage. Herein, a systematic investigation of Li/Na atom adsorption and diffusion on Sc_2C planes was performed based on density functional calculations. The metallic character of pristine and adsorbed Sc_2C ensures desirable electric conductivity, which indicates the advantages of 2D Sc_2C for Li/Na ion batteries. In addition, the diffusion barriers are as low as 0.018 and 0.012 eV for Li and Na, respectively, which illustrates the high mobility and cycling ability of Sc_2C. In particular, each formula unit of Sc_2C can adsorb up to two Li/Na atoms, which corresponds to a relatively high theoretical capacity of 462 or 362 $mAhg^{-1}$. The average electrode potential was calculated to be as low as 0.32 and 0.24 V for stoichiometric Li_2Sc_2C and Na_2Sc_2C, respectively, which makes Sc_2C attractive for the overall voltage of the cell. Herein, our results suggest that Sc_2C could be a promising anode candidate for both lithium-ion and sodium-ion batteries.

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2D MXenes for Theranostic Nanomedicine

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Abstract:

Great and interdisciplinary research efforts have been devoted to the biomedical applications of two-dimensional (2D) materials, owing to their unique planar-structure and prominent physiochemical properties. The emerging 2D MXenes, a family of ultrathin atomic nanosheet materials derived from MAX phase ceramics, are currently booming as novel inorganic nanosystems for biologic and biomedical applications.[1] The metallic conductivity, hydrophilic nature, and other unique physiochemical performances make the 2D MXenes possible to meet the strict requirements of biomedicine.[2] Here, we introduce the very recent progresses and novel paradigms of 2D MXenes for state-of-the-art biomedical applications, focusing on the design/synthesis strategies, therapeutic modalities, diagnostic imaging, biosensing, antimicrobial and biosafety issues. It is highly expected that the elaborately engineered ultrathin MXenes nanosheets will become one of the most attractive biocompatible inorganic nanoplatforms for multiple and extensive biomedical applications to profit the clinical translation of nanomedicine.[3]

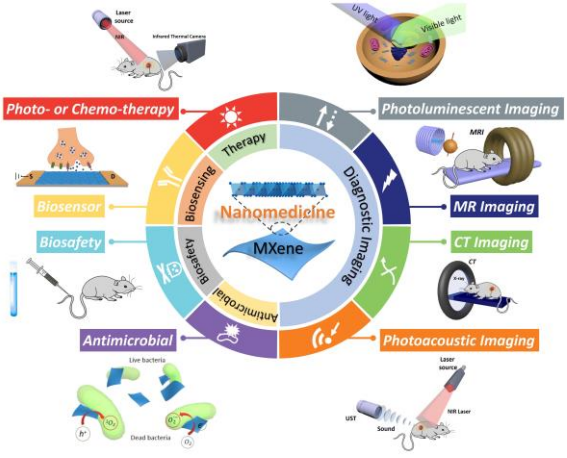

Figure 1. Summary of emerging 2D MXenes used in nanomedicine.

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Highly Compressible MXene/Melamine Sponge Electrode for High Performance Supercapacitors

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Abstract:

The preparation of elastic electrode with high compressibility and facile fabrication processes is one of the most popular hotpots especially for supercapacitors, battery, biological electrodes and sensors, yet still facing great challenges. [1] Here, a series of novel designed three-dimensional superelastic and durable sponge electrodes have been synthesized through introducing melamine foam as skeleton then dip-coating with MXene solution followed by, which is prepared through selectively etching Al layers from a Ti_3AlC_2 (MAX) precursor. [2, 3] The merits of porous structure and great mechanical properties of melamine foam candidate it as an ideal substrate with large surface area restricting the restacking of $Ti_3C_2T_x$ sheet, meanwhile facilitating the transportation of electrolyte ions very smoothly as well. As-obtained MXene sponge exhibit high specific capacitance of 112F g^{-1} and excellent stability with 92% retain its initial capacitance after 1000 charging-discharging cycles. As compressible electrodes, the compression capacity of the MXene sponge electrode are also investigated with almost full recovery after 1000 compression-release cycles at 80% formation. What's intrigue, on the account of strong hydrogen bonding between matrix and MXene, the sponge electrodes exhibit steady electrochemical performances maintaining during compressive cycling. Thus we have provided an available strategy for designing and fabricating high electrochemical activity compressible electrodes, which is convinced beneficial a lot for future applications areas like catalyze platform and piezoresistive sensors.

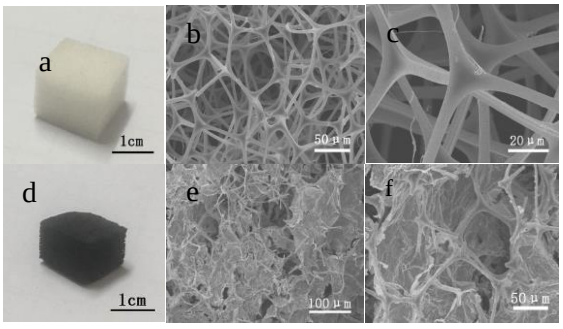

Figure 1. Optical and SEM images of the original melamine sponge (a, b, c) and corresponding MXene coated sponge (d, e, f) at different scales.

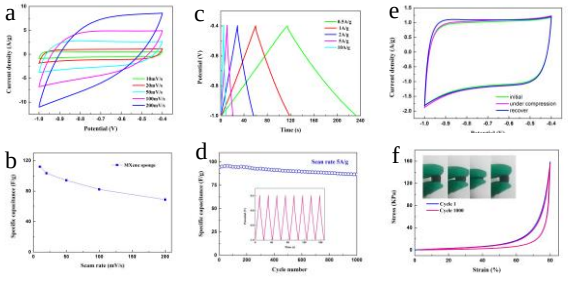

Figure 2. Electrochemical and mechanical performance of MXene sponge. (a) CV curves at different scan rates. (b) Specific capacitances at different scan rates. (c) Charge-discharge curves at different current density. (d) Cycling stability of the sponge at a current density of 5A/g. (e) CVs at a scan rate of 20mV/s before, under and after compressing of the sponge. (f) Stress–strain curves for the sponge from compression tests.

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MXene and Wearable Energy Storage

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Abstract:

Wearable technology is posed to provide the human body with a new interface and seamless experience to interact with the latest technologies, thereby attracting tremendous academic research and investment from relevant industries. However, the wearability and operation of current wearable technologies is often limited by the unsatisfactory material properties such as flexibility and durability, and rigid electronic components such as energy storage devices. Current miniaturisation approaches of these bulky and rigid energy storage devices also fall short in providing sufficient energy density. New applications can emerge if energy storage devices are made wearable and functional in various conditions.[1,2] Relevant challenges for making MXene-based wearable fibre-shaped energy storage device that can operate under various conditions need to be addressed by first understanding the processability of MXene in order to fabricate supercapacitors in fibre- or yarn-format. Meanwhile, energy density (capacitance) and power density (charge/discharge rate capability) of these fibre-shaped supercapacitors have to reach a level to compete with conventional energy storage devices. $Ti_3C_2T_x$ MXene with excellent electrical conductivity and high volumetric capacitance is a promising candidate for building wearable supercapacitors with high energy density. Rapid ion diffusion and high conductivity of MXene can compensate for the low ionic conductivity of the electrolyte and large resistivity of the fibre-shaped devices. Preliminary results from our group have shown that novel MXene-based yarn can deliver unprecedented high energy density.[3,4] However, further developments such as on suitable electrolyte for MXene fibre-shaped device, new scalable fabrication technique are required to access MXene's full potential in yarn-shaped supercapacitor.

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ab initio Computational Screening of 2D Double Transition Metal Carbides (MXenes) as Electrocatalysts for Hydrogen Evolution

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Abstract:

Hydrogen (H_2), as a clean green fuel with high specific energy, is one of the most promising energy carriers to substitute the finite coal and oil resources [1]. Finding a suitable electrocatalyst for the large scale production of hydrogen is vital. MXenes, due to their many excellent properties, such as a large specific surface area, metallic conductivity, fast transfer of ions and hydrophilic surface, have been explored as potential catalysts for the hydrogen evolution reaction (HER) [2].

We used density functional theory calculations to explore the thermodynamic stability and screen optimum catalysts that would promote hydrogen evolution reaction among the 24 two-dimensional double transition metal carbides (MXenes). By calculating the Gibbs free energies for hydrogen adsorption (ΔG_H) on $M'_2M''C_2O_2$ and $M'_2M''_2C_3O_2$ at 1/8 ML coverage of H^*, most of the MXenes fall on the left side of the volcano, indicating that the interaction between hydrogen and the double transition metal carbides is generally strong. The Gibbs free energy for hydrogen adsorption on 11 oxygen terminated Mo and Ti based bimetal carbide MXenes is close to 0 eV, and so these are predicted to be the most promising nonprecious HER electrocatalysts. Among them, the Gibbs free energy of $Mo_2NbC_2O_2$ shows a near-zero value of 0.003 eV. This value is lower than the theoretical values of the highly efficient HER catalysts, such as Pt (ΔG_H=0.09 eV) [3]. Furthermore, adding transition metal atoms on basal plane can adjust the H-O bond strength and engineer the HER overpotential close to the optimal value, 0 V. Overall, this investigation confirms that the double transition metal carbides, as a new family of MXenes, are promising electrocatalysts for HER.

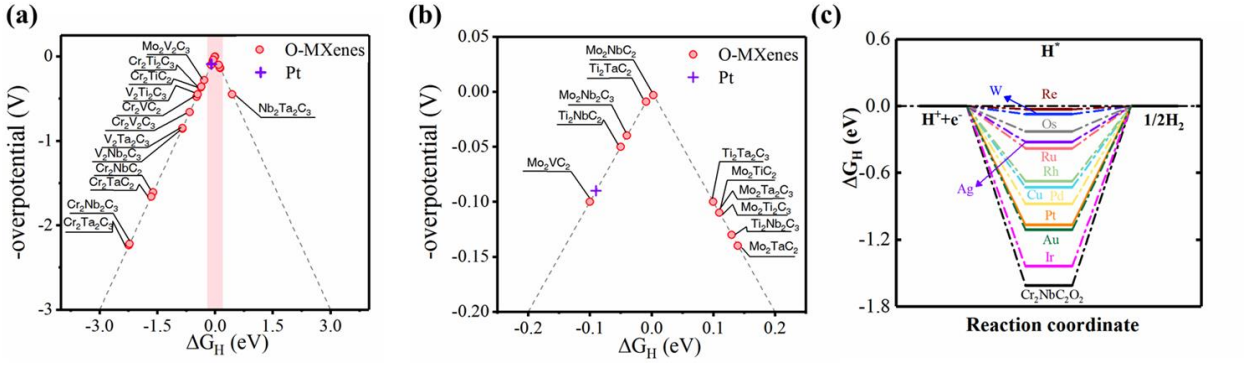

Figure 1. (a) HER volcano plot with the theoretical overpotentials for the O-MXenes. (b) The zoomed-in portion of the top of the volcano, for 24 ordered double transition metals carbides, there are 11 kinds of O-MXenes that are candidates for HER. (c) The calculated free energy diagram for hydrogen evolution of doped with Re, W, Os, and other elements and pristine $Cr_2NbC_2O_2$.

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Ti_3C_2 MXene co-catalyst on Ag_3PO_4 for enhanced visible-light photocatalytic activity

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Abstract:

MXene, a novel family of 2D early-transition metal carbides, nitrides, and carbonitrides, has been successfully demonstrated as a co-catalyst for enhancing the photocatalytic activity of a number of photocatalysts[1-3]. In the paper, we showed a feasible strategy of hybrid materials to enhance photocatalytic activity of the Ag_3PO_4/Ti_3C_2 hybrid materials that were fabricated by the electrostatically driven self-assembly process. The morphology, structure, and optical properties of the pristine Ag_3PO_4 and Ag_3PO_4/Ti_3C_2 were characterized in detail, and results revealed that the as-prepared hybrid materials featured Ag_3PO_4 nanoparticles with uniformly assembled Ti_3C_2 nanosheets. With the optimal Ti_3C_2 content, the resultant Ag_3PO_4/Ti_3C_2 hybrid materials exhibited a remarkable enhanced visible light photocatalytic degradation of papermaking wastewater, far exceeding that of bare Ag_3PO_4 nanoparticles. The synergistic effect between Ag_3PO_4 and Ti_3C_2 is contributed to the enhancement of photocatalytic activity, which can improve the separation of photogenerated electron-hole pairs. This work demonstrates the potential of MXene family materials as a co-catalyst to construct highly efficient photocatalysts.

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Synthesis of Ti_3C_2 at a relatively low temperature and its application in supercapacitor

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Abstract:

Ti_3C_2, produced by selectively etching aluminum from MAX Ti_3AlC_2, is a promising two-dimensional MXene material used for chemical researches, however, the synthesis of Ti_3AlC_2 is mostly at high temperature with high energy consumption and equipment requirement. For the first time, we report a novel approach for the synthesis of Ti_3AlC_2 from Ti_2AlC and TiC mixture at a relatively low temperature. Applied the Ti_3C_2 produced from as prepared Ti_3AlC_2 in supercapacitor, the d-Ti_3C_2/NF (2D delaminated Ti_3C_2 sheets/3D Ni foam) composite electrode exhibits a high specific capacitance up to 654 F g^{-1} at 1 A g^{-1} and good cycling stability. An asymmetrical supercapacitor with d-Ti_3C_2/NF composite as a positive electrode, bulk Ti_3C_2 (b-Ti_3C_2) as a negative electrode and 6 M KOH as electrolyte, exhibits a maximum energy density of 18.1 Wh kg^{-1} (at 397.8 W kg^{-1}) and excellent cycling stability (80.6% after 5000 cycles). The results indicate that d-Ti_3C_2/NF composite is a promising electrode material for practical energy storage devices. The introduced approach in this study may open a door for the synthesis of MAX materials at relatively low temperatures with lower energy consumption and equipment requirement, greatly widening the applications of MXene materials in energy storage and conversion.

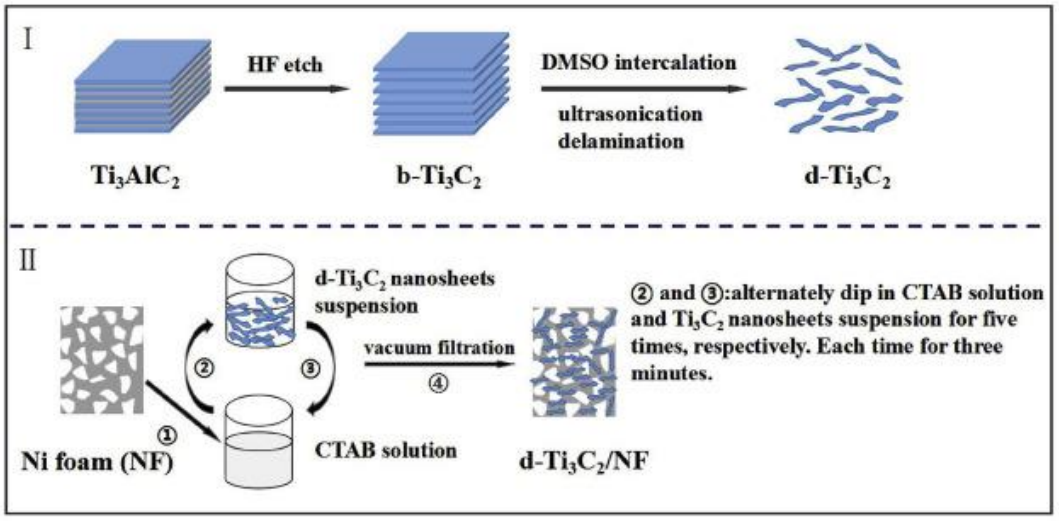

Fig. 1. Schematic illustration of (I) the preparation of d-Ti_3C_2 nanosheets and (II) fabrication of d-Ti_3C_2/NF composite.

Three dimensional MXenes ($Ti_3C_2T_X$) /graphene hybrid aerogel supported Pt nanoparticles for electrocatalysts of direct methanol fuel cells

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Abstract:

The design and construction of nanostructured platinum-based electrode catalysts with high activity at low cost are important for their large-scale applications in fuel cells[1-2]. MXene is a new kind of 2D materials and can be used as electrode support materials because of their hydrophilic surface, metallic conductivity, as well as rich surface chemistries[3-4]. In this work, we employ a bottom-up method to fabricate small-sized Pt nanoparticles (NPs) strongly coupled on 3D porous MXene/graphene hybrid aerogels (denoted as Pt/MG) as anode catalysts for direct methanol fuel cells (Figure 1). Impressively, the as-obtained Pt/MG catalysts possess large surface area, interconnected porous networks, and uniform Pt NPs (Figure 2). As a result, the optimum Pt/MG exhibits excellent catalytic activity, good poison tolerance and reliable long-term stability toward the methanol oxidation reaction, which are superior to those for traditional Pt/carbon black (Pt/C), Pt/carbon nanotubes (Pt/CNT) and Pt/graphene (Pt/G) catalysts.

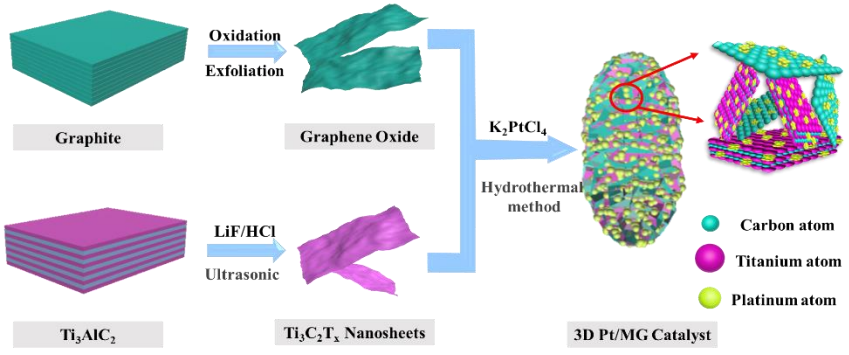

Figure 1. Illustration for the preparation of Pt/MG.

