TOPICAL REVIEW

Harnessing the unique properties of MXenes for advanced rechargeable batteries

Deobrat Singh1,5, Vivekanand Shukla2,5, Nabil Khossossi1,3, Abdelmajid Ainane1,3 and Rajeev Ahuja1,4

1 Condensed Matter Theory Group, Materials Theory Division, Department of Physics and Astronomy, Uppsala University, Box 516, 75120 Uppsala, Sweden
2 Department of Microtechnology and Nanoscience (MC2), Chalmers University of Technology, SE-412 96 Gothenburg, Sweden
3 Laboratoire de Physique des Matériaux et Modélisations des Systèmes, (LP2MS), Unité Associée au CNRST-URAC 08, Faculty of Sciences, Department of Physics, Moulay Ismail University, Meknes, Morocco
4 Applied Materials Physics, Department of Materials Science and Engineering, Royal Institute of Technology (KTH), S-100 44 Stockholm, Sweden
5 These authors contributed equally to this work.

E-mail: rajeev.ahuja@physics.uu.se

Keyword: MXene, rechargeable batteries, metal-ion batteries, lithium–sulfur (Li–S) batteries, two-dimensional (2D) materials, Van der Waals heterostructure

Abstract

In recent years, two-dimensional MXenes have been emerged as potential electrode materials for rechargeable batteries due to their unique properties such as exceptional safety, significant interlayer spacing, environmental flexibility, large surface area, high electrical conductivity, and excellent thermal stability. This review examined all of the recent advances in the field of MXenes and their composites (hybrid structures), which are found to be useful for the electrochemical applications of advanced rechargeable batteries. The main focus of this review is on metal-ion batteries and lithium–sulfur (Li–S) batteries. It is intended to show that the combination of recent improvements in the synthesis and characterization, greater control of the interlayer distance, and new MXene composites, together serve as an emerging and potential way for energy storage applications.

1. Introduction

Since the isolation of graphene in 2004, the importance of two-dimensional (2D) graphene-like materials has been growing significantly in the scientific community owing to their outstanding features such as excellent mechanical, electronic, and optical properties, and their exciting potential for various practical applications. Given their high surface-to-volume ratio, 2D materials (2DMs) offer high specific surface areas to enable full utilization of all accessible sites as effective electrode materials. As a result, the exposed contact area is significantly enhanced within the electrodes and electrolytes, and also the pathways for the transport of charges are reduced. These characteristics of excellent electrochemical properties make them suitable candidates for various energy storage applications. The key appeal of 2D material is the property that makes them naturally suited for a type of integration that is not so much possible with any three-dimensional (3D) material, forming heterostructures by stacking 2DMs together in the form of lateral vertical device, doping flexibility, nanoconstructions, and several others. Over the last decade, a considerable research has been carried in identifying new 2DMs, mainly by focusing on mono elemental and those containing double elements such as, graphene, [1] silicene, [2] germanene, [3] phosphorene, [4] transition metal dichalcogenides (TMD), [5] transition metal oxides (TMD) [6]. Among the family of 2DMs beyond graphene, transition-metal carbides, carbonitrides, and nitrides also called MXenes materials [7–12] have attracted much interest. Their general chemical formula is M_{n+1}X_nT_x with n = 1, 2, 3 or 4, where M is Transition-metal, X represents carbon and/or Nitrogen-atom, and T is hydroxyl (OH), oxygen (O), or fluorine (F) [13–15]. The transition-metal carbide Ti_3C_2T_x was the first 2D MXene successfully synthesized...
using aqueous fluoride-containing acidic solution to etch down to a few layer and further exfoliated with water and other organic solutions in 2011 [7]. Ti₃C₂Tₓ manifested unique structural and electronic properties in both the experiments and theoretical modeling. A year after this ground-breaking research, universal etching of Al from many other MAX phases gave rise to the new family of 2DMs known as MXenes. Until now numerous MXenes have been successfully synthesized, including 2D Vanadium Carbide (Vₓ₋₁XₜTₓ) [16] and Niobium Carbide (Nbₓ₋₁XₜTₓ) [17]. It has become the broadest category of 2DMs and is still growing significantly due to the range of various elemental configurations and prospective applications [18–23]. Their exciting properties and utilization in number of applications have been reported in various published reviews recently [24–30].

Motivated from the stimulating properties and suitability in energy storage application, in this review, we will focus on alkali-ion and unexplored Li–S batteries electrode applications of pristine phases and heterostructures of MXenes. We start by introducing the family of the layered MAX phases with the aim of better understanding of the MXenes and their synthesis with the various functional groups such as oxygen (−O), hydroxyl (−OH) and/or fluorine (−F). We would simultaneously focus on the importance of computational design of MXenes in the prediction of new members of the family and their heterostructures, as well as toward the better understanding of their physical and chemical properties at an atomic-scale (section 2). In sections 3 and 4, we outline recent cutting edge works related to the development of MXene with enhanced performance for rechargeable battery electrode applications such as lithium-ion, non-lithium ion, and lithium-sulfur batteries. We will review the effect their surface functionalization and heterostructure in order to achieve high storage capacity and high safety battery performance, focusing on physical and chemical characterization, computational modeling, and electrochemical properties. Finally, section 5 is dedicated to summary and highlighting the critical challenges in developing MXene and their heterostructures for alkali-ion and Li–S battery applications.

2. MXenes: structure, synthesis and properties

2.1. Structure

In 1960s, hundreds of new carbides and nitrides were identified by Hans et al in Vienna [31], but these phases remained unexplored for nearly 30 years until 1990s. Later Barsoum and El-Raghy synthesized Ti₃SiC₂, which showed remarkable electronic and thermal conductivity with a suitable combination of ceramic and metallic properties [32]. Further, synthesis of Ti₄AlN₃ suggested that these phases shared a basic structure, which was later designated the acronym ‘Mₓ₋₁AXₜₓ phases’ ( n = 1, 2, 3, etc) or ‘MAX phases’. M is a transition metal (mostly group 13 and 14 elements), A stands for group IIIA or IVA elements, and X is C/N [33, 34]. The MAX phases constitute a significant group of currently > 130 diverse compositions, vast majority of which crystallizes in hexagonal structure with the P6/3/mmc space group or other derivatives [35]. Figure 1 shows the schematic crystal structures of MAX phase materials. The structure is comprised of MX₆ octahedra, with pure Al layers. The main difference separating these three different MAX phases, viz. n = 1, 2, or 3, is in the number of M layers (2–4) between the A layers. They are assigned as 211, 312, and 413, sequentially [36–38].

The exposure of the chemically active exterior metals layer of a MAX phase causes surface terminations. This further can remove the ‘A’ element from the bulk MAX phases and result in the mono or few layers of MXene, which is described in figure 1. The schematic picture of 2D-MXenes consist of different variants of monolayers. MₓX is the tri-sublayer structure, where the carbon/nitrogen (X) atom is sandwiched in between two metal (M) atom layers in a hexagonal unit cell. There are also M₁X₂ and M₁X₃ sheets, as shown in figure 1. Besides these, there are possibilities of double transition metal MXenes. This contains a sandwiched configuration of X between two different transition metals ‘M and M’, and these metals can be randomly distributed [11, 39, 40]. It is well understood that outer metal atoms would play a vital role in deciding the surface behavior of these MXenes. Since the metal atom generally has coordination number six, it is quite natural to expect that the transition metals in MXenes favor making six chemical bonds with the neighboring atoms [41, 42]. Hence, for environmental stability, these MXenes have functionalization at the outer metal atoms, further tuning their properties. It is experimentally perceived that the outer layers are often terminated with F, O, and/or OH groups, and these group’s ratios and distributions strongly depend on the synthesis methods [15, 43–45].

2.2. Synthesis

For the bulk MAX phases synthesis, we recommend readers go through the literature [18, 46–50]. We focus only on its 2D counterpart. In general, MAX phases have stronger interaction in between the layers than...
Figure 1. Crystal structure of the M$_2$AX (211), M$_3$AX$_2$ (312), and M$_4$AX$_3$ (413) phases in the right column, further removal of A element gives the 2D MXenes in the central column as M$_2$X, M$_3$X$_2$, and M$_4$X$_3$ after HF etching and exfoliation. Recent experimental and theoretical examples are tabulated in the third column for all the three phases. Brown color balls are X(C/N), blue color balls manifests A(Al/Si) and Light blue color stand for the transition metals.