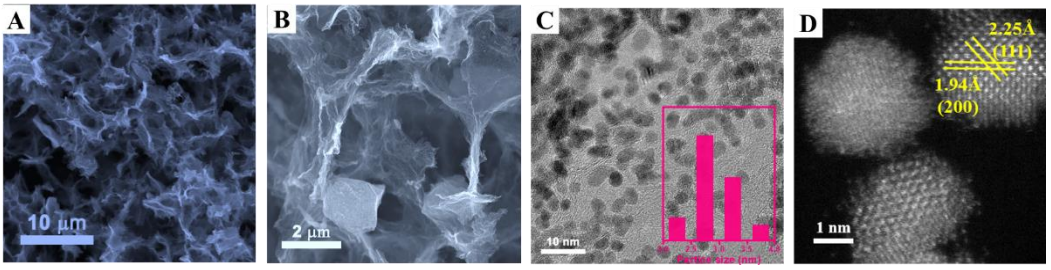

Figure 2. Typical (A-B) FE-SEM, (C-D) HR-TEM images of the 3D Pt/MG architecture.The inset in (C): Pt NP size distribution.

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Multiscale MXene Topographies Programmed by Transfer-Free Mechanical Deformations

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Abstract:

Complex surface topographies emerge in ultrathin two-dimensional (2D) materials undergoing large mechanical deformations. Previous research has explored the approaches of creating complex textures based on 2D materials by conducting multiple deformations on various substrates, which suffer from complex transferring processes and limited productivity. Therefore, transfer-free, programmable and scalable fabrication of multi-scale microstructures of 2D titanium carbide (MXene) has posed a great challenge and not been investigated. Herein, a simple and scalable approach is developed by first depositing MXene ink onto an inflated latex balloon followed with subsequent multi-stage deflations at varying rigidification temperatures. The transfer-free mechanical deformations enable the programmable fabrication of multiscale MXene topographies with controllable characteristics. By controlling the temperature of deflation, the latex substrate can be softened or rigidified and thus tune the mechanical mismatch between latex substrate and MXene nanocoating, leading to the formation of hierarchical MXene structures. With specific rigidification temperatures and deflation sequences applied, multi-generational architectures with structural "memory" effect can be programmed, which was only achievable for multi-transfer processes previously. Meanwhile, the feature size and orientation order of crumples generated at each deflation step can be finely tuned by adjusting the applied pre-strain and deflation direction, respectively. As a demonstration, hierarchical multi-generational MXene microstructures with various characteristics have been fabricated, which show superhydrophobicity and high electrochemical activity with promising applications in anti-fouling substrates, stretchable electronics, barriers and actuators.

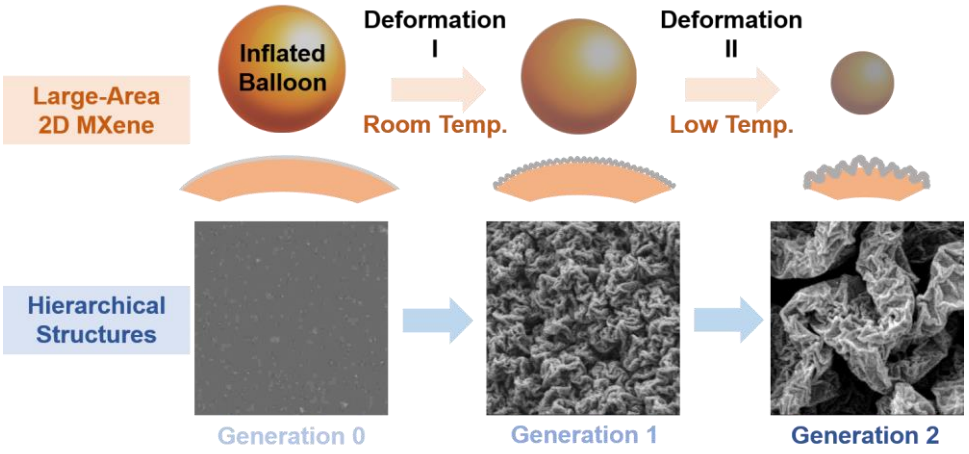

Figure 1. Schematic illustration of fabricating the multiscale MXene topographies by transfer-free mechanical deformations.

Densely-populated isolated single Co-N site for efficient oxygen electrocatalysis

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Abstract:

Atomically dispersed transition metal confined with nitrogen on carbon support have been demonstrated great electrocatalytic performance, but extremely low concentration of metal atoms (usually below 1.5 %) is necessary to avoid aggregation through sintering which limit their mass activity. Here we report a salt-template method to fabricate densely-populated, mono-dispersed cobalt (Co) atoms on a nitrogen-doped graphene-like carbon support, and achieving dramatically higher site fraction of Co atoms (~15.3 %) in the catalyst and demonstrating excellent electrocatalytic activity for both oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) in an alkaline solution. The atomic dispersion and high site fraction of Co provide large electrochemically active surface area (ECSA) of ~105.6 m2/g, leading to very high mass activity for ORR (~6.92 A/mgCo at 0.8V vs RHE: reversible hydrogen electrode), almost 27 times higher than that of the state-of-the-art benchmark Pt/C catalyst (0.26 A/mgPt under similar conditions). It also demonstrates an outstanding mass activity for OER (1.38 A/mgCo). The Zn-air battery based on this bifunctional catalyst exhibites high energy density of 945 Wh kgZn-1 as well as remarkable stability. In addition, both density functional theory (DFT) based simulations and experimental measurements suggest that the Co-N4 sites on the carbon matrix are the most active sites for the bifunctional oxygen electro-catalytic activity.

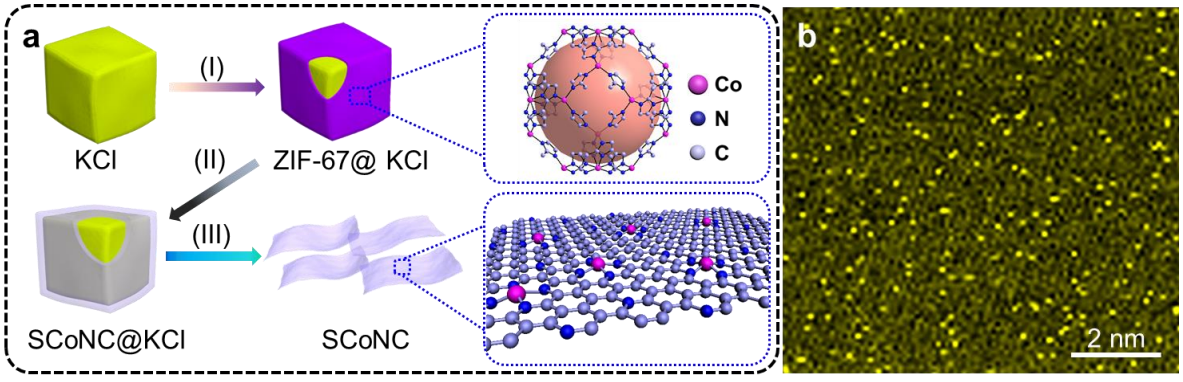

Figure 1. a) Schematic illustration of the synthetic procedure of the SCoNC catalysts. b) HAADF-STEM image of SCoNC, where the white dots were Co atoms.

References:

[1] J. Wu, H. Zhou, Q. Li, M. Chen, J. Wan, N. Zhang, L. Xiong, S. Li, B. Y. Xia, G. Feng, M. Liu, L. Huang*. Adv. Energy Mater., No. aenm.201900149. (under review)

Ultralight Ti_3C_2/MoS_2 foams for broadband microwave absorption

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Abstract:

In this work, ordered lamellar Ti_3C_2 /MoS_2 architectures were designed to satisfy the demand of lightweight and high efficiency for electromagnetic (EM) microwave absorption materials. The hybrid foams were synthesized by self-assembly and in-situ thermal decomposition of ammonium tetrathiomolybdate (ATM). The MoS_2 in-situ grown on the surface of Ti_3C_2 can not only avoid the restack of sheets, but also improve the impedance match and enhance the internal reflection of EM wave. As a result, the free standing foams exhibit excellent EM absorption performance superior to most of the current foam-based counterparts. The EAB covers the whole X band at the thickness of 3.1mm with density of only about 0.004g/cm^3. And its specific EM absorption performance (SMAP = RL (dB)/Thickness (cm)/Density (g cm^{-3})) value can reach 42142.85 dB cm^{-2} g^{-1}. This study evidence that the combination of Ti_3C_2 and dielectric materials like MoS_2 have great potential in EM wave absorption field.

Nitrogen-doped MXene electrodes for high-performance supercapacitors

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Abstract:

MXene is a new discovered family of exfoliated transition metal carbides and/or nitrides, processing excellent electrical conductivity and hydrophilic property. MXene has been demonstrated as a promising electrode material for supercapacitors, and extensive effort has been devoted to further improve its electrochemical properties. In our recent work[1], nitrogen-doped two-dimensional MXene (N-$Ti_3C_2T_x$) was synthesized by post-etch annealing $Ti_3C_2T_x$ in ammonia as a promising electrode material for supercapacitors. The concentrations of nitrogen can be rationally controlled to produce N-$Ti_3C_2T_x$ materials with 1.7-20.7 at.% of nitrogen by simply tuning the annealing temperatures from 200 °C to 700 °C. The introduction of nitrogen as a heteroatom in the $Ti_3C_2T_x$ structure leads to a remarkable increase of the c-lattice parameter of MXene sheets from 1.92 nm in $Ti_3C_2T_x$ to 2.46 nm in N-doped ones upon ammonia treatment at 200 °C. More interestingly, the resultant doped MXene materials under optimized condition exhibited drastically improved electrochemical capacitances of 192 $F \cdot g^{-1}$ in 1 M H_2SO_4 and 82 $F \cdot g^{-1}$ in 1 M $MgSO_4$ electrolyte (Figure 1), which are remarkably higher than those of the un-doped $Ti_3C_2T_x$ materials (34 F·g-1 in 1 M H_2SO_4 and 52 $F \cdot g^{-1}$ in 1 M $MgSO_4$).

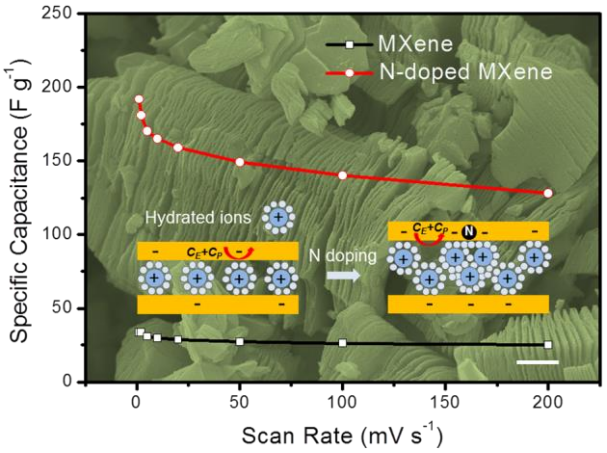

Figure 1. Capacitive performance and possible charge storage mechanism in N-doped MXene.

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Study of the ion intercalation between the MXene membranes for the water membrane application

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Abstract:

MXenes showed great promise as gas separation and water purification membranes. It was proposed that MXene can reject ions by both charge and size sieving mechanisms(1, 2). Generally, it is expected that the interlayer spacing between the MXene nanosheets acts as a trap for the ions and the negatively charged surface of MXene allows for spontaneous intercalation of cations form aqueous salts. However, detailed ion sieving mechanism through the layered MXene sheets hasn't been fully explored. We aim to have a clear and thorough understanding of the water/ions intercalation between the MXene layers by using an advanced spectroscopic characterization techniques. Ions with different charges and hydration radios are expected to have different interaction pattern with MXene. Here we use study the entrapment of various cations. In this work we use in situ XRD-DSC system and in situ environmental SEM to investigate the effect of dehydration and temperature variation on the interlayer spacing of MXene membrane. XRD and SEM have revealed different intercalation patterns with ions and insignificant changes to interlayer spacing of MXene with water, as compared with graphene oxide membrane where a pronounced swilling/contraction was observed with increasing/decreasing humidity. Hence, this study not only allows to understand the ion sieving mechanism of MXene, but also will help to understand and perhaps to help improving the stability MXene membranes stability in aqueous media applications.

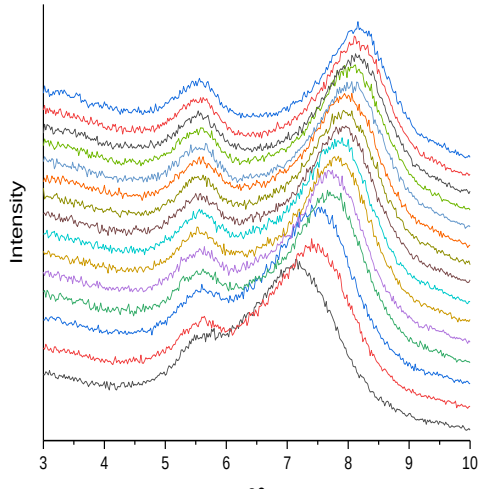

Figure 1 XRD analysis shows the 002 peak shift with increasing the temrature from room temperature to 300 °C.

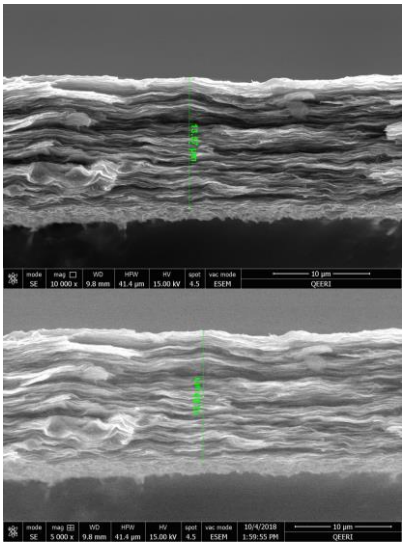

Figure 2 in-situ SEM image with varying relative humidity from a) 25 to b) 90.

References:

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Multi-Wall Carbon Nanotubes Connected MXene as a Binder-Free Electrode for the High Performance Supercapacitor

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Abstract:

In this study, we develop a new method for high performance electrode fabricated by multi-wall carbon nanotube (MWCNT) homogenously connected with $Ti_3C_2T_x$ particles based on the catalysis of nickel and aluminum layered double hydroxide (Ni-Al LDH), which can be directly applied on the carbon cloth as a binder-free flexible electrode for supercapacitor. Electrochemical property was significantly enhanced due to the CNT maintained the original multilayer structure of MXene, bridged the pathways for electron transport between each individual particle, and provided extra-capacitance for supercapacitors. MXene-CNT electrode exhibits the areal specific capacitance of 440.9 mF cm^{-2} at a discharge current of 5 mV/s, and keeping increased retention after 16000 cycles at 10mA cm^{-2}. On this basis, it is proved that our solid-state supercapacitor retains desirable electrochemical performance, leading to the expectation of great promise for flexible supercapacitor and other energy storage devices.

Improving the Properties of 2D Titanium Carbide Films by Thermal Treatment

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Abstract:

$Ti_3C_2T_x$, as one of the most important two-dimensional transition metal carbides, has been widely attracting researchers because of its superb hydrophilicity and excellent specific surface area. However, some of its properties cannot satisfy the requirement of making flexible electronic devices very well, such as electrical conductivity, flexibility and stability in atmospheric environment. Herein, a simple method is proposed to further improve these properties of $Ti_3C_2T_x$ films. After thermal treatment at 300 degrees under argon protection, the resultant films reveal lower sheet resistances, which probably reduce to 1/15 of the previous level. The resistance decreases more for films with higher thickness. Besides, the flexibility and stability of $Ti_3C_2T_x$ also have been greatly enhanced. Based on the characterization of scanning electron microscope and X-ray photoelectron spectroscopy, its mechanism is disclosed. The densification of film structure, the removal of residual organic matter as well as the reduction of terminal groups, such as -F and -OH result in the variation in electrical, mechanical and chemical properties of $Ti_3C_2T_x$. $Ti_3C_2T_x$ films with sheet resistance as low as 1.5 Ω sq^{-1} and enhanced stability and flexibility is obtained through a facile low temperature thermal treatment, which show great potential to fabricate supercapacitors, transparent conductive film and flexible sensor.

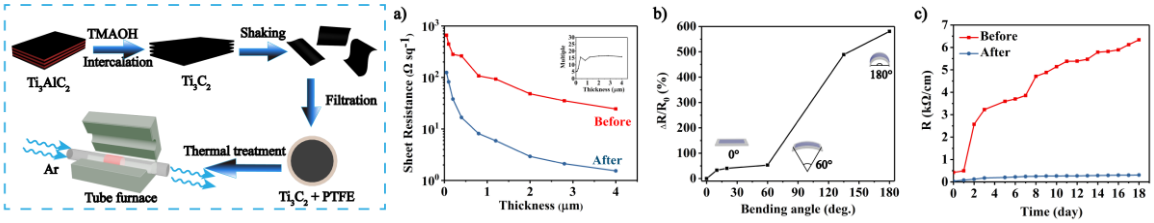

Figure 1. Schematic of $Ti_3C_2T_x$ nanosheets intercalated with TMAOH and thermal treatment process. a) Sheet resistances of $Ti_3C_2T_x$ films with different thicknesses before and after thermal treatment. The inset shows the specific reduction multiple of sheet resistances after thermal treatment. b) Bending test of $Ti_3C_2T_x$ film after thermal treatment. c) Continuous resistance monitoring of $Ti_3C_2T_x$ films before and after thermal treatment.

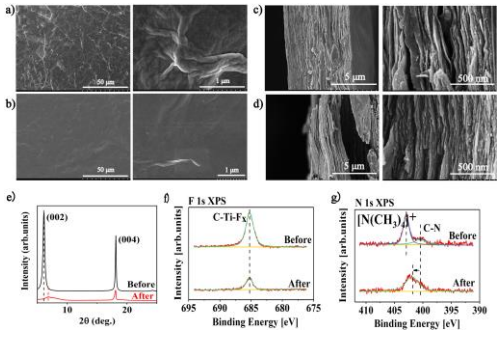

Figure 2. a, b) Top-view SEM images before (a) and after (b) thermal treatment. c, d) Cross-sectional SEM images before (c) and after (d) thermal treatment. e) XRD patterns before and after thermal treatment. f) F 1s g) N 1s XPS spectra before and after thermal treatment.

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Molecular Dynamics Simulation and Comparison of 2D Materials: MXene Mo_2C *vs.* transition metal dichalcogenide Mo_2S

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Abstract:

Two-dimensional (2D) Mo_2C and 1T-Mo_2S are typical MXene and transition metal dichalcogenide (TMP), respectively. Both of them show high stability [1] and electrical conductivity [2, 3], acting as electrodes of energy storage devices such as supercapacitor. Since they also have similar 2D structures, comparison of their performance in supercapacitors with the same electrolyte is helpful for understanding their underlying mechanism of electrical energy storage.

In this poster, molecular dynamics (MD) simulations of 2D Mo_2C and 1T Mo_2S with different interlayer spaces have been conducted to compare and analyze their capacitive performance, in particular the charging dynamics, when adopted as supercapacitor electrodes. The results show that with the same interlayer space, Mo_2C has much quickly charging response than 1T MoS_2. To reach similar charging response, the interlayer space of 1T MoS_2 needs to be increased. It reveals that the initial ionic distribution in slit of Mo_2C is wider than that of 1T MoS_2 with the same interlayer space, which could be helpful for the ionic intercalation or deintercalation during the charging process. Different ionic intercalation or deintercalation paths of Mo_2C and 1T MoS_2 were found by analyzing the changing of ionic distribution between layers during charging process, which could result in different charging responses and is found to be affected by the surface property and interlayer space significantly. Briefly, our simulations show that the Mo_2C has better charging performance compared with 1T MoS_2 with the same interlayer space, and with increased interlayer space, the charging performance of 1T MoS_2 could also be improved.

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MXene and MXene-derived materials for high performance metal-ion batteries and capacitors

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Abstract:

Recently, a hybrid energy storage device called capacitor battery or alkali-metal ion capacitor have be designed to bridge the gap of alkali-metal ion batteries and supercapacitors. Usually, the capacitor battery is constructed from a capacitor-type electrode and a battery-type electrode. Many ion intercalated materials such as $LiMn_2O_4$, MnO_2 and $Li_4Ti_5O_{12}$ are explored as battery-type electrode for capacitor batteries and present capable electrochemical performance. However, the investigation of the capacitor-type electrode is mainly focused on the activated carbon due to its electrochemical double-layer capacitance.

In this work, we designed and fabricated MXene capacitor-type electrode for the capacitor battery. The electrochemical performance of $Ti_3C_2T_x$ MXene material was investigated as electrode for rechargeable aqueous capacitor with Li_2SO_4 and Na_2SO_4 electrolyte, respectively. In addition, both $LiMn_2O_4$//$Ti_3C_2T_x$ Li-ion capacitor battery and MnO_2//$Ti_3C_2T_x$ Na-ion capacitor battery are design and assembled for the first time. Such a low-cost and environmental friendly hybrid system exhibited a high capacity, good rate capability and out-standing cycling performance.

Moreover, we use the graphene oxides (GO) as an inductive agent to obtain the MXene-derived TiO_2 nanoparticles. Meanwhile, GO nanosheets are reduced to RGO and connected by TiO_2 to form a sheet structure. Serving as anode materials, the TiO_2/RGO present high capacity, remarkable rate ability and long cycling performance for both Li and K ion batteries. The superior electrochemical performance is attributed to short ion diffusion path due to the small particle size (15-25 nm) and highway for electron transport provided by RGO. In addition, RGO motivates the capacitive contribution, resulting in enhanced capacity and better rate performance. Meanwhile, the electrochemical kinetics of Li/K ions storage is investigated by quantitative kinetics analysis. This work demonstrates a possibility to introduce the capacitive capacity to realize rapid ion storage and improve the cycling stability, providing a new strategy to design capable electrode for metal ion batteries

References:

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Two-dimensional MXene membrane tailored by Ni^{2+} for hydrogen permeation

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Abstract:

With the development of separation technology, there is growing concern about hydrogen purification. In this work, MXene were tailored by Ni^{2+}, and vacuum-assisted filtration was applied to assemble the Ni-MXene laminates on the surface of Al_2O_3 hollow fiber. Then Ni-MXene/Al_2O_3 composite membranes were prepared by vacuum drying. The composite membranes exhibit excellent gas separation performance for H_2/CO_2 mixture. At room temperature, the separation factor was 432, and permeance of hydrogen was 4.68×10^{-8} mol m^{-2} s^{-1} Pa^{-1}. This may be due to Ni^{2+} was well combination with MXene laminates, realizing the delicate tuning of interlayer spacing of MXene nanosheets.

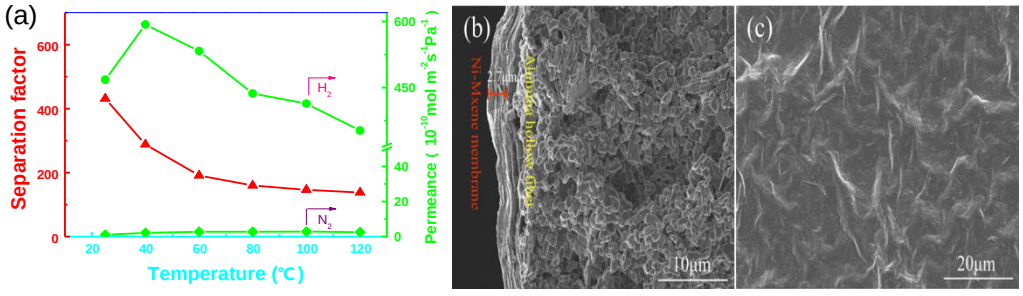

Figure 1. (a) H_2/CO_2 separation performance of composite membrane as a function of function of temperature. SEM image of the cross-section (b) and surface (c) of the Ni-MXene /Al_2O_3 composite membrane.

References:

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3D $Ti_3C_2T_x$ aerogel modified separators for long cycling stability Li-S batteries

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Abstract:

The rational structure design to multifunctional modified separator materials is critical for excellent electrochemical performance of lithium-sulfur (Li-S) batteries. Herein, we designed the titanium carbide ($Ti_3C_2T_x$) aerogel functionalized separators with a three-dimensional (3D) interconnected hierarchical porous network structure to greatly improve electrochemical performance of Li-S batteries. This special 3D aerogel structure avoids the problem that the 2D materials are stackable and can expose more active sites, thus exhibiting a prominent adsorption effect to polysulfide and effectively suppressing the shuttle effect so as to improve cycle stability of Li-S batteries. In addition, $Ti_3C_2T_x$ aerogel has excellent electrical conductivity and porous network structure, which facilitates the transportation of electrons and ions and accelerates the redox reaction kinetics, so as to improve the utilization of active materials and exhibit excellent rate performance. It has been proved that the cells with 3D $Ti_3C_2T_x$ aerogel modified separators have higher initial discharge specific capacity(1487mAh g^{-1} at 0.1C) (1C=1.675mAh g^{-1}) than those with 2D stackable freeze-dried $Ti_3C_2T_x$ functionalized separators and can still achieve a high discharge specific capacity of 670mAh g^{-1} at a high current density of 2 C. Importantly, the cells with 3D $Ti_3C_2T_x$ aerogel modified separators have an ultra-low capacity decay rate of 0.037% per cycle at 1C current density for over 1500 cycles, demonstrating outstanding cycle stability and long cycle life.

Interlayer structure control of laminated MXene thin films for highly sensitive and selective VOC gas sensors

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Abstract:

MXenes are a family of two-dimensional (2D) transitional metal carbides/nitrides with very high electrical conductivity (~10,000 S/cm), and a high density of surface functionalities. Such a unique combination renders MXenes a powerful candidate for gas sensors, as it is required that sensing channel materials possess both high conductivity and strong gas molecule binding sites. In this presentation, laminated MXene thin films and their application as highly sensitive gas sensors will be discussed. Assembled Ti_3C_2 MXene films were able to detect ppb-level volatile organic compound (VOC) gases at room temperature, which is critically important for therapeutic applications. The signal-to-noise ratio (SNR) of Ti_3C_2 gas sensors reached over 350 for ethanol at room temperature, being more sensitive than any other reported 2D material. Furthermore, sodium ions were deliberately intercalated into the interlayers of MXene films to enhance the selectivity of MXene gas sensors toward VOCs. Metal ions allowed the selective intercalation of ethanol gases over CO_2 gases to swell the MXene interlayers, which was confirmed by *in-situ* XRD analyses. By precisely controlling the concentration of intercalated sodium ions in the MXene interlayer, VOC selectivity was increased by 20 times compared to gas sensors based on pristine MXene film.

References:

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Fabrication of $Ti_3C_2T_x$ MXene/CeO_2 nanocomposites for high-performance electromagnetic wave absorption

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Abstract:

Two-dimensional transition metal carbides/carbonitrides (MXenes), has excellently potential applications in the field of electrochemistry owing to its high conductivity and fast charge transporting speed. To the best of our knowledge, despite some progress achieved in the synthesis of $Ti_3C_2T_x$ MXene, studies on the microwave properties of $Ti_3C_2T_x$ MXene and MXene-Derived Nanocomposites remain few. Herein, the composites of $Ti_3C_2T_x$ MXene/CeO_2 with different CeO_2 contents had been synthesized successfully via HF etching treatment and in-situ formed approach. The microwave absorption mechanism of these materials was investigated. Moderated complex permittivity and desirable higher complex permeability presented for the $Ti_3C_2T_x$ MXene/CeO_2 composite, resulting in strong microwave attenuation ability and good impedance matching property. Attributing to the multiple layer structure, the dielectric property of $Ti_3C_2T_x$ MXene/CeO_2, and the synergistic effect between the $Ti_3C_2T_x$ and CeO_2, the as-prepared composites possessed a specific microwave absorbing behavior. This work offers a new route for fabricating novel electromagnetic wave absorbers, and the fine balance among lightweight, broad band, and small thickness of the MXene/CeO_2 nanocomposites makes them promising in the field of electromagnetic wave absorption.

References:

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Robust 3D $Ti_3C_2T_x$ MXene/C Hybrid Foam/Epoxy Nanocomposites with Superior Electromagnetic Interference Shielding Performances

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Abstract:

With the increasingly severe electromagnetic pollution, the demand for electromagnetic interference (EMI) shielding materials with lightweight, excellent mechanical properties and high shielding effectiveness (SE) has become more and more urgent. In this work, few-layered $Ti_3C_2T_x$ MXene was prepared by ionic intercalation and sonication-assisted method. Then the novel porous three-dimensional (3D) MXene/C hybrid foam (MCHF) was prepared by sol-gel method followed by thermal reduction treatment. MCHF/epoxy EMI shielding nanocomposites were prepared by a vacuum-assisted impregnation and curing process. When the mass fraction of MCHF was 4.25 wt% (MCHF-4.25), MCHF-4.25/epoxy EMI shielding nanocomposite exhibited the optimal comprehensive properties, with electrical conductivity of 184 S/m, EMI SE (X-band) of 46 dB, Young's modulus 3.96 GPa and hardness of 0.31 GPa. Compared with the nanocomposite without the addition of MXene, the electrical conductivity was increased by 3.1×10^4 times, EMI SE was increased by 480%, and Young's modulus and hardness were improved by 13% and 11%, respectively. The electromagnetic waves dissipated by multiple reflection and reabsorption in the highly conductive network and converted into thermal energy. The unique three-dimensional conductive network of MCHF would greatly widen the applications of MXene/polymer-based nanocomposites in the field of EMI shielding.

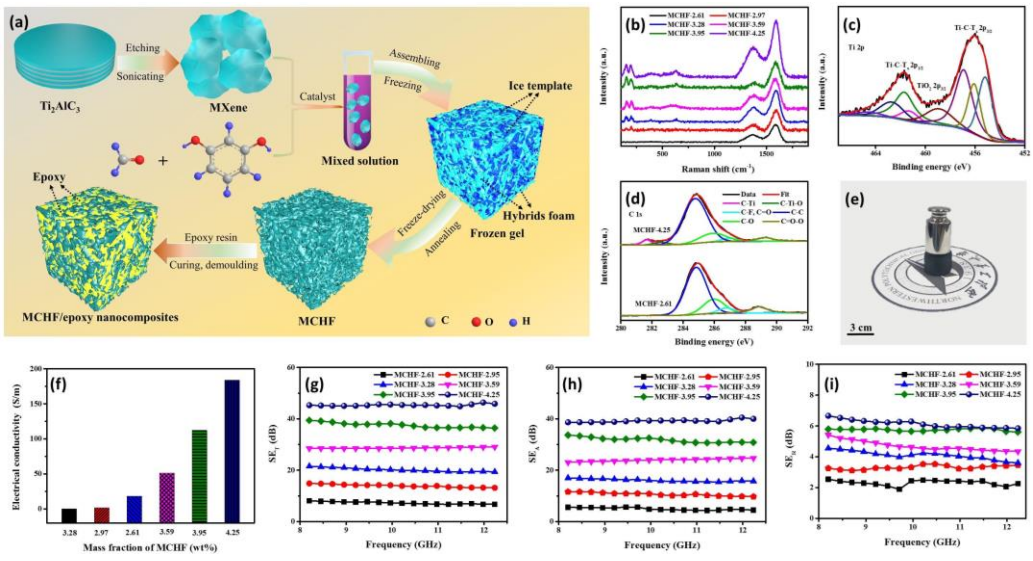

Figure 1 (a) Fabrication process for MCHF/epoxy nanocomposites; (b) Raman spectra of MCHF; (c) Ti 2p spectra of MCHF-4.25 and (d) C 1s spectra of MCHF-2.61 and MCHF-4.25; (e) A 200 g of counterweight supported by MCHF-4.25; (f) Electrical conductivities of the MCHF/epoxy nanocomposites measured at room temperature; (g) SE_T, (h) SE_A and (i) SE_R for MCHF/epoxy nanocomposites at X-band, respectively.

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Strain Sensors with a High Sensitivity and a Wide Sensing Range Based on a $Ti_3C_2T_x$ (MXene) Nanoparticle-Nanosheet Hybrid Network

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Abstract:

Wearable strain sensors have attracted considerable research efforts due to their promising applications in intelligent human/machine interactions, disease diagnosis, personal health care and so forth. However, sensitivity and stretchability, which are the two most critical performance indicators, are mutually constrained, due to their opposite requirements on the sensing material structure. Complicated microstructures of sensing materials and substrates have been designed to balance the two performance, whereas mainly relying on sacrificing either one. To develop strain sensors with both high sensitivity (gauge factor (GF) > 100) and broad strain range (> 50%) is still a grand challenge.

Herein, we fabricated a strain sensor based on a unique $Ti_3C_2T_x$ nanoparticle-nanosheet hybrid network. Through constructing the hybrid structure, the working range was enlarged by 7-10 times with the high sensitivity being maintained. The sensor exhibited high sensitivity (GF from 178.4 to 1176.7) over the entire broad range (0-53%), as well as super low detection limit (0.025%) and good cycling durability (over 5000 cycles). Such high sensitivity (GF 178.4) at the small strain region (0-5%) has seldom been reached for strain sensors with wide sensing range (over 50%) to the best of our knowledge.

The synergetic motion of nanoparticles and nanosheets was mainly responsible for the high performance, of which the migration of nanoparticles generated holes and microcracks, leading to noteworthy variation of resistance, while nanosheets wrapped and bridged the detached nanoparticles, forming bunched conductive clusters and constraining the rapid propagation of the microcracks. The constrained micro-crack propagation mechanism was proposed, which may reveal an ideal solution to reconcile the conflict between sensitivity and stretchability.

Manganese Dioxide Nanowires In-Situ Decorating 2D Titanium Carbide (MXene) as High-Performance Anode for Asymmetric Supercapacitor with Impressive Energy Density

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Abstract:

Two-dimensional (2D) MXenes nanomaterials have been broadly applied in supercapacitors, lithium ion batteries and other energy storage devices due to their unique structure as well as high electric conductivity. However, MXene nanosheets easily get agglomerated and stacked as the large surface energy. To solve the above-mentioned problem, we introduced well-ordered manganese dioxide (MnO_2) nanowires to decorate $Ti_3C_2T_x$ nanosheets by a facile liquid phase co-precipitation method with the aid of polyethylene glycol surfactant. $Ti_3C_2T_x$ was initially modified by polydopamine (PDA) coating to ensure the homogeneous distribution of MnO_2. Owing to the synergistic effect between MnO_2 nanowires and $Ti_3C_2T_x$ backbone, $Ti_3C_2T_x$@α-MnO_2 electrode yielded superior electrochemical performances with a high specific capacitance of 341.2 F g^{-1} with an excellent cycling stability up to 10 000 cycles at a high current density of 3 A g^{-1}. Additionally, asymmetric supercapacitor has been developed employing $Ti_3C_2T_x$@α-MnO_2 composite as positive electrode and activated carbon (AC) as negative electrode in aqueous Na_2SO_4 electrolyte. The prototype device was cycled reversibly in the voltage range of 0~1.8 V, also it manifested maximum energy and power densities of 76.9 W h kg^{-1} and 12 130.5 W kg^{-1}, respectively. These encouraging results show enormous possibilities for applications in high energy density storage systems.

Fabrication of MXene thin film and its electromagnetic shielding properties

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Abstract:

MXenes, a new class of 2D materials, are transition metal carbides, carbo-nitrides and/or nitrides synthesized from corresponding parent MAX phase as a result of etching in acidic environment. $Ti_3C_2T_x$, the representative candidate of this family owes high electrical conductivity, lightweight and easy processability; meeting the critical requirements for an efficient electromagnetic interference (EMI) shielding material. EMI which can cause the malfunctioning of electronic devices and pose a hazard impact on human should be mitigated to make the electronic devices electromagnetically compatible. [1] Although MXene has shown good EMI shielding properties at micro-scale thickness ranges, it has been limited to reveal potential of ultrathin MXene films. In this study, we present the fabrication of various nano-meter thick large area MXene thin films prepared by interfacial self-assembly [2], and their basic electrical, optical and EMI shielding properties. A uniform multi-layer MXene film yields efficient EMI SE and excellent specific shielding effectiveness per unit areal mass density. Moreover, we also investigate the EMI shielding mechanism of nano-meter thin MXene film and prove it by theoretical studies.