graphite, bulk black phosphorus, and MoS$_2$ [51–54]. The simple mechanical (scotch tape) method has difficulty in providing monolayer MXenes. The best suitable way to exfoliate monolayers and the colloidal solution of mono or few-layer is the delamination technique. Within a few years of the initial announcement in 2011, MXenes have already grown as an established class of 2DMs with exceptional possibilities in variation of chemical composition and highly tunable properties [7, 55–57]. The chemical or structural properties of MXenes are directly associated with the structural order in the bulk phases [7]. There are several steps to synthesize MXene from these bulk MAX phases, described as below:

$$\text{Ti}_3\text{AlC}_2 + 3\text{HF} \rightarrow \text{Ti}_3\text{C}_2 + \text{AlF}_3 + 3/2\text{H}_2 \quad (1)$$

$$\text{Ti}_3\text{C}_2 + 2\text{H}_2\text{O} \rightarrow \text{Ti}_3\text{C}_2(\text{OH})_2 + \text{H}_2 \quad (2)$$

$$\text{Ti}_3\text{C}_2 + \text{HF} \rightarrow \text{Ti}_3\text{C}_2\text{F}_2 + \text{H}_2. \quad (3)$$

Due to the strong metallic M–A bond, it has not been possible to isolate the M$_{n+1}$X$_n$ layers and get MXenes by mechanical shearing of MAX phases. Nevertheless, M–A bonds are chemically reactive compared to the more robust M–X bonds, which makes a selective etching of A-layers possible. This selective etching is the central requirement for MXenes synthesis. In the process of MAX to MXene conversion, the etched layers are substituted by various termination groups T$_x$, such as hydroxyl (–OH), oxygen (–O) or fluorine (–F) [7, 18]. The material recovered after etching thus consists of M$_{n+1}$X$_n$T$_x$ multilayers attached by hydrogen and/or Van der Waals (vdW) bonds. The most used, suitable, and highly selective etchant solution for this etching is hydrofluoric acid (HF). Aluminium layers are etched by the HF from MAX phases to synthesize the MXene. The reaction occurs in this process is given in equation (1), where HF first etches the MAX phase and form the few-layer or MXene clays and AlF$_3$ and releases H$_2$. In the presence of water, one can get OH functionalized MXene, and there is also a possibility of formation of Ti$_3$C$_2$F$_2$ during the process, as described in equations (2) and (3). The details of etching conditions for a different type of beyond Al-containing MAX phase can be found in the literature [11, 18, 38, 58–64]. Overall, different MXenes can be synthesized under different etching conditions, which further gives a different quality. However, when the atomic weight of metal atoms is high, then longer time and stronger enchat solution are required due to the M–Al bonding.
HF has highly corrosive nature, it can penetrate through the skin and harm the bones and muscle tissues. That is why an alternative to a strong HF solution should be used where possible, or one should minimize the concentration of HF. The most common alternative is the etching with a mixture of hydrochloric acid (HCl) and fluoride salt. This was first reported by Ghidiu et al., where they used it in situ experiment using lithium fluoride (LiF) and HCl on Ti3AlC2, and a similar result was achieved [48]. In this experiment, they concluded that the presence of proton and fluoride ions are necessary conditions for the etching process and MXene synthesis. Metal-halide presence leads to the intercalation of cations (such as Li+) and water in MXene layers. This increases the interlayer spacing among the MXene layers and also weakens the interlayer interaction. There have been other favorable alternatives such as sodium fluoride (NaF), potassium fluoride (KF) and NH4F with different HCl concentrations [16, 65]. Ammonium hydrogen bifluoride (NH4HF2) also used to synthesize thin epitaxial Ti3AlC2 films and powders [66]. In addition, there is an F-free etching method with an electrolyte mixture of NH4Cl and tetra-methylammonium hydroxide (TMOAH) used on Ti3AlC2 with more than 40% yield [67]. Tengfei et al reported another promising F-free hydrothermal method was based on the Bayer process [68]. Recently, Cl-terminated Ti3C2Tx and Ti3CTx MXenes have also been synthesized from of these compounds in the presence of ZnCl2 Lewis acidic solution [69].

Aside from Al etching; there have been reports of Si etching from the Si based MAX phase precursors like Ti3SiC2 with the use of HF and hydrogen peroxide (H2O2) solution [70]. Nitride MXene such as Ti3N2Tx has been also synthesized in the molten eutectic mixture of KF, LiF, and NaF at 550°C, under argon (Ar) environment [71]. V2NTz and Mo2NTz, have been realized by the ammoniation of carbide counterpart at 600°C [72]. Chemical etching leaves the byproduct of synthesis, such as AlF3 salts, which has to be washed out from the yield. Hence it may need to be washed several times with water, which can functionalize the MXene with –OH [7] as it can be seen in equation (2). Acid-prewash with HCl or sulfuric acid (H2SO4) is also used to dissolve salts such as AlF3 or LiF [71]. Further, the delamination process is used to exfoliate the MXene from the resultant. The suitable molecule intercalation can widen the gap in the interlayer space, weaken the interaction, and enables the exfoliation of multilayer MXene into a single layer nanosheet at a reasonably large scale [73]. For example, such as dimethyl sulfoxide (DMSO), isopropylamine, tetrabutylammonium hydroxide, chlorine hydroxide, n-butylamine, and urea can all be used to intercalate and followed by sonication to produce MXenes [74–76]. In the case of Ti3C2Tx, interlayer spacing goes from 9.8 to 17.6 Å with DMSO intercalation and in other example, Nb2CTx is reported to be exfoliated via the intercalation of iso-propylamine [17, 73]. Readers are suggested to go through the references for specific methods and information about the delamination process [15, 77].

2.3. Theoretically predicted MXenes

The advancement of state-of-the-art, high-throughput theoretical methods has enabled the prediction of thousands of new possibly stable materials amongst hundreds of thousand of potential combinations with the capability to effectively screen the multivariate chemical species of compounds [78–81]. The growing interest in MXenes as a new 2DMs class has fueled research to identify new phases. Due to the bottleneck in the synthesis of new 2DMs, computational efforts continue to expand, covering the prediction of materials and widening the field of their possible utilization [30]. Although computational calculations have predicted many promising 2DMs, only a few dozen of them have experimentally been realized. Still, high throughput calculations give us liberty and support for trying new kinds of materials, which further motivates experimentalists to focus their efforts to synthesize these materials. Henceforth, theoretical strategies are needed that would make it plausible to describe the electronic structure of MXenes and their heterostructures and suggest the new members of the MXene family at a fundamental level. Various high-performance calculations have been performed on the properties and composition of MXenes lately [82]. Nathan et al have recently used elemental information and data from high-throughput density functional theory (DFT) computations [83] to apply the positive and unlabeled machine learning approach on 2D transition metal carbides, carbonitrides, nitrides, and their layered parent MAX phases. In their work, they identified 20 different MAX phases with a high possibility of experimental realization, which can be exfoliated to produce MXene sheets. Examples include Hf3C3N, Ta3N5 and Sc3C2, and so on. In another work, a new form of MAX phase, Cr4Ti4AlC2 with a sandwiched Ti-layer between two outer chromium carbide layers in a M2AX2 structure, was calculated to be dynamically stable [40, 84]. Another study based on ab-initio DFT predicted and verified the stability of new, ordered, double-M MXenes phases. These have stoichiometry like M′/M/M′/C3, where M′ is the exterior layer metal and M′ is the internal layer metal [11]. These metals can be Ti, V, Nb, Ta, Cr, or Mo. In all these cases, carbon atoms occupy the octahedral sites between the M′ and M′. Besides this, all these MXene can have several termination groups such as O, OH, or F. Several theoretical predictions of nitride MXenes with various configurations and applications have also been reported [85–88]. Although, only a few of the nitride MXenes like V2NTz, Ti2N3T2 have been experimentally synthesized till now [71, 89]. However, the theoretical discovery does not guarantee that the
corresponding MXene sheets can be synthesized, even they are energetically and thermodynamically stable in calculations. The main challenge is to find a suitable etchant. Although this gives the impression that various new MXenes would be synthesized in the future, opening the possibility of expansion of the family.

2.4. Electronic properties
The MAX phase’s striking characteristics emerge from their layered structural arrangements and the mixed nature of metallic-covalent (M–X) bonds united with M–A bonds that are comparatively weak compared to the former one [18, 35, 46, 47, 90]. These exceptional combinations make MAX phases suitable for a broad range of applications, varying from sensors, electrical contacts, microelectromechanical systems, protective coatings, and many more [28, 39, 91]. The electronic structures of the first few MXene phases were established rapidly [92–94]. Similar to MAX phases, most of the pristine MXenes have a metallic electronic structure. In DFT calculations, Ti3C2 was found to be metallic, but further the functionalization of this MXene can effectively change the electronic structure from metal to semiconductor [7, 13]. The electrical conductance of Ti3C2Tx has attained 3250 S m⁻¹, which is eventually higher than that of graphene (2500 S m⁻¹) [52, 95]. An extensive DFT investigation was performed by Kazari et al for various metal nitride M₂N (M = Sc, Ti, Cr, Zn, Nb, Ta) and metal carbide M₂C (M = Cr, Ti, Zr) with the saturation of metal atoms with O, OH, and F [41, 96]. Theoretically, it has been suggested that both F and OH groups affect the electronic structure of MXenes in the same order because they withdraw only one electron from the surface. On the other hand, O termination is different and has the capability of also reporting two electrons from the surface to be stabilized [10]. Sulfur (S) terminated nitride MXenes also reported for metallic behavior and good electrochemical properties [86]. Most of the functionalized MXenes were found to be metallic and magnetic with some exceptions. Only a handful of them, such as Sc₂CT₂ (T = O, F, OH), Cr₂CT₂ (T = OH, F), and Ti₂CO₂ are semiconductors, whereas Cr₂NT₂ (T = O, F, OH) and Cr₂CT₂ (T = F, OH) are magnetic [97, 98]. However, all these MXenes mentioned above have indirect bandgap, excluding Sc₂C(OH)₂, which has a small direct bandgap [10]. Lee et al studied the strain effect on Sc₂CO₂, which suggest that with the increase in tensile strain, the bandgap gradually decreases [99]. At a critical tensile strain, the indirect bandgap changes to a direct one. External electric field can also tune the gap from indirect-to-direct bandgap [100, 101]. The electronic properties have been experimentally verified for selected MXene such as Ti₃C, Ti₃C₂, Mo₃C [102–105].