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Ti_3C_2 MXene-polystyrene composites for tunable EMI shielding Properties

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Abstract:

Recent growth and innovation in electronics and telecommunication have revolutionized modern era by facilitating human beings. In the meantime, this dramatic upsurge in the number of electronic devices has introduced electromagnetic interference (EMI) pollution; a kind of disturbance causing the malfunctioning of highly integrated circuits. Two dimensional materials with minimal thickness, ease of processing and most importantly absorption dominant EMI shielding capability are strongly needed. 2D transition metal carbides and/or nitrides (MXenes) have shown great potential towards EMI shielding application. [1] Herein, we report synthesis of Ti_3C_2 MXene/polystyrene composite films with different beads size to achieve the desired EMI shielding efficiency. Owing higher electrical conductivity, MXene@PS heterogeneous structure of micro-meter thickness shows excellent EMI SE with major absorption contribution in the microwave frequency range (X-band). Total shielding efficiency along with EM waves' absorption capability of the composite films are optimized by different PS beads size. Composite films with smaller beads size possess higher dielectric domain density (larger surface area) and reveal better EMI shielding.

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Screening surface structure of MXenes by high-throughput computation and vibrational spectroscopic confirmation

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Abstract:

Functionalized MXenes hold promises in a variety of applications in which the dispensable functional groups are mixed. The functionalization is spontaneously realized through competitive adsorption of active species on the MX matrix during the acid etching process of MAX phases. Nevertheless, the knowledge of proportion and distribution of functional groups on MXenes, i.e., surface structures, is still limited. By high-throughput computation screening, ground-state stable structures of four kinds of typical MXenes – Ti_2CT_x, $Ti_3C_2T_x$, Nb_2CT_x and $Nb_4C_3T_x$ (T = O, F, and OH) with mixed functional group compositions are figured out for the first time. The multi-component functional group patterns definitely demonstrate an obvious feature of spatial mixing at a given component. However, the heterogeneous structure has a near linear dependence on the functional group components in terms of free energy. Most functionalized MXenes are dynamically stable except for Nb_2CF_2 and $Nb_2C(OH)_2$ due to their competing displacive counterparts. Last but not the least, Raman spectra of the four kinds of MXenes confirm the predicted stable surface structures of MXenes. This study provides a clear fundamental basis for understanding the surface structures of MXenes.

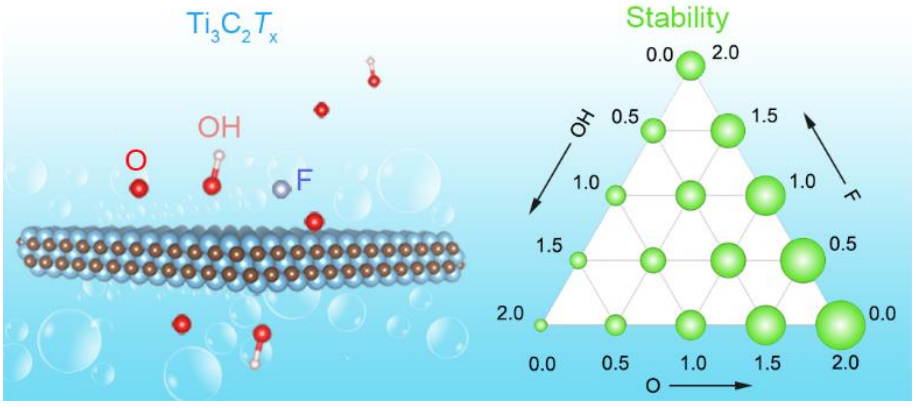

Figure 1. Relative stability bubble plots for (a) $Ti_3C_2O_xF_y(OH)_z$. The bubble size represents the relative stability of a certain MXene.

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Effective Removal of Anionic Re(VII) by Surface-Modified Ti_2CT_x MXene Nanocomposites: Implications for Tc(VII) Sequestration

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Abstract:

Environmental contamination by ^{99}Tc(VII) from radioactive wastewater streams is of particular concern due to the long half-life of ^{99}Tc and high mobility of pertechnetate[1]. Herein, we report a novel MXene-polyelectrolyte nanocomposite with three-dimensional networks for enhanced removal of perrhenate, which is pertechnetate simulant[2]. The introduction of poly(diallyldimethylammonium chloride) (PDDA) regulates the surface charge and improves the stability of Ti_2CT_x nanosheet, resulting in Re(VII) removal capacity of up to 363 mg g−1, and fast sorption kinetics. The Ti2CTx/PDDA nanocomposite furthermore exhibits good selectivity for ReO4− when competing anions (such as Cl− and SO42−) coexist at a concentration of 1800 times. The immobilization mechanism was confirmed as a sorption-reduction process by batch sorption experiments and X-ray photoelectron spectroscopy. The pH-dependent reducing activity of Ti_2CT_x/PDDA nanocomposite toward Re(VII) was clarified by X-ray absorption spectroscopy. As the pH increases, the local environment gradually changes from octahedralcoordinated Re(IV) to tetrahedral-coordinated Re(VII). The overall results suggest that Ti_2CT_x/PDDA nanocomposite may be a promising candidate for efficient elimination of Tc contamination. The reported surface modification strategy might result in applications of MXene-based materials in environmental remediation of other oxidized anion pollutants.

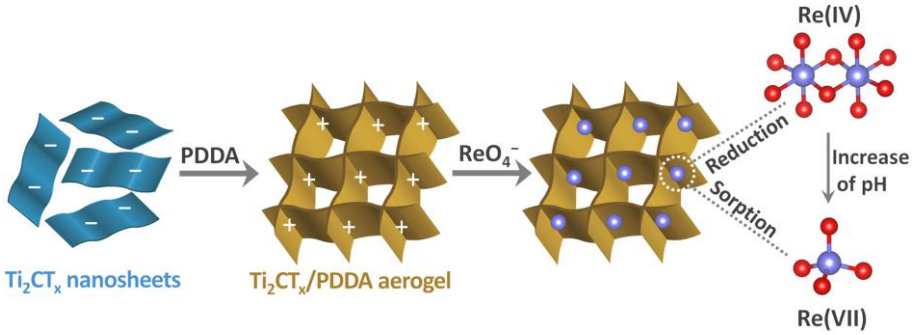

Figure 1. Surface modification of Ti_2CT_x nanosheets with cationic polyelectrolyte for efficient removal of Re(VII) and corresponding mechanism study.

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Superlithiated Polydopamine Derivative/MXene composite as High-Performance Anode for Lithium-Ion Batteries

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Abstract:

Due to the unique layered structure, metallic conductivity and low diffusion barrier for Li^+, the two-dimensional (2D) transition-metal carbides and carbonitrides called MXenes have caused widespread concern for lithium ion battery (LIB) anodes. However, the multilayer tightly stacked structure and low specific capacity have hampered the applications of MXenes in lithium ion batteries. Herein, we synthesize a PDA300/$Ti_3C_2T_x$ composite through in-situ polymerization on the surface of $Ti_3C_2T_x$ nanosheets to improve the Li-ion accessibility by increasing the interlayer space and boost its specific capacity by introducing superlithiated polydopamine derivative (**Figure 1a**). The PDA300/$Ti_3C_2T_x$ composite electrode exhibits high-capacity and high-rate electrochemical performance. The specific capacities of PDA300/$Ti_3C_2T_x$ can reach 1190 mAh g^{-1} at 50 mA g^{-1}, and 550 mAh g^{-1}at 5 A g^{-1}, respectively (**Figure 1b**). Furthermore, a capacity retention is about 82% after 1000 cycle at 1 A g^{-1}, demonstrating the good cyclic stability of PDA300/$Ti_3C_2T_x$ electrode (**Figure 1c**). The excellent lithium storage performance is highly associated to the unique two-dimensional nanostructure and high conductivity of $Ti_3C_2T_x$ substrate, and the superlithiation process of the unsaturated carbon-carbon bonds in the PDA300.

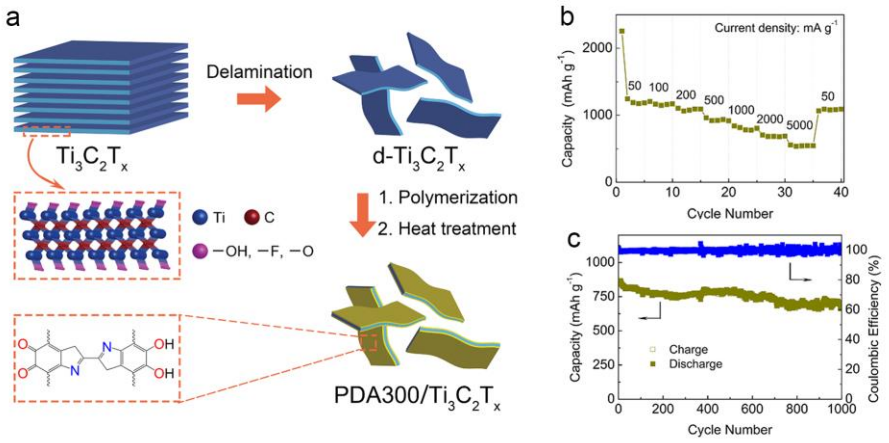

Figure 1. (a) Scheme illustration of the fabrication route of the PDA300/$Ti_3C_2T_x$ composite. (b) Rate performance of PDA300/$Ti_3C_2T_x$. (c) Cycling performance of PDA300/$Ti_3C_2T_x$ at a current density of 1 A g^{-1}.

Acknowledgements:
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"MXene" inspired fabrication of graphene-based materials for high-performance sodium ion capacitors

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Abstract:

MXenes, produced by selectively etching MAX phase, have been attended much interest since initial successful synthesis. Hydrofluoric acid, fluoride salts with hydrochloric acid are selected as the etching agent. MXenes have Heteroatom functional groups with hydrophobicity and metallic conductivity. MXenes with metallic conductivity, hydrophilic surfaces, and reversible intercalation of cation makes most work focusing on electrical and electrochemical properties since its unique structure. The lower ion diffusion coefficient refer to the lower resistance in ions like sodium, lithium diffuse in interlayers. Therefore, MXene is the ideal material for electrochemical energy storage.

For sodium-ion storage, Metal sulfides have superior kinetics by taking advantage of the easy electrochemical reaction between metal sulfur bonds and Na-ion. Now, we plan to study sodium-ion hybrid capacitors used graphene as electrode material drawing on these methods of MXene. The procedure consist of: Treating graphene with a suitable modifier, followed making sulphur atoms intercalate into interlayer by thermal diffusion to Increase layer spacing after annealing will be chosen. Coupling graphene-based composites with counter electrode material, assembled half cells and sodium ion hybrid capacitors. In our view, it has better electrochemical performance.

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Enhanced electrochemical performances of organ-like Ti_3C_2 MXenes/polypyrrole composites as supercapacitors electrode materials

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Abstract:

A novel organ-like Ti_3C_2/PPy nanocomposite has been synthesized via in-situ polymerization of pyrrole monomers to form well-defined and uniformly dispersed polypyrrole nanoparticles on the organ-like Ti_3C_2 nanosheets under a low temperature. The microstructures and electrochemical properties of Ti_3C_2/PPy composites with the different mass ration of PPy and Ti_3C_2 were studied by means of measurement. The analyses reveal that organ-like Ti_3C_2/PPy nanocomposite exhibits the highest specific capacitance of 184.36 F g^{-1} at 2 mV s^{-1} and keeps excellent cycling stability almost 83.33% capacitance retention after 4000 charging-discharging cycles at 1 A g^{-1}. Notably, the high specific capacitance and excellent cycling stability are mainly attributed to the combination of organ-like Ti_3C_2 nanosheets with electric double-layer capacitor (EDLCs) mechanism and PPy nanoparticles with pseudocapacitance behavior, which take advantages of the synergistic effect between different electrode materials and different energy storage mechanisms to improve the electrochemical performance. The organ-like Ti_3C_2 as framework limits the growth of PPy, prevents the stacking of PPy, and promotes structural stability of Ti_3C_2/PPy nanocomposite. Additionally, the intercalation of homogeneous PPy nanoparticles expands the interlayer spacing of Ti_3C_2, and the highly aligned polymer chains can afford more pathways for electrolyte ions diffusion and charge transfer, therefore increasing the specific capacitance and decreasing the charge transfer resistance. And most of all it has shown a low-cost and convenient way to fabricate large-scale Ti_3C_2/PPy nanocomposites which has great potential and promising prospect as electrode materials for supercapacitors.

Facile synthesis SnO_2 nanoparticle-modified Ti_3C_2 MXene nanocomposites for enhanced lithium storage application

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Abstract:

SnO_2 nanoparticle-modified Ti_3C_2 MXene (SnO_2-Ti_3C_2) nanocomposites have been synthesized via hydrothermal method and subsequently used as anode material for lithium-ion batteries (LIBs) with enhanced electrochemical performance. The results of the microstructure analysis indicate that the introduction of SnO_2 nanoparticles enlarged the d-spacing of Ti_3C_2 layers and increased the Li storage. Meanwhile, SnO_2 nanoparticles improve the electrochemical performance based on the alloying mechanism. Electrochemical results reveal that SnO_2-Ti_3C_2 nanocomposites can greatly improve the reversible capacity compared with pure $Ti_3C_2T_x$ particles. Remarkably, SnO_2-Ti_3C_2 nanocomposites show outstanding initial capacity of 1030.1 mAh g^{-1} at 100 mA g^{-1}, and the capacity can remain about 360 mAh g^{-1} after 200 cycles. The SnO_2-Ti_3C_2 nanocomposites demonstrate a stable cycle performance and high reversible capacity for lithium storage.

Preparation of TiO_2/Ti_3C_2 Nanocomposites by One-Step Hydrothermal Method and Its Photocatalytic Activity

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Abstract:

In this study, TiO_2/Ti_3C_2 nano composites were successfully synthesized by a simple one-step hydrothermal method. The phase composition and microstructure of TiO_2/Ti_3C_2 composites were analyzed by XRD, SEM, TEM and BET, and their photocatalytic properties were tested. The composite is obtained by growing TiO_2 crystal particles on two-dimensional layered Ti_3C_2. The composite material combines the excellent photocatalytic performance of TiO_2 and the good electron transporting property of Ti_3C_2. This combination facilitates the rapid separation and transmission of photogenerated carriers which are generated under illumination conditions, and achieves the purpose of accelerating photocatalytic degradation of organic dyes. The results show that the photocatalytic degradation efficiency of TiO_2/Ti_3C_2 composites is significantly better than that of Ti_3C_2 and TiO_2.

Organ-like Ti_3C_2 MXenes/polyaniline composites by chemical grafting as high-performance supercapacitors

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Abstract:

We demonstrated a novel and convenient synthesis of amino-Ti_3C_2/polyaniline (N-Ti_3C_2/PANI) composites as high-performance supercapacitors electrode by chemical bonding between organ-like N-Ti_3C_2 and PANI chains, which were successfully deposited on FTO-glass substrates by a facile two-steps electrochemical reactions. Owing to effective chemical bonds between PANI chains and N-Ti_3C_2 layers, and well-defined Ti_3C_2 layers profiting from organ-like structures, it could afford the rapid pathways for charge/ion transfer and prevent the restacking of Ti_3C_2 layers. Herein, the effects of the electrochemical time of aniline, morphology, structure and electrochemical properties of organ-like N-Ti_3C_2/PANI composites were explored. Experimental results show that N-Ti_3C_2 can act as active sites to combine with the amine nitrogens of PANI chains and promote the growth of aniline monomers on the interlamination and surface of Ti_3C_2 layers. PANI possesses the good pseudocapacitance behavior which can enhance surface area and interlaminar spacing of the Ti_3C_2 MXenes. The N-Ti_3C_2/PANI composites achieve the maximum area capacitance as high as 228 mF cm^{-2} at a scan rate of 5 mV s^{-1}, and almost 85 % capacitance retention is obtained after 1000 charging/discharging cycles. Moreover, the facile synthesis of organ-like N-Ti_3C_2/PANI composite can provide a convenient and green strategy to prepare promising electrode materials for supercapacitors.

Tuning the excellent mechanical property and high EMI shielding performance of MXene film by interface engineering

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Abstract:

High-performance EMI shielding materials with lightweight and flexibility are highly desired to attenuate the electromagnetic interference.[1-3] The development of MXene-based electromagnetic interference shielding materials with simultaneous good performance stability, high-strength and excellent EMI shielding remains a grand challenge to this day. Herein, we report on fabrication of mechanically strong and high-performance EMI shielding $Ti_3C_2T_x$ composite film by incorporating of conducting polymer PEDOT:PSS and sulfuric acid post-treatment to achieve strong interface interaction between $Ti_3C_2T_x$ sheets. The tensile strength of sulfuric acid post-treated $Ti_3C_2T_x$/PEDOT:PSS composite film with only 30 wt% PEDOT:PSS is up to 38.6 MPa (45% increment when compare to that of $Ti_3C_2T_x$ film), while its shielding effectiveness with thickness of ~ 6 μm is up to 37 dB, which achieves a good balance between EMI shielding performance and mechanical properties. Moreover, there is no significant deterioration in the EMI shielding performance of composites after damp and heat test for over 48 hours, which shows excellent performance stability in harsh environment. This study provide a strategy to fabricate mechanically strong and high-performance EMI shielding MXene film, which is highly promising for applications in portable and wearable smart electronics.

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Ultrasmall Sized-SnS Nanosheets Vertically Aligned on Carbon Microtubes for Sodium-Ion Capacitors with High Energy Density

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Abstract:

Sodium ion hybrid capacitors (SHCs) using battery-type and capacitor-type electrodes, are designed to obtain both high energy and power densities[1, 2]. However, the anode materials commonly cannot meet the high capacity and rapid charging/discharging stability requirements[3]. With the help of sandwiched design, herein novel porous carbon microtubes are sandwiched by vertical ultrasmall sized-SnS nanosheets (SnS/aCMT) via combined solvothermal and thermal-treatment approaches (**Figure 1**). The three-dimensional interconnected SnS nanosheets network grown on both sides of the hollow carbon microtubes could greatly prevent their aggregation and facilitate the ions transport, which endows the anode material with improved specific capacity and structural stability. As a result, the SnS/aCMT electrode presents high capacity (517 mA h g^{-1} at 0.1 A g^{-1}) and remarkable rate capability (306 mA h g^{-1} even at 5 A g^{-1}) as well as long cyclic stability with 88.7% retention over 500 cycles. Furthermore, a SHC assembled by using SnS/aCMT as the anode and aCMT as the cathode, presenting a high energy density of 115 Wh kg^{-1} in the voltage range of 0.5–4.0 V and stable long-cycling performance.

Figure 1. Schematic illustration of the preparation process of SnS/aCMT and assembled sodium hybrid capacitor.

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Design of Biomimetic MXene-base Electrocatalytic Nitrogen Fixation Materials

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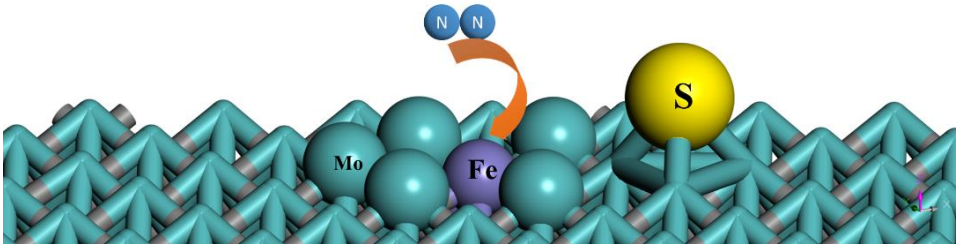
Abstract:

In order to design an efficient nitrogen-fixing electrocatalyst, MXene with excellent electron transport performance was selected as the base material to construct the composite structure. On the surface of the material, we used FeMo cofactor structure of nitrogenase for reference, and constructed similar structure by doping and loading monoatoms to optimize the performance of electrocatalytic nitrogen fixation. At the same time, we analyzed the competitive relationship between HER and NRR on the surface of materials, and proposed a new strategy to effectively improve the efficiency of NRR.



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Research Progress of SnSe-Base Composite Two-Dimensional Transition Metal Carbides Material Thermoelectric Film Properties

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Abstract:

As a material for converting thermal energy into electrical energy, thermoelectric materials have attracted more and more attention. SnSe is a material with high thermal power superiority, especially its b-c plane of β phase, its electric power is higher than other plane. Accronding to the thermoelectric figure of merit ZT=S2σT/k, where S is the Seebeck coefficient, σ is the conductivity, and the thermal conductivity, we know that SnSe has poor mechanical properties and high thermal conductivity, so its thermoelectric properties will be not goo[1]. which is a semiconductor, its thermal conductivity is low. We use SnSe as a base material, compound it with it, cast it into a film by casting, and anneal it at 400-600 °C. we can get SnSe-Base Composite Two-Dimensional Transition Metal Carbides Material Thermoelectric. The conductivity, the Seebeck coefficient and the thermal conductivity of the film were measured, and the thermoelectric figure of merit was found to be improved. We have selected several different types of Two-Dimensional Transition Metal Carbides Material (Ti_2CT_x、Ti_2NT_x、Nb_2CT_x ect) to study the effects of different Two-Dimensional Transition Metal Carbides Materials on the thermoelectric properties of the materials and found that their thermoelectric properties have improved[2].

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Mechanical Properties and Corrosion Behavior of $Ti_3(Al_{1-x},Ga_x)C_2$ solid solution

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Abstract:

Nearly dense and almost single-phase bulk $Ti_3(Al_{1-x},Ga_x)C_2$ (x = 0, 0.1, 0.2, 0.3, and 0.4) materials were fabricated by hot-pressing method using Ti, Al, TiC, and Ga as raw materials. The lattice parameters, microstructure, and mechanical properties of the $Ti_3(Al_{1-x},Ga_x)C_2$ ceramics were investigated in detail. The results indicated that the lattice parameters (especially the c axis) decreased with the substitution of Al by Ga. The dependence of the mechanical properties on the Ga content was a single-peak type. The $Ti_3(Al_{0.7},Ga_{0.3})C_2$ ceramic possessed the optimal mechanical performance and its Vickers hardness, flexural strength, and fracture toughness reached the values of 7.87 GPa, 403.17 MPa, 7.74 $Mpa \cdot m^{1/2}$, respectively, due to the solid solution effect. On the other hand, due to the activation of Al by Ga, the stripping energy of Al layers is greatly reduced, so it provides a new method for the preparation of MXene by substitution of the A-sublattice in MAX phase. Therefore, studying the mechanical properties and corrosion behavior of $Ti_3(Al_{1-x},Ga_x)C_2$ solid solution is of great significance.

Phase transition induced unusual electrochemical performance of V_2CT_X MXene for aqueous zinc ion battery

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Abstract:

Non-battery behavior related phase transition of electrode is usually not favorable for any batteries because it results in performance degradation all times. Here we demonstrate a zinc ion battery (ZIB) with an unusual capacity enhancement even within 18000 cycles by employing V_2CT_X MXene as the cathode, enormously differing from all the reported counterparts with capacity degradation initiated within hundreds of cycles. The dominated mechanisms are determined to be MXene delamination and an unexpected phase transition during cycling. Both the original cathode and secondary derivate contribute to capacity simultaneously, resulting in the unusual capacity enhancement. Consequently, an unprecedent specific capacity of 508 mAh g^{-1} (highest for all reported ZIBs) and high energy density of 386.2 Wh kg^{-1} are realized. Also, the quasi-solid-state batteries fabricated can output stably at -20 ℃ and in bending, twisting, stabbing and cutting conditions. Our work brings a new breakthrough approach, that is, utilizing "unstable" electrode materials, which should usually be avoided, to achieve continuously enhanced performance of a battery. The idea to use both original and secondary materials for energy storage may be developed to be a general method to achieve extraordinary cycling stability of batteries.

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Atomic Sn^{4+} Decorated into Vanadium Carbide MXene interlayers for Superior Lithium Storage

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Abstract:

Ion intercalation is an important way to improve energy storage performance of two dimensional materials. However dynamic energy storage process in such layered intercalations is rarely studied, mainly due to the lack of effective *operando* methods. Here we demonstrate a unique atomic Sn^{4+} decorated vanadium carbide (V_2C) MXene not only exhibiting highly enhanced lithium ion battery (LIB) property up to 1284.6 mA h g^{-1} at 0.1 A g^{-1}, but also possessing outstanding rate performance and superior cyclic stability due to the expanded interlayer and formation of V-O-Sn bonding. More importantly, in combination with *ex-situ* tests, our *operando* X-ray absorption fine structure (XAFS) measurements are performed to explore the dynamic mechanism of V_2C@Sn MXene electrode in LIB. The results clearly reveal the valence changes of vanadium (V), tin (Sn) and positive contribution of oxygen (O) atoms during the charging/discharging process, confirming their contribution for lithium storage capacity. The stability of intercalated MXene electrode is also *in-situ* observed and understood.

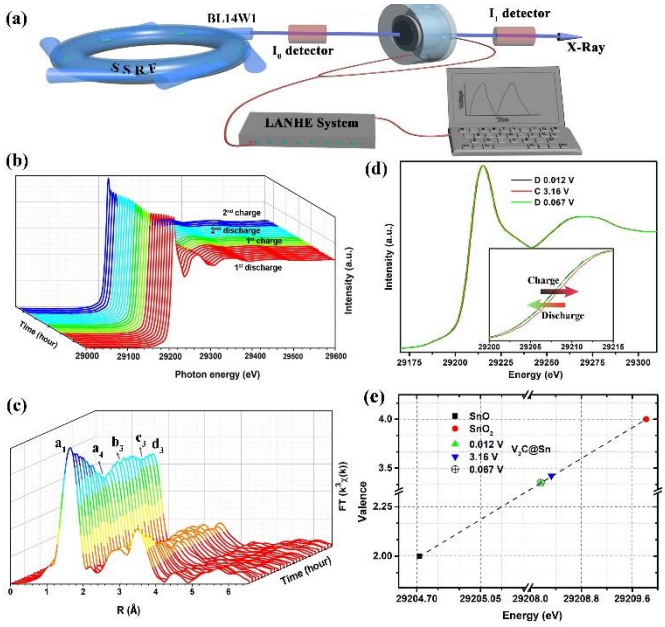

Figure 1. Operando Sn K-edge XAFS study for V_2C@Sn MXene electrode**.** (a) Schematic diagram of the *operando* XAFS testing environment. (b) *In-situ* Sn K-edge XAFS spectra. (c) Fourier-transformed Sn K-edge EXAFS spectra corresponding to (b). (d) Normalized XANES spectra of Sn K-edge at different voltages, inset: enlargement of the absorption edge. (e) Chemical valence of Sn atom in SnO, SnO_2, and V_2C@Sn electrode.

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Synthesis and characterization: From MAX phase V_4AlC_3 to MXene $V_4C_3T_x$

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Abstract:

Recently, MXenes, a new class of 2D nanomaterials, have been widely investigated because of their advantages, such as special microscopic morphology, flexible tunability in element composition, hydrophilicity, metallic nature, high charge-carrier mobility, and favorable mechanical properties. 2D MXenes used as electrochemical electrodes or electrocatalysts have shown superior performance and have made significant impact in the field of energy storage and conversion as well advanced catalysis. However, the numbers of MXenes (about 30) are much less than that of their precursor compounds (more than 70). It is important and necessary to synthesize new MXenes to expand their family and applications in other fields. Very recently, we have successfully synthesized single phase V_4AlC_3 and by selectively etching Al layers from V_4AlC_3 in hydrofluoric acid at 55℃ we also have obtained corresponding MXene $V_4C_3T_x$, which have been confirmed by XRD, SEM, EDX, TEM, and XPS characterizations. Large interlayer spacing (~ 0.466 nm) and specific surface (~ 52 $m^2 g^{-1}$) can be obtained in V_4C_3 MXene via adding sufficient ball-milling treatment on precursor V_4AlC_3. Furthermore, good conductivity, hydrophilicity, and thermostability, as well as abundant valence states (V^{2+}, V^{4+}, and V^{5+}) have also been found in MXene $V_4C_3T_x$. Based on the abovementioned features, $V_4C_3T_x$ will be widely used in energy storage and conversion fields.

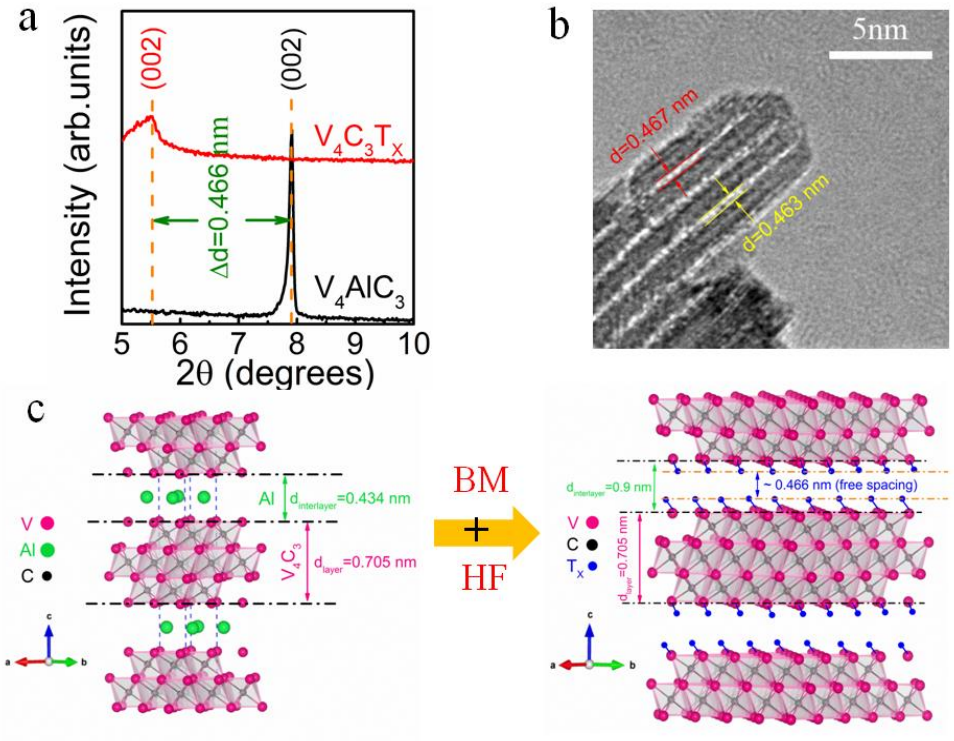

Figure 1. (a) XRD diffraction patterns for the MAX phase V_4AlC_3 and the MXene $V_4C_3T_x$; (b) The cross-section HRTEM images of the MXene $V_4C_3T_x$; (c) The schematic diagram of the crystal structure for MAX phase V_4AlC_3 before and after HF treatments (MXene $V_4C_3T_x$). T_x stands for the surface functional groups, such as -O, -OH, and/or -F; BM stands for the ball milling.

Controllable preparation of MXene-derived two-dimensional porous carbon nanosheets for high-performance supercapacitors

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Abstract:

Two-dimensional (2D) porous carbon materials have attracted intense researching interest for supercapacitors (SCs) due to their high aspect ratio and large surface area. Herein, we propose an exfoliation-self assembly-chlorination route for preparing ultrathin MXene-derived carbon (MDC) nanosheets and 2D-2D MDC-ordered mesoporous carbon (MDC-OMC) by using layered MXene as the template and precursor. Due to the large intersheet space of exfoliated layered MXene, the as-prepared carbon materials exhibit large specific surface areas and hierarchical porosity. These features significantly improve the ion-accessible surface area for charge storage and shorten the ion transport length in thin dimension. As a result, these 2D carbon nanosheets materials show high specific capacitances and remarkable high power capabilities when used as electrode materials for SCs. The method described here provides a new route to prepare 2D electrode materials from bulk precursor, thus exploiting their full potentials for energy-storage devices.

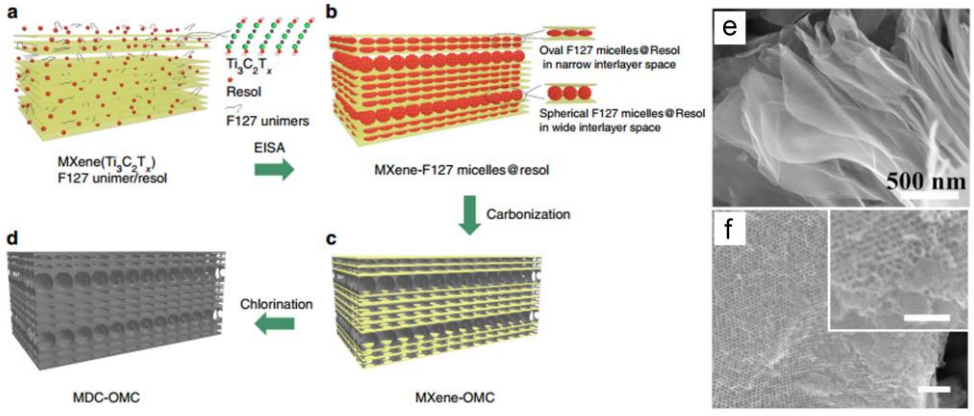

Figure 1. Schematic illustration of the synthetic route: preparation of the (a) MXene/F127 unimer/resol mixture, (b) MXene-F127 micelles@resol composite, (c) MXene-OMC composite and (d) MDC-OMC composite. SEM images of MDC and MDC-OMC composite.

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$Bi_4O_5Br_2$/monolayer-Ti_3C_2 composite with enhanced visible-light photocatalytic activity

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Abstract:

$Bi_4O_5Br_2$ is a photocatalyst with open layered structure, indirect photoelectron-hole transition and excellent response to visible light[1], but it still has serious problem of photogenicelectron-hole pair recombination. MXenes, with its advantages of good conductivity, anisotropy and high carrier mobility, can be used as a cocatalyst of $Bi_4O_5Br_2$ to accelerate the separation of photogenerated electrons and holes[2]. Therefore, we constructed $Bi_4O_5Br_2$/monolayer-Ti_3C_2 composite in order to obtain higher visible light catalytic activity. $Bi_4O_5Br_2$/monolayer-Ti_3C_2 composite was synthesized using a simple precipitation method. Additionally,the visible Photocatalytic degradation tests of sulfamethoxazole (SMX) show that $Bi_4O_5Br_2$/monolayer-Ti_3C_2 composite had higher photocatalytic activity than pure $Bi_4O_5Br_2$,and when the composite amount of Ti_3C_2 was 0.165wt‰, the visible Photocatalytic degradation had the best effect(Fig.2). The result suggest that $Bi_4O_5Br_2$/monolayer-Ti_3C_2 composite constructed an effective transmission channel of photogenic electron holes, which could transfer the photogenic electrons migrated from $Bi_4O_5Br_2$ to Ti_3C_2 rapidly. Therefore, it can effectively promoted the separation of photogenic electron hole pairs, increased the carrier life, and thus obtained higher photocatalytic activity.