Furthermore, the multiple-metal-atom MXenes open the possibilities for a range of potential applications, owing to their lower symmetry and the capability to choose combinations of metal atoms, which tailors the chemical and electronic properties. Dong et al predicted possible spintronic materials with robust ferromagnetism in Ti₃MnC₂Tx independent of surface functionalization, similar in oxidized H₂MnC₂O₂ and H₂VC₂O₂ [106]. Lately, Sun et al investigated a series of surface-metal and termination-dependent metal–insulator transitions in TiCrN₂ and TiMN₂ with Ti as the middle layer [107]. Mo₃TiC₂Tx, Mo₃Ti₂C₃Tx, and Cr₂TiC₂Tx were experimentally realized and manifested to have distinct electrochemical properties from that of the conventional single-metal Ti–C based MXenes [11, 108]. Besides these, Tao et al designed a new i-MAX phase in 2017 with stoichiometry (Mo₂/Scₓ/2)₃AlC, with in-plane chemical ordering of the Sc and Mo atoms [62]. Selective etching made it possible to remove both the Al and Sc atoms and resulted in 2D MXene Mo₂/AlC sheets. The initially characterized capacitance showed the value of 1153 F cm⁻³ and 339 F g⁻¹, which exceeds those of Mo₂C by 65% and 28%, respectively. Khazaee et al predicted that certain combinations of i-MXenes may display semiconducting nature, due to the lack of centrosymmetric, and can exhibit piezoelectric properties [109]. i-MXenes can be advantageous for properties that are profoundly surface geometry dependent. We also encourage readers to go through the literature for mechanical properties of the MXenes [43, 71, 98, 110, 111].

3. 2D MXene based electrodes for rechargeable batteries
High performance demands on electrochemical energy storage systems have become increasingly important. Unquestionably, the efficiency of rechargeable battery electrodes depends largely on the successful design and implementation of electrode materials. The specifications for potential energy storage materials consist of: (a) good reversible redox-reaction; (b) easy access to electrolyte ions; (c) sufficient number of adsorption sites; (d) high electrical conductivity. Over the last few years, a large number of 2DMs have demonstrated considerable benefits in the area of electrochemical energy storage owing to both their large surface area as well as their relatively fast ion transport pathway. With only a single or few atomic layers thickness, multiple surface active sites and excellent mechanical characteristics, 2DMs fulfill the challenges of electrochemical energy storage technologies, especially rechargeable batteries. As mentioned in the previous section, roughly 20 different types of MXene have been successfully synthesized and many important breakthroughs have been achieved in the energy storage area, owing to their outstanding and distinctive structure.
high-conductivity, high ionic-diffusion and other advantages compared to other 2DMs. Based on the 2D features as well as superior electrical conductivity of MXene materials, they represent an alternative for high-performance electrochemical rechargeable batteries including metal-ion and Li–sulfur batteries. In this context, it is of utmost necessity to survey and summarize the most recent progress of MXenes as promising battery electrodes.