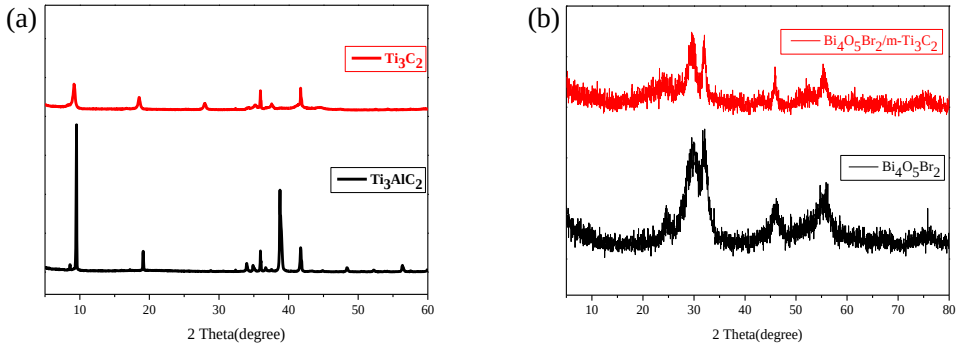

Fig.1 XRD patterns of (a) Ti_3AlC_2, m-Ti_3C_2 and (b) $Bi_4O_5Br_2$,$Bi_4O_5Br_2$/m-Ti_3C_2

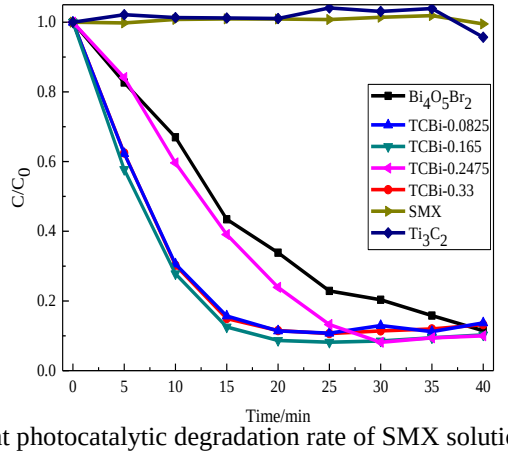

Fig.2 Visible-light photocatalytic degradation rate of SMX solution over different sample

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The sodium storage mechanism of nitrogen-doped mesoporous carbon sphere

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Abstract:

The capacitive contribution of nitrogen-doped mesoporous carbon sphere (NMCSs-800) is obtained around 53% at 0.5 mV/s (Figure 4a, 4b and 4c). The capacitive contribution increases with the increasing of scan rate (40% at 0.1 mV/s to 70 % at 1.4 mV/s, Figure 4d), manifesting that the high ratio of capacitive contribution is beneficial to the rate performance. Moreover, the results support both adsorption-pore-filling [1, 2] and insertion mechanism [3] for Na^+ storage in hard carbon. Moreover, the position of G-band shows gradually red-shift from open circuit potential (OCP,) to 0.4 V and 0.02 V in the discharge process (Figure 4e and 4f) because that Na^+ intercalants endowing electrons to the hard carbon [4, 5], manifesting that the intercalation of Na^+ dominates at 0.3 V to 0.02 V. Meanwhile, the intensity of D-band exhibits a dramatic change during the GCD process, verifying that the defects in the NMCSs-800 is reduced due to the adsorption of Na^+ ion on defects during the discharge process. Therefore, the slope region above 0.3 V is attributed to the adsorption of Na^+ and the slope region of 0.3 V-0.02 V is ascribed to both the adsorption and intercalation of Na^+.

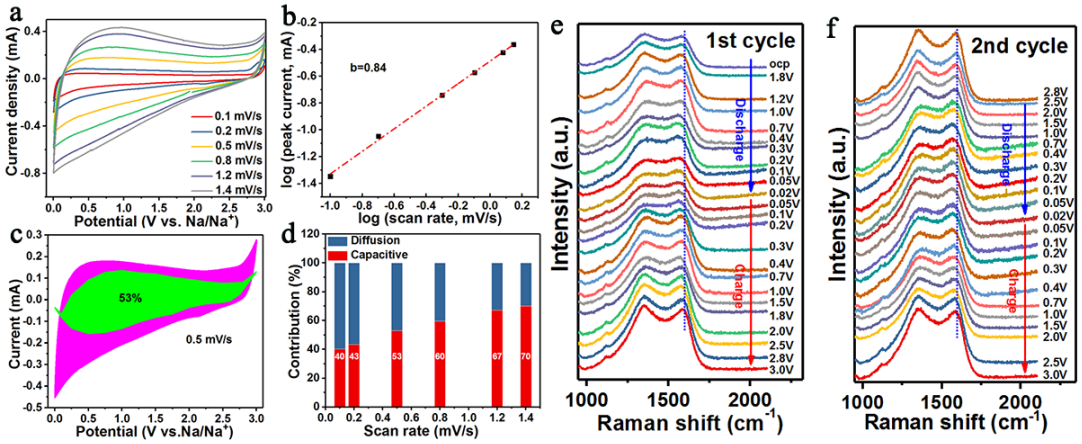

Figure 1. Kinetic analysis of NMCSs-800 electrode for Na^+ ion storage: a) CV curves at different scan rates; b) log (scan rate)-log (peak current) profile; c) capacitive (yellow) and diffusion-controlled (pink) contribution to Na^+ storage of NMCSs-800 at 0.5 mV/s; d) Normalized contribution ratio of diffusion-controlled (blue) and capacitive (red) capacities at various scan rates. In-situ Raman spectra of NMCSs-800 for SIBs at the e) first cycle and f) the second cycle with the current density of 200 mA/g (532 nm laser excitation).

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Multifunctional 2D CuSe monolayer nanodevice

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Abstract:

In a very recent experimental work, a graphene-like CuSe monolayer (ML) was realized. Motivated by this success, we performed first-principles calculations to investigate its electronic transport and photoelectronic properties. We find that the CuSe ML shows a strong electrical anisotropy, and its current-voltage (*I*–*V*) curves along the zigzag and armchair directions are noticeably different. The CuSe ML also displays a useful negative differential resistance (NDR) effect along the both directions when the bias is beyond 1.0 V. Moreover, it has a large photon absorption to orange light. Our study suggests that CuSe ML is a multifunctional material and has various potential applications in electrical-anisotropy-based, NDR-based, and even optical nanodevices.

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3D MXene/graphene Hybrid Aerogels for High-performance Electromagnetic Interference Shielding

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Abstract:

Two-dimensional (2D) transition metal carbides/carbonitrides (MXenes) integrating versatile surface chemistry and considerable electrical conductivity are promising materials for various potential applications.[1] However, the easy restacking of 2D nanosheets results in increased contact resistance and poor dispersion in polymer matrices when they are employed as conductive nanofillers in functional nanocomposites.[2] Given this, we developed a mild hydrothermal method to assemble 2D MXene into 3D architecture which can act as the conducting pathway for polymer nanocomposite. The resultant MXene-based aerogel, combined with the well-retained intrinsic structure of MXene and aligned core-shell structure, shows promising electrical conductivity as high as 1085 S m^{-1}. When used as conductive networks in shielding materials, the aerogel endows epoxy nanocomposite with remarkable electrical conductivity (695.9 $S \cdot m^{-1}$), and the electromagnetic interference shielding effectiveness of the nanocomposite exceeds 50 dB with maximum value of 56.4 dB over X-band. The building of 3D MXene-based architecture opens new avenue for the application of MXene in various fields.

Acknowledgements：

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High-performance Polydimethylsiloxane/$Ti_3C_2T_x$ (MXene) Nanocomposite Foam for efficient electromagnetic interference shielding

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Abstract:

Lightweight and compressible electromagnetic interference (EMI) shielding polymer nanocomposites are urgently required to solve increasingly serious electromagnetic pollutions.[1] Two-dimensional transition metal carbides and nitrides (MXenes), especially $Ti_3C_2T_x$, are ideal candidates for constructing highly efficient conduction networks in polymer matrices due to their intriguing layered structure and high electrical conductivity.[2,3] Herein, compressible and electrically conductive and lightweight polydimethylsiloxane (PDMS)-coated MXene foams are fabricated by preforming three-dimensional (3D) MXene aerogel architectures assisted with sodium alginate followed by coating a thin layer of PDMS to enhance stability and durability of the porous architecture. Consequently, the lightweight aerogel achieves an outstanding conductivity of 2211 S/m and a high EMI shielding efficiency of 72 dB. Moreover, the PDMS coating effectively endows the 3D conductive network with excellent compressibility and durability. The PDMS-coated MXene foam with only 6.1 wt% of MXene shields over 99.99% of incident electromagnetic waves and reserves its high EMI shielding efficiency after 500 compression cycles. Therefore, the lightweight, compressible and conductive PDMS-coated MXene foam is promising for applications in EMI shielding gaskets, wearable electronics, sensors and other specific areas.

Acknowledgements:

Financial support from the National Natural Science Foundation of China (51673015, 51373011, 51533001), the National Key Research and Development Program of China (2016YFC0801302), and the Fundamental Research Funds for the Central Universities (BHYC1707B) is gratefully acknowledged.

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Flexible and Stretchable Electrically Conductive MXene/Natural Rubber Nanocomposite Film for Efficient Electromagnetic Interference Shielding

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Abstract:

Flexible and stretchable thin electromagnetic interference (EMI) shielding materials are in great demand due to their versatile adaptable capability to complex various surfaces, especially in the next-generation foldable and wearable electronics.[1] However, it remains a great challenge to simultaneously achieve outstanding EMI shielding efficiency and satisfactory stretchability and flexibility due to the susceptibility of conductive networks under complicated deformations. Herein, we report a facile approach for fabricating electrically conductive $Ti_3C_2T_x$/natural rubber (NR) nanocomposite film with superb EMI shielding performance through a vacuum filtration process by using the same charge to ensure the uniform dispersion of MXene nanosheets and NR latex. The resultant nanocomposite with a thickness of 196 μm shows an excellent conductivity of 500 S/m and outstanding EMI shielding effectiveness of 29.9 dB at 3.10 vol%. At the same time, the tensile strength and Young's modulus of the nanocomposite film are significantly increased by 463.3% and 425.5% as compared to those of pristine NR. The excellent stretchability and elasticity make the film ultimately retain its original electrical and EMI shielding performances even after long-term stretching and folding deformations.[2,3]

Acknowledgements:

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Preparation of Thin Sheet Ti_3C_2 and In-situ Construction Mechanism and Electrochemical Properties of Low-Dimensional Derivatives

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Abstract:

Ti_3C_2 has been widely used in lithium-ion batteries, supercapacitor and other energy storage fields because of its unique two-dimensional layered structure. In general, people obtain Ti_3C_2 by selective etching of Ti_3AlC_2 with HF. However, HF is harmful to human health. At the same time, the F^- on the surface of the material after HF etching will lead to the decrease of electrochemical performance. In my study, HCL+LiF was used to corrode Ti_3AlC_2 and continuous ultrasonic of a physical peeling method to acquire thin sheet Ti_3C_2 which specific surface is larger and beneficial to improve its electrochemical performance. In addition, according to research show that adding the transition metal oxides into MXene is an effective way to improve its electrochemical properties. Among them, TiO_2 is one of the most widely studied electrode materials which has the advantages of high availability, convenient synthesis, low cost and so on.[1] Herein, on the basis of Ti_3C_2 of thin sheet structure, the surface of Ti_3C_2 was slowly oxidized by OH^- and oxygen-containing functional groups by pouring into NaOH/KOH(aq.) and alkaline etching in room temperature so that TiO_2 were grown in situ. This work not only studies the in-situ growth mechanism of Ti_3C_2 and its low-dimensional derivatives, but also provides a simple method for the preparation of Ti_3C_2/TiO_2 composites with excellent electrochemical performance.

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Monolayer Sc_2CO_2: a promising candidate for SO_2 gas sensor or capturer

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Abstract:

With the rapid development of modern industry and the intensively increasing of air-pollution, it is highly desirable yet challenging to develop new functional gas-sensing materials for achieving high-performance gas sensors especially for toxic SO_2 so far[1]. Recently, two-dimensional (2D) MXenes have attracted tremendous attention because of their fascinating physical and chemical properties[2]. Therefore, we have explored the gas-sensing performance of M_2CO_2 (M=Sc, Hf, Zr, Ti) monolayers in more detail, by means of first-principle calculations. It is found that monolayer Sc_2CO_2 outperforms the others as a promising candidate for SO_2 gas sensor or capturer, with high selectivity and sensitivity, controllable capture, or reversible release by applying external tensile strains or E-fields[3]. This can be ascribed to the distinctive findings: (1) Monolayer Sc_2CO_2 stands out for molecular SO_2 physisorption with the desirable interaction strength and excellent stability, coupled with prominent modifications in electronic band structures and appreciable charge transfer; (2) A sharply increased electronic conductivity upon SO_2 adsorption manifests monolayer Sc_2CO_2 highly sensitive to SO_2 molecule. (3) In-plane tensile strains or external vertical electronic fields can effectively modulate the interaction strength of molecular SO_2 adsorbing on Sc_2CO_2, and thereby realize the controllable capture or reversible release of toxic SO_2 gas.

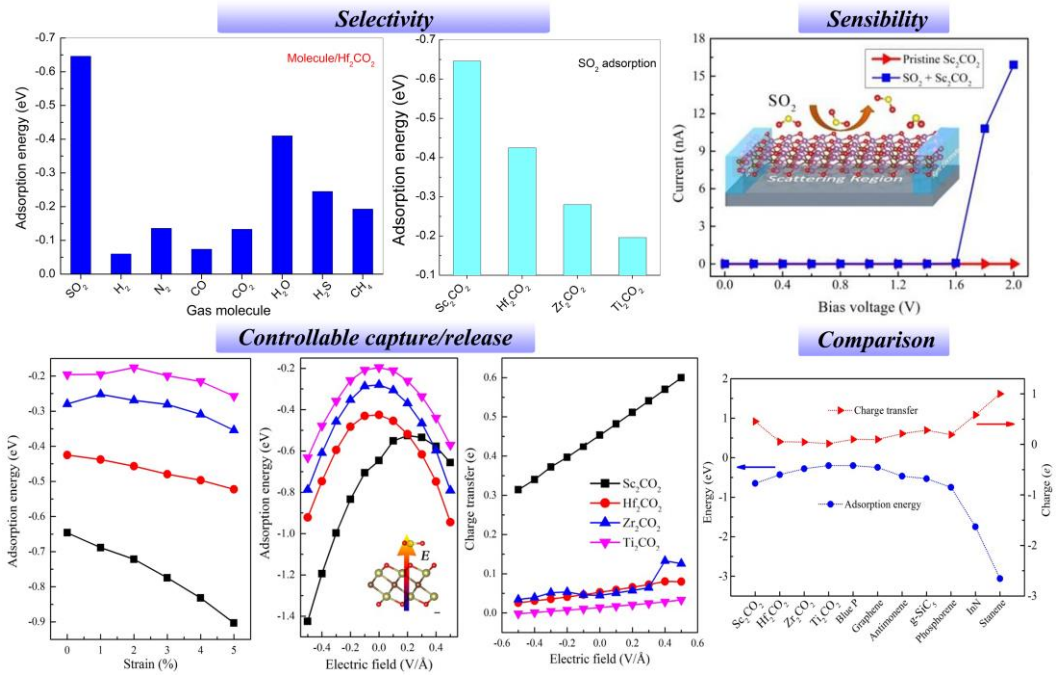

Figure 1. An illustration for the gas-sensing properties of monolayer Sc_2CO_2 toward SO_2 molecule, along with the key results for SO_2 molecule adsorbed on various nanosheets for comparison (right-down panel).

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Strong and Biocompatible Poly(lactic acid) Membrane Enhanced by $Ti_3C_2T_z$ (MXene) Nanosheets for Guided Bone Regeneration

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Abstract:

Herein, strong and biocompatible $Ti_3C_2T_z$-enhanced poly(lactic acid) (PLA) nanocomposite membranes were prepared. The interface of the $Ti_3C_2T_z$ nanosheets with the hydrophobic PLA matrix was mediated using n-octyltriethoxysilane (OTES). The optimized ultimate tensile strength of the OTES-$Ti_3C_2T_z$/PLA nanocomposite membrane was 72 MPa (33% higher than that of a pure PLA membrane). The addition of $Ti_3C_2T_z$ enhanced the biological properties of the membrane, including the *in vitro* adhesion, proliferation, and osteogenic differentiation of MC3T3-E1 mouse preosteoblasts.

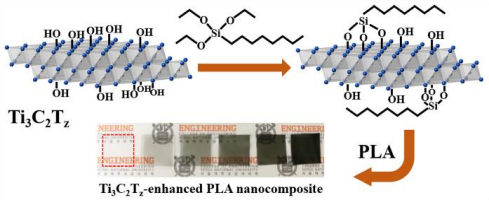

Figure 1. N-octyltriethoxysilane was used to mediate the interface between $Ti_3C_2T_z$ nanosheets and poly(lactic acid).

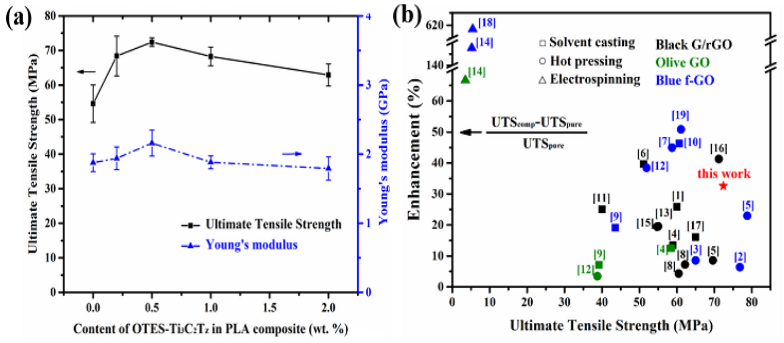

Figure 2. (a) UTS and Young's modulus of pure PLA and OTES-$Ti_3C_2T_z$/PLA nanocomposite membranes; **(b)** Comparison of UTS and its enhancement of OTES-$Ti_3C_2T_z$/PLA nanocomposite membrane in this work with those of the membranes which were enhanced by graphene (or reduced GO), GO, and functional group modified GO from the references. [1-4]

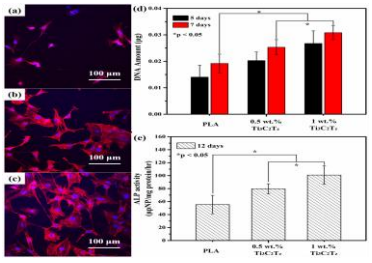

Figure 3. Typical CLSM images of adherent MC3T3-E1 cells on pure PLA and OTES-$Ti_3C_2T_z$/PLA nanocomposite membranes: **(a)** pure PLA, **(b)** 0.5 wt. %, **(c)** 1 wt. %; **(d)** DNA assay for the determination of cell viability after 5-day and 7-day incubation; **(e)** ALP assay for the determination of cell differentiation after 12-day incubation.

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First-principles study on the formation mechanisms and properties of $Ti_3C_2O_2$-MXene with N dopants

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Abstract:

In recent years, two-dimensional materials have shown great application potential and broad development prospects in the field of supercapacitors, due to their large surface area, flexible layered channels and tunable electronic structures [1]. Among them, transition metal carbide/nitride nanosheets (MXenes) were discovered by researchers at Drexel University, by selectively etching the *A* layer of the ternary layered compound material MAX, who possess better conductivity and stacking density [2]. In order to further improve some properties of MXenes, introducing dopants (nitrogen sulfur, boron and phosphorus) is an effective method. However, there are few studies on the tailoring of MXenes at this moment, while in graphene materials, the dopants can effectively improve the electrochemical performance of graphene-based supercapacitors [3].

The present work aims at revealing the formation mechanisms and properties of $Ti_3C_2O_2$-MXene with N dopants using DFT simulation, thereby guiding the tailoring of MXenes for their potential applications in supercapacitors or batteries. Two different types of configurations have been taken into consideration: substitutions and adhesions, while the previous ones include nitrogen substitutions for carbon and oxygen atoms. The geometry optimization results suggest that substitution atoms have insignificant impacts on the structure of $Ti_3C_2O_2$ substrate, while the nitrogen adhesion forms strong bond with surrounding Ti and oxygen atoms. The density of states of these three models have been studied, which suggest that the conductivity of $Ti_3C_2O_2$-MXene gets worse with nitrogen substitutions, and the opposite trend occurs when nitrogen adheres on the surface. Moreover, the third configuration, with a nitrogen substitution for oxygen atom, is found to be beneficial for adsorbing Li atoms, with the largest adsorption energies.

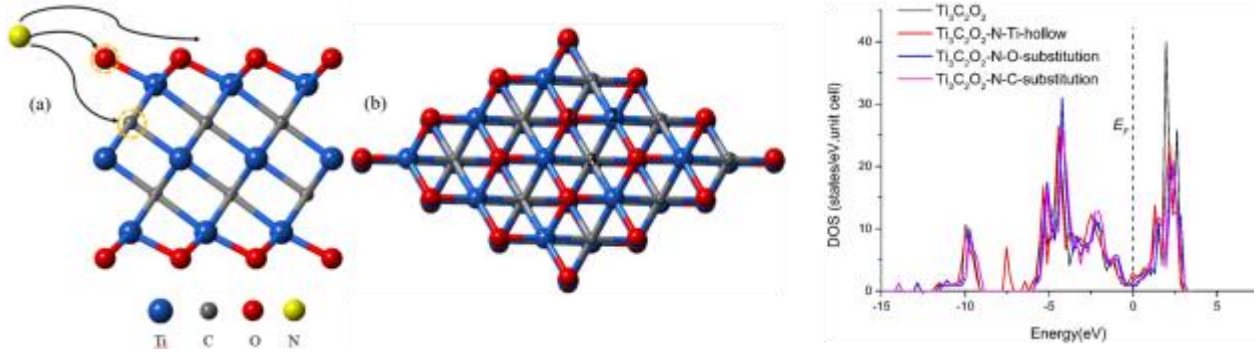

Figure 1. Models and properties of $Ti_3C_2O_2$ with N substitutions or adhesion studied in this work: (a). projection along c axis; (b). projection of the basal plane; (c). density of states.

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Thionine Functionalized MXene based fibers as high capacity and flexible Supercapacitors

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Abstract:

Fiber-shaped supercapacitors (FSCs) are promising energy storage candidates for micro and wearable electronics. The scalable fabrication of fiber electrodes with high electrical conductivity and excellent energy storage performance for use in FSCs remains an open problem [1]. Here, an easily scalable one-step wet-spinning approach is reported to fabricate highly conductive fibers using hybrid formulations of thionine/$Ti_3C_2T_x$ MXene nanosheets. This approach produces fibers with a high conductivity of ≈500 S cm^{-1}. The as-fabricated metal-free symmetric device exhibits a very high specific capacitance of ~380 F g^{-1} at 1 A g^{-1} which is about two times higher than pristine Ti_3C_2Tx. We report outstanding flexibility along with excellent capacitance retention of with 96% when cyclically stretched to 100% strain. This scalable approach provides an effective strategy to fabricate high-performance flexible supercapacitors and facilitates progress toward fiber-based energy storage in sustainable energy future.

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Ecotoxicological evaluation of the MXenes superficially modified with ceramic and noble metal nanoparticles

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Abstract:

The number of investigations regarding the application of 2D nanosheets of MXenes in different technological areas is growing rapidly. Different surface modifications of MXenes have been introduced to date in order to tailor their properties. As a result, surface-modified MXenes could be released in the environment from filtration membranes, adsorbents, or photocatalysts. On the other hand, assessment of their environmental impact is practically unexplored[1]. The pristine expanded 2D sheets of the Ti_3C_2 MXene phase were modified with Al_2O_3/Ag, SiO_2/Ag, and SiO_2/Pd nanoparticles using the sol-gel method and extensively characterized by antibacterial properties. The preliminary ecotoxicological assays considered green algae (*Desmodesmus quadricauda*) as well as two higher plants: sorghum (*Sorghum saccharatum*) and charlock (*Sinapis alba*). Modifications of the pristine Ti_3C_2 MXene with SiO_2/Ag or SiO_2/Pd made it more phytotoxic; this effect was not observed for Ti_3C_2/Al_2O_3/Ag. Germination inhibition was lower with modified nanoproducts compared with the pristine Ti_3C_2 MXene. Our experiments with the representatives of green algae and selected higher plants have shown that modification of pristine Ti_3C_2 MXene with metal oxide and/or metal nanoparticles can potentially influence its effect on the community of the primary producers in the natural environment. We have also indicated nanocomposite structures that were characterized by a lack of toxic effect.

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2D-2D Mn_3O_4-MXene as a flexible anode for Li-ion battery

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Abstract:

Transition metal oxides, such as Mn_3O_4, are promising anode materials due to their ultrahigh theoretical capacity in lithium-ion batteries (LIBs). Mn_3O_4, however, is hampered by the poor electronic conductivity and volume expansion during the electrochemical process, resulting in irreversible capacity fade and poor cyclic stability. $Ti_3C_2T_x$-MXene, as a novel two-dimensional transition metal carbide, possess the metallic electrical conductivity (~4000 S cm^{-1}), excellent flexibility and hydrophilic surface which is an ideal material to improve the electrochemical performance. Herein, the Mn_3O_4-MXene hybrid flexible films with 2D-2D nanostructure are assembled by vacuum filtration of layered $Ti_3C_2T_x$-MXene and 2D-Mn_3O_4. The MXene nanosheets in the composite can not only efficiently buffer the volume change of Mn_3O_4 nanosheets, but also preserve the high electronic conductivity. In addition, Mn_3O_4 nanosheets coupling with MXene, will also greatly enhance the electrochemical performance due to increased structure stability and charge transfer rate. The 2D-2D nanostructure is beneficial for ions and electrons to access their surface, enabling a fast conversion reaction and structure stability. As a result, the hybrid film shows the superb flexibility and extremely high specific capacity of 996.7 mAh g^{-1} at 0.05 A g^{-1} in LIBs. Moreover, it also exhibits excellent rate performance with 500.5 mAh g^{-1} at 1 A g^{-1} and marvelous cycle stability with a capacity retention of 99.8% after 1000 cycles.

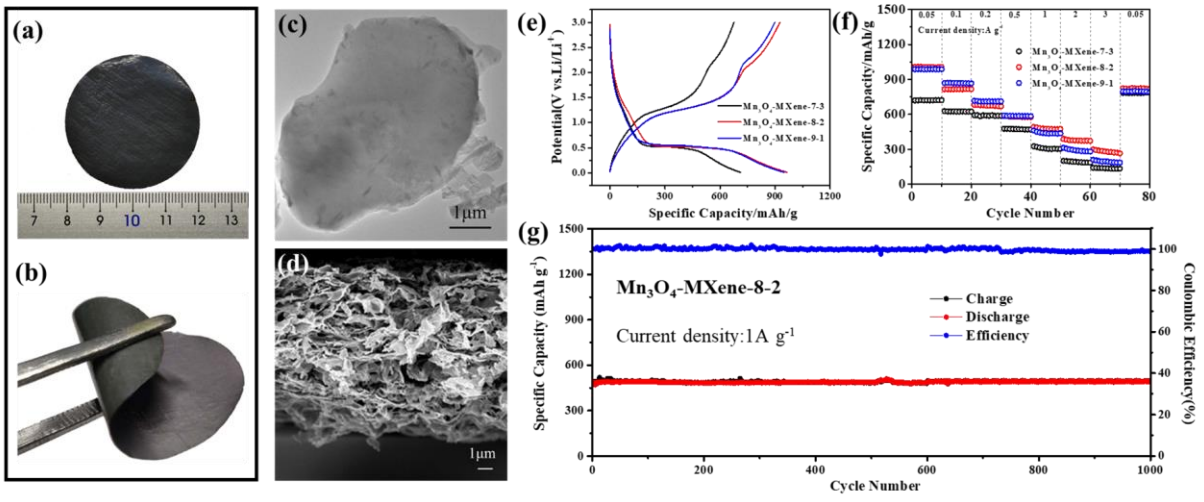

Figure 1 (a) Digital photographs of the Mn_3O_4-MXene-8-2 films. (b) Digital photographs showing flexible, free-standing Mn_3O_4-MXene hybrid films. (c) TEM images of the 2D-Mn_3O_4. (d) Cross sectional SEM images of the Mn_3O_4-MXene-8-2 films. (e) Discharge-charge curves at 0.05 A g^{-1} and (f) rate performance of the samples. (g) Cyclic performance at 1 A g^{-1} of the Mn_3O_4-MXene-8-2.

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Carbon Nanotubes Enhance Flexible MXene Films for High-Rate Supercapacitors

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Abstract:

MXene, as a new family of 2D material with metallic conductivity, has attracted great attention as a promising electrode material for supercapacitors. However, the aggregation and self-restacking of 2D nanosheets hinders the ion transfer. In our work, flexible and conductive MXene/carbon nanotubes (CNTs) hybrid film was prepared through a simple vacuum filtration of the suspension of MXene and CNTs for supercapacitors. The inserted CNTs between MXene nanosheets can effectively prevent the MXene nanosheets from restacking, which leads to a considerably increased interlayer spacing enabling more electrochemical active sites to become accessible. The resulting hybrid films exhibited excellent performance when working as electrodes for supercapacitors in 1 M H_2SO_4 electrolyte. The free-standing MXene/CNTs-5% electrode displays a high capacitance of 300 F g^{-1} at 1 A g^{-1} with superior rate performance (67% capacitance retention even at an ultrahigh current density of 500 A g^{-1}) and excellent cyclic stability (91.5% capacitance retention after 10,000 cycles at 20 A g^{-1}), demonstrating great potential as an electrode material for flexible, portable and highly integrated supercapacitors.

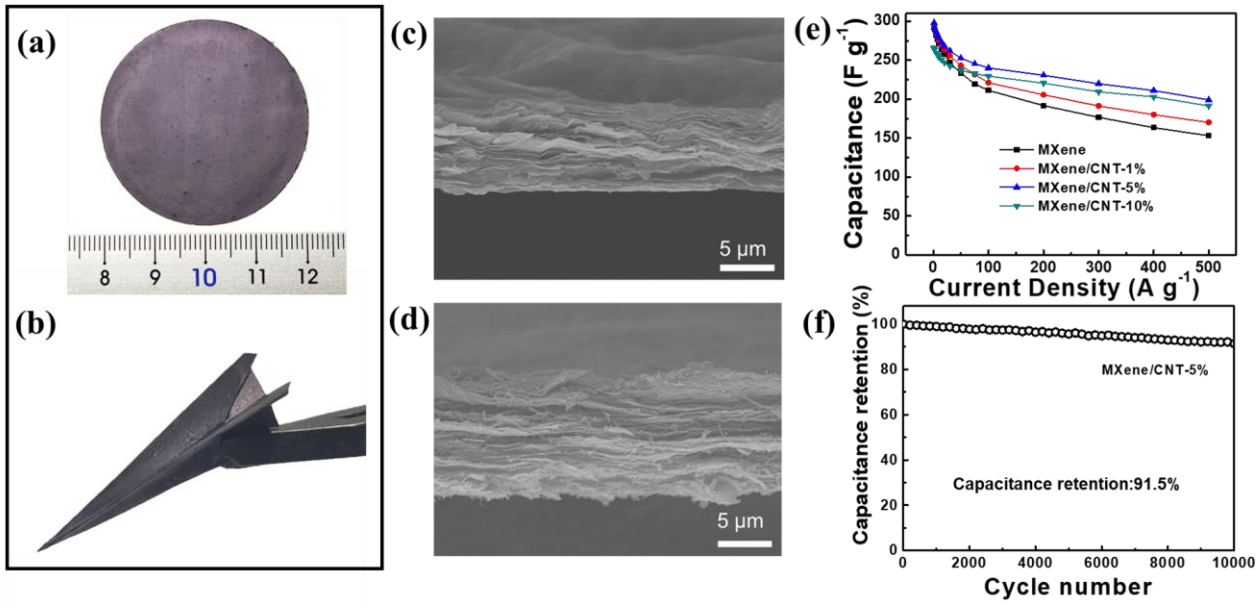

Figure 1 (a) Top-view and folded digital photo of MXene/CNT-5% films. Cross-sectional SEM images of (c) MXene and (d) MXene/CNT-5% film. (e) Rate capability of MXene/CNT films in 1 mol L^{-1} H_2SO_4. (f) Cyclic performance at 20 A g^{-1} of the M/CNT-5% film in 1 mol L^{-1} H_2SO_4.

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MXene-bonded flexible hard carbon film as anode for stable Na/K ion storage

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Abstract:

Hard carbon (HC) is a promising anode material for sodium ion batteries (SIBs) and potassium ion batteries (PIBs), but the cycle performance is still not satisfactory for practical application, due to the volume change during the insertion/extraction process of Na^+ or K^+.[1] Moreover, the poor flexibility of the conventional HC anodes prepared through coating method cannot satisfy the requirement of flexible devices.[2,3] Herein, we propose a very simple but powerful strategy to fabricate flexible HC electrode with excellent structure and cycle stability for SIBs and PIBs by using $Ti_3C_2T_x$ MXene as a multi-functional buffer binder. By vacuum-assisted filtration of evenly dispersed solution of HC and MXene, the obtained MXene-bonded HC films are flexible, free-standing and can be directly used as anodes for SIBs and PIBs. The elimination of all the inactive components, including polymer binders, conductive additives and current collectors, makes the HC-M films show superior electrode capacity to the conventional polymer-bonded HC electrode. What's more, in the MXene-bonded HC film, HC particles are embedded in the conductive MXene sheets. The MXene sheets construct 3D network, which can effectively stabilize the electrode structure and buffer the volume expansion of HC during the charge/discharge process, leading the excellent cycle performance. Compared with the conventional PVDF-bonded HC electrode, the MXene-bonded HC films exhibit enhanced electrode capacity and cycle stability as anodes of both SIBs and PIBs. The HC-M-2:1 film can deliver a high Na-storage capacity of 368.5 mAh g^{-1} at 30 mA g^{-1} with no capacity decay after 1500 cycles. For PIBs, in which the volume expansion is more serious, the HC-M-2:1 film can show a capacity retention of 84% over 100 cycles, superior to conventional HC-PVDF electrode (36.8%). Benefiting from the 3D conductive network, the MXene-bonded HC film electrodes also present improved rate capability, indicating MXene is a very promising multi-functional buffer binder for next-generation flexible secondary rechargeable batteries.

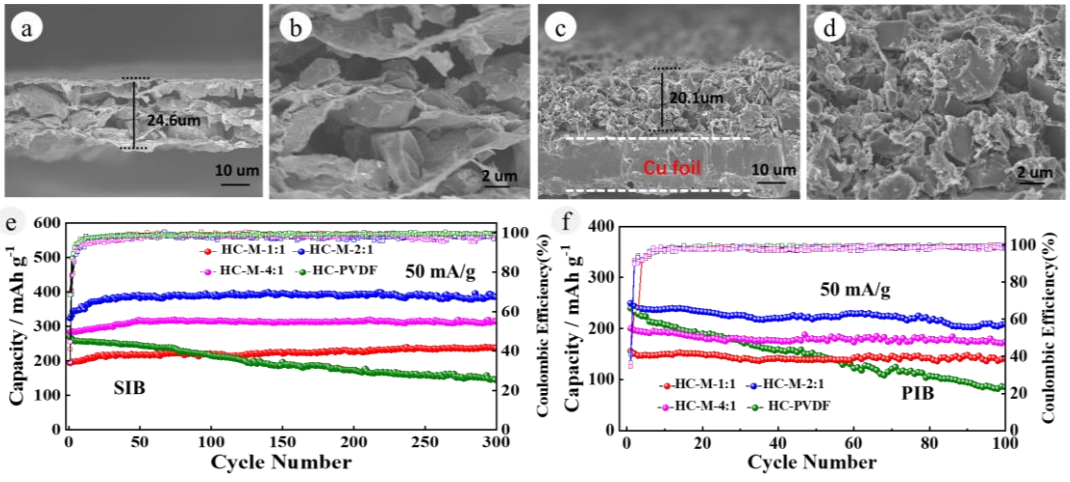

Figure 1 SEM images of (a, b) MXene-bonded HC film and (c, d) conventional PVDF-HC electrode coating on the Cu foil current collector, comparison of cycle stability of two kinds of HC electrode in (e) SIBs and (f) PIBs.

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Adsorption Properties of Ti_2CT_x MXene for Rhodamine B

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Abstract:

Water pollution is one of the growing issue that pose a serious threat both to aquatic and terrestrial species. In particular, direct release of industrial dyes in the aquatic system has been found to associate with server health detriments. Among the many reliable remediation approaches, the adsorption technology is most preferable due to simplicity, applicability at preparative scale and affordability [1]. To achieve the maximum potential, the surface area and functionalities of adsorbent material are crucial factors. Thus, the nature and engineering of adsorbent is the key parameters in designing ultra-adsorbent materials.

In this context, MXene, a relatively new 2D material with excellent hydrophilicity besides large surface area and abundant tunable functionality has shown tremendous potential compared to graphene based competitors [2]. In this contribution, we report the synthesis of ultra-thin MXene nanosheets, which have been tested for adsorptive removal of Rhodamine B (RhB) dye. The MXene sheets were prepared using acid-etching technique subsequently producing lamellar-like structure, and abundant surface bound oxygen-moieties (Fig.1a). The MXene sheets demonstrated excellent removal capability, with maximum RhB adsorption capacity of 3047 mg/g (Fig.1b) and equilibrium setting time of 1 min. The excellent adsorptive behavior of MXene sheets was experimentally proven to be attributed to the synergic combination of favorable forces such as chemical adsorption (ion exchange) and physical adsorption (electrostatic interaction, hydrogen bonding, van der Waals force). The present study serves as a step onward to understand MXene adsorption mechanism and its practical consideration as a suitable alternative to graphene.

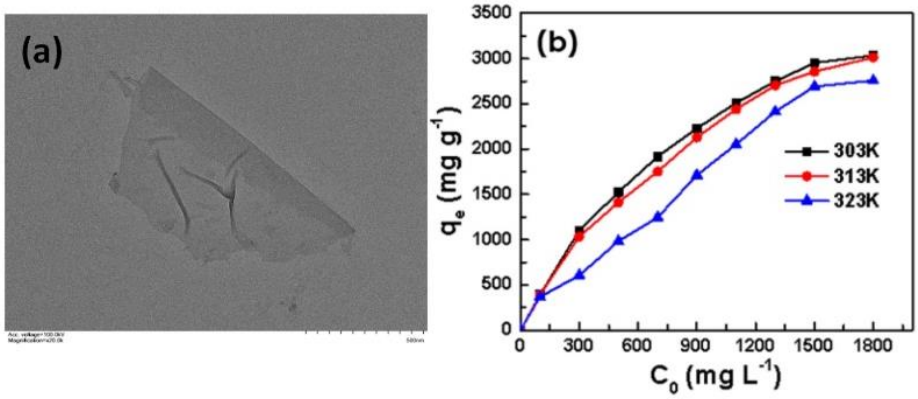

Figure 1 (a) The TEM of the Ti_2CT_x nanosheets; and (b) corresponding adsorption capacities at different concentration of RhB dye.

Reference

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MXene as a multi-functional buffer binder promises Si@C electrode with excellent stability for lithium ion batteries

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Abstract:

Silicon is regarded as a promising anode material for lithium ion batteries due to its ultrahigh theoretical capacity (~ 4200 mAh g^{-1}), natural abundance, and low working potential (~ 0.4 V vs. Li+/Li), but the poor conductivity and large volume expansion during lithiation/delithiation process hinder its practical application. Here, using 2D conductive MXene as a multi-functional buffer binder, we report a novel strategy to fabricate MXene-bonded Si@C film through a simple vacuum filtration method, which is free-standing, flexible and can be directly used as anodes for LIBs. In the film, MXene constructs a 3D conductive network with Si@C nanocomposites embedded within. The loose structure and the developed porosity create much spaces to buffer the large volume expansion of Si@C nanoparticles during the lithiation/delithiation process, making the MXene-bonded Si@C film exhibits much superior cycle stability to the conventional CMC- and PVDF-bonded Si@C electrode. Moreover, as a conductive binder, the metallic conductive MXene endows the MXene-bonded Si@C film has outstanding conductivity (hundreds time higher than the conventional CMC- and PVDF-bonded Si@C electrodes), while the loose and porous structure facilitates ion transporting, resulting in much enhanced rate performance, and demonstrating its great potential as an electrode for flexible lithium-ion batteries.

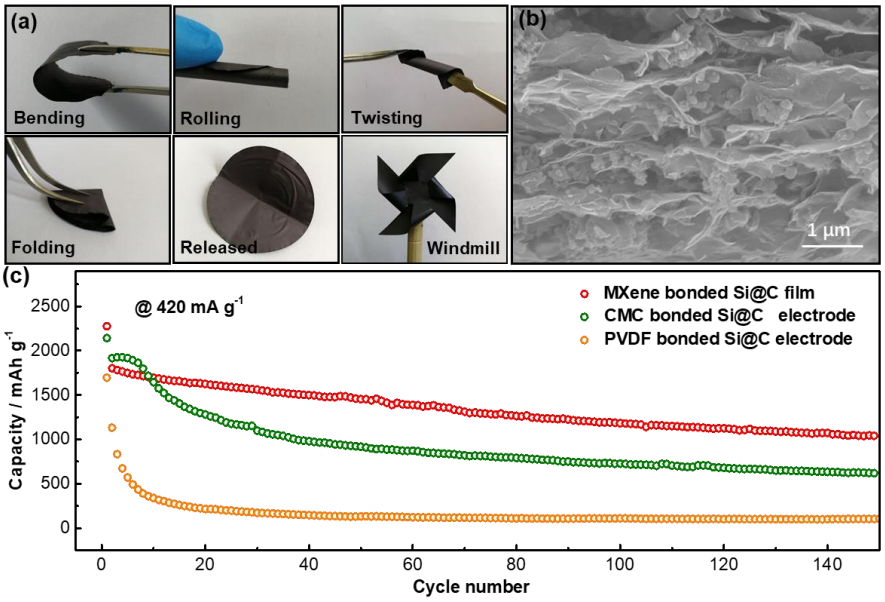

Figure 1 (a) Digital images for the appearance and flexibility (bending, rolling, twisting, folding, and folding into a windmill) of the MXene-bonded Si@C film.; (b) High-magnification section SEM image of the MXene-bonded Si@C film; (c) Cycle performance of the MXene-bonded Si@C film, CMC-bonded Si@C electrode, and PVDF-bonded Si@C electrode.

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2D MXene nanosheets enable small-sulfur electrode to be flexible for lithium-sulfur batteries

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Abstract:

Lithium-sulfur batteries are one of the most promising energy storage devices with high energy density, but their practical application is hindered by the serious capacity fading due to the shuttle effect resulting from the migration of polysulifdes during charge-discharge. Using small sulfur molecules (S_{2-4}), in place of conventional cyclo-S_8, as cathode material is an efficient method to fundamentally eradicate the shuttle effect [1, 2]. To satisfy the demands of flexible electronic devices, in this paper, two-dimensional (2D) MXene nanosheets were used as the conductive binder and flexible backbone to combine with S_{2-4}/carbon composite, fabricating a flexible small-sulfur electrode for lithium-sulfur batteries. The 2D MXene nanosheets with excellent conductivity can not only provide the flexibility for the electrode, but also construct the conductive network for fast charge transfer. As a result, the flexible S_{2-4} electrode exhibits superior electrochemical performance, which has a capacity of 1029.7 mAh g^{-1} at 0.1 C and maintains 946.7 mAh g^{-1} after 200 cycles with 91.9% retention. Besides, a capacity of 502.3 mAh g^{-1} is obtained at 2 C current density. This electrode is promising for flexible lithium-sulfur batteries, and the application of MXene as a conductive binder and flexible backbone in lithium-sulfur batteries offers an effective method to achieve both flexibility and high performance.

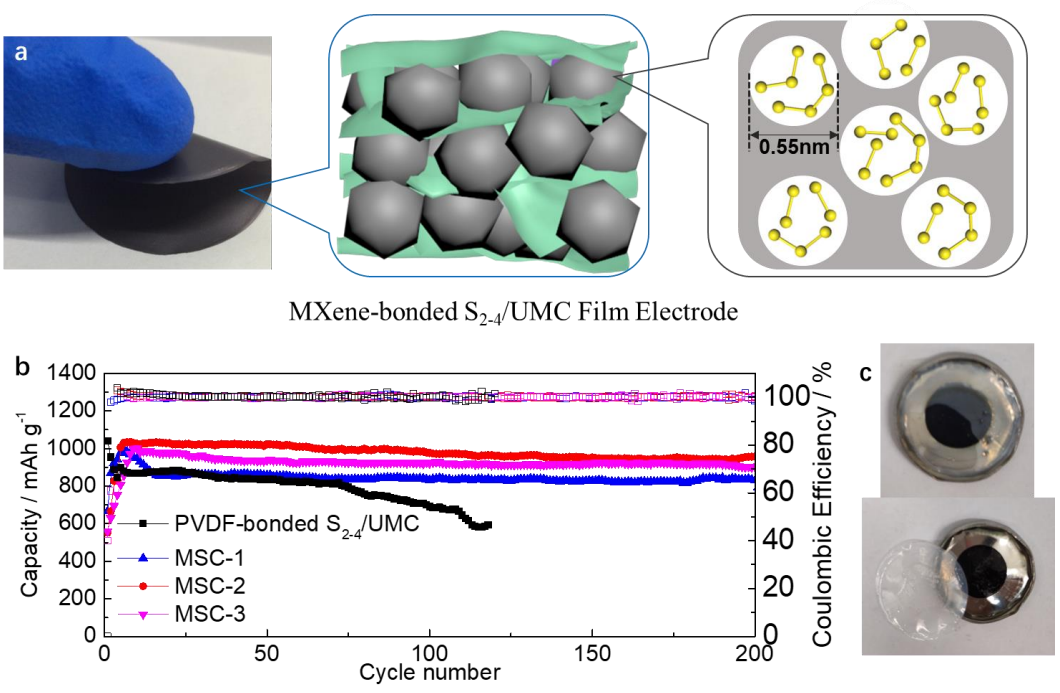

Figure 1 (a) the schematic of the flexible MXene-bonded S_{2-4}/UMC (MSC) film electrode, (b) the cycle performance of the MSC electrode and traditional PVDF-bonded S_{2-4}/UMC electrode, (c) pictures of the separator and the MSC electrode after 100 cycles at 0.1 C.

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Nano-ZnS/MXene Hybrid for Stable Lithium Storage

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Abstract:

Zinc sulphide is considered as one of the most promising class of anode materials for lithium-ion batteries. However, like other transition metal sulfide materials, the huge volume expansion, accompanied with structural collapse and unsatisfied electric conductivity upon continuous cycling, always lead to inferior rate capability and severe cycling fading[1]. In this work, we prepared a well-designed heterogeneity of ZnS/MXene composite by in-situ growth method using 2D MXene nanosheets with good conductivity. The ZnS nanoparticles, serve as the spacer to prevent the MXene nanosheets from restacking, thus preserving the active areas from being lost. The MXene nanosheets, in turn, not only enable reversible electron and ion transport at the interface but also prevent the ZnS nanoparticles from aggregation during lithiation/delithiation. After 300 cycles, a large capacity (701 mAh g^{-1}) is retained under voltage 0.01V-2.5V. The ZnS/MXene composite also delivers good rate capabilities (407 and 245 mAh g^{-1} at 1 and 2 A g^{-1}). As far as I know, this is the first work studying the ZnS/MXene composite for lithium-ion batteries.

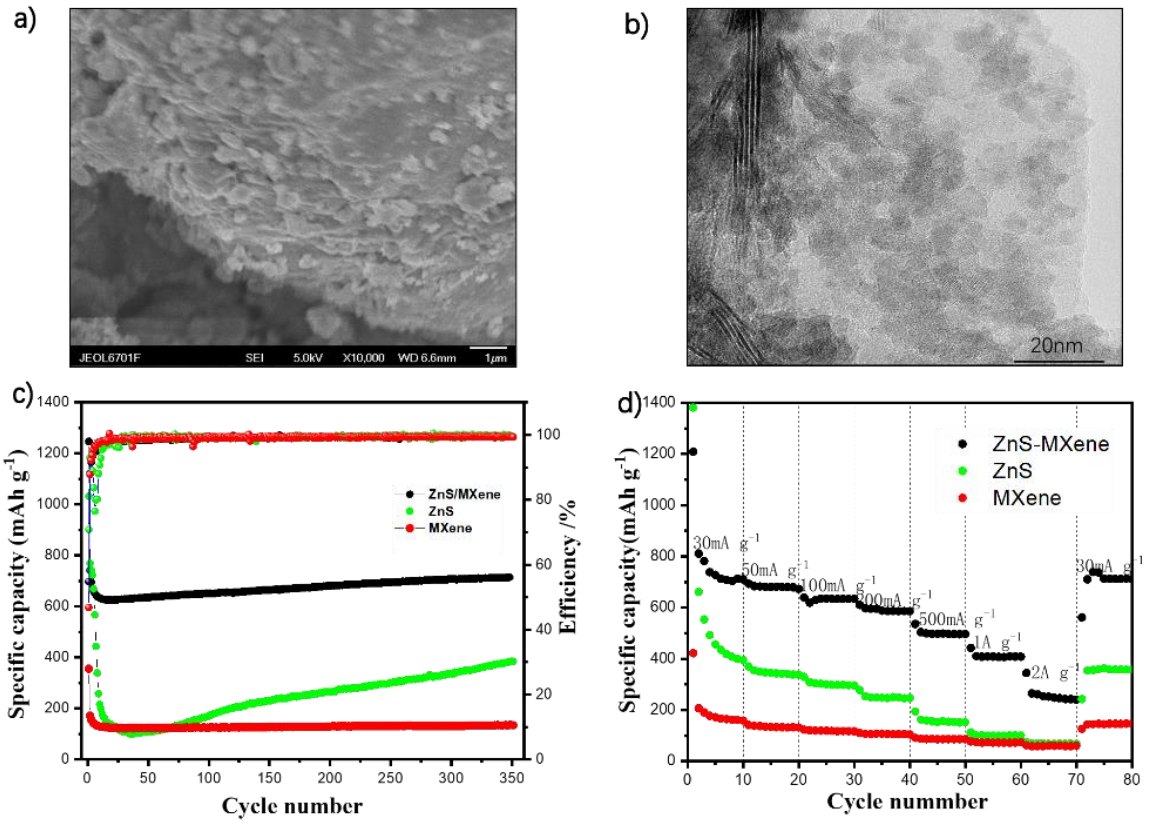

Fig.1 (a) SEM of ZnS/MXene; (b) HR-TEM of ZnS/MXene; (c) cycle and (d) rate performance of ZnS/MXene.

References:

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Flexible 3D Porous MXene Foam for High Performance Lithium ion batteries

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Abstract:

Two-dimensional (2D) transition metal carbides and nitrides, named MXene, are promising materials for energy storage, but suffer from the aggregation and restacking of the 2D nanosheets, which limits their electrochemical performance. Here, in order to prevent the aggregation and achieve the full potential of the MXene nanosheets, a 3D MXene foam with developed porous structure is established via a simple sulfur-template method. Similar to the stacked MXene film, the 3D porous MXene foam is freestanding, flexible and highly conductive, which can be directly used as the anode of lithium ion batteries. Furthermore, the 3D porous architecture of the MXene foam provides enlarged surface area and loose structure, offering massive active sites to enhance the lithium storage capacity. Moreover, the foam structure facilitates the electrolyte infiltration for fast Li^+ transfer and faradaic redox reaction. As a result, the flexible 3D porous MXene foam exhibits significantly enhanced capacity (455.5 mAh g^{-1} at 50 mA g^{-1}) compared to the stacked MXene film (35.4 mAh g^{-1}), excellent rate property even at ultrahigh current density (133.3 mAh g^{-1} at 10 A g^{-1} and 100 mAh g^{-1} at 18 A g^{-1}), and superior ultralong-term cycle stability (220 mAh g^{-1} at 1 A g^{-1} after 3500 cycles). This work not only demonstrates the great superiority of the 3D porous MXene foam, but also proposes the sulfur-template method for controllable constructing of the 3D foam from 2D nanosheets at a relatively low temperature.

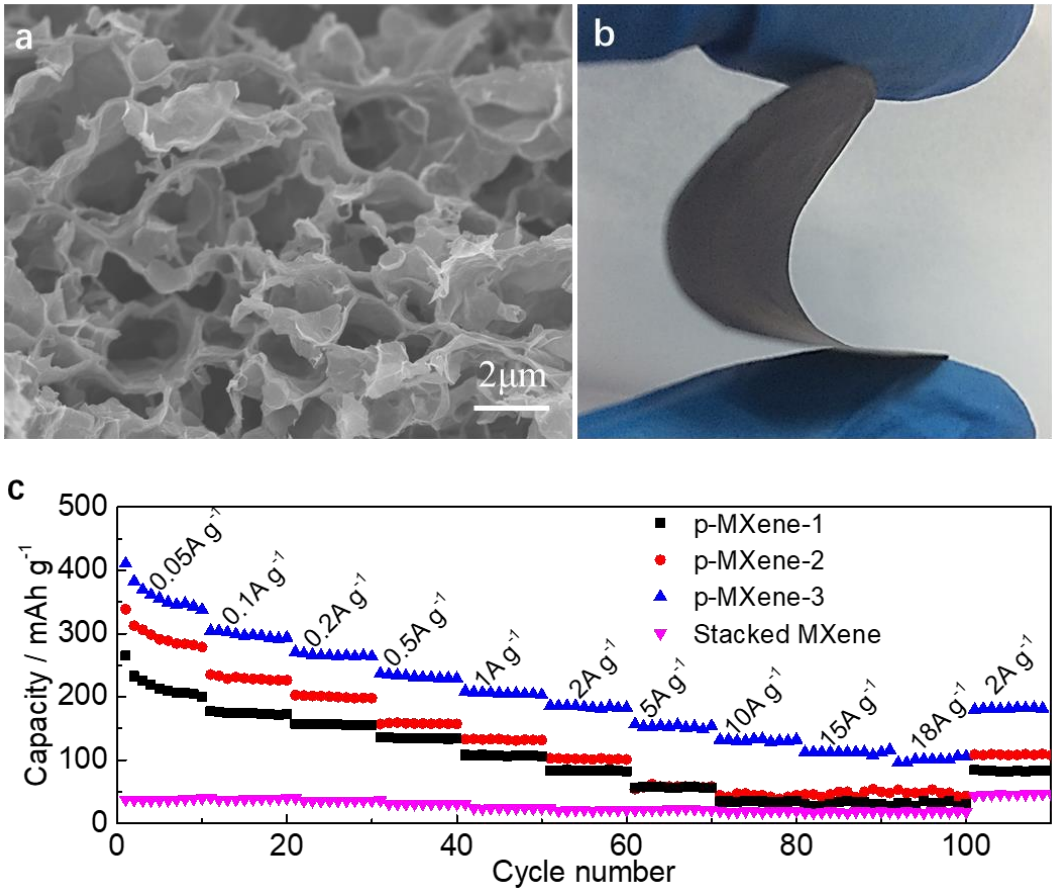

Figure 1 the SEM image (a) and the digital photo (b) of the flexible 3D porous MXene foam, and (c) the rate performances of the 3D porous MXene foam electrode with different sulfur-template contents.

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