3.1. 2D MXene for alkali metal-ion batteries
In recent years, a large amount of computational and experimental researches have been carried out in order to design new materials for negative electrodes in Li-ion and non-Li-ion batteries, with high storage capacity, high safety performance and low volume expansion (summarized lists of MXenes materials in figure 2). Among the family of 2DMs which have attracted a lot of interest 2D \( \text{M}_{n+1}X_n \) MXenes (with \( n = 1–3 \), M: transition-metal, X: Carbon and/or Nitrogen-atom and T: hydroxyl, oxygen or fluorine) has been reported to be the upcoming promising alternatives for graphite 2DMs as anodes (see figure 2), owing to their unique properties including great carrying capacity, a huge surface area with more space for the intercalation of alkali metal ions, as well as the surface activity derived from the transition-metal surface terminated by OH-, O- or F-groups [18, 19, 23, 23, 112]. In this section, we will highlight some recent breakthroughs achieved in metal-ion batteries by focusing on the electrochemical efficiency of MXenes as a negative electrode.

Interesting progress has been achieved through the experimental process. It was established on the basis of gravimetric capacity that bare 2D \( \text{M}_{n+1}X_n \) MXenes with \( n = 2 \) are more promising and can store a high number amount of metal-ions per gram compared to bare \( \text{M}_2X_2 \) and \( \text{M}_3X_3 \) layers. Naguib’s group have studied the possibility of using \( \text{Ti}_3C_2 \) and \( \text{Ti}_2\text{C}_2\) layers as anode for Li-ion batteries and concluded \( \text{Ti}_3C_2 \) exhibits a gravimetric capacity about 50% higher than that of \( \text{Ti}_3\text{C}_2 \) [73, 113]. It was further determined in the case of \( \text{Ti}_3C_2 \) that lithiation/delithiation peaks are located at 1.6–2.0 V relative to Li\(^+\)/Li with a gravimetric capacity of 225 mAhg\(^{-1}\) [113] and that the gravimetric capacity of \( \text{Ti}_3\text{C}_2\text{T}_x \) is about 1.5 times greater than that of \( \text{Ti}_3\text{C}_2\text{T}_x \) [73]. Subsequently, niobium and vanadium carbides, namely \( \text{Nb}_2\text{C} \) and \( \text{V}_2\text{C} \), have been
tested as electrode materials for Li-ion batteries showing ability to handle high charge/discharge rates with reversible capacities of about 170–260 mAh g⁻¹ at 1 C in the case of the Nb₂C layer, and 100–125 mAh g⁻¹ at 10 C in the case of the V₂C layer [9]. Tang et al have reported the feasibility to use Ti₃C₂ monolayer with its F- and OH-functionalized surfaces as a promising active materials for Li-ion batteries. Adopting DFT they have found that Ti₃C₂ sheet has outstanding electrochemical characteristics when used as anode for Li-ion batteries, such as significant adsorption energies of about −0.504 eV/Li-atom, low diffusion barrier of 0.07 eV, low profile insertion of 0.62 V vs. Li/Li⁺ and corresponding theoretical specific capacity of 320 mAh g⁻¹ compared to Ti₃C₂F₂ (130 mAh g⁻¹) and Ti₃C₂(OFH₂) (67 mAh g⁻¹). Xie et al systematically explored using theoretical calculations combined with experiments, the interaction between Li-ion and different functionalized 2D transition-metal carbides including Sc₂C, Ti₃C, Ti₃C₂, V₂C, Cr₂C₃, and Nb₂C [11, 114]. They have found that the capacity of Li-ion storage is mainly dependent on the type of surface functional groups and that the O-terminated MXenes exhibit the highest specific capacities (see table 5). Additionally the computed Li-diffusion barriers confirm great Li-mobilities [86]. Based on the fact these materials exhibit a high conductivity, the Li-ion can form reversible multi-layer ion intercalation, which manifest high theoretical specific capacity (see table 5).

MXenes also demonstrated encouraging performance in terms of specific capacity and stability for non-lithium ion batteries. Table 4 summarizes the capacity and stability in non-lithium ion battery applications of Ti₃C₂Fₓ [19, 115–119]. Xie et al have investigated a family of 2D transition metal carbides for promising anodes in non-Li ion batteries including Na, K, Mg, Ca, etc by using both DFT and experiments [120]. They have found that the O-functionalized surface and bare MXenes present a great theoretical specific capacity and proved to be promising anode materials for non-li ion batteries. Furthermore, Vivek et al have modeled recently the S-functionalized nitride MXenes, namely Ti₃NₓS₂ and VₓCᵧNₓSₓ and their possibility to use as active materials in Li- and Na-ion batteries by using first principle modeling [86]. Based on the fact these materials exhibit a high conductivity, the Li-ion can form reversible multi-layer ion intercalation, which manifest high theoretical specific capacity (see table 5).

Zinc-hybrid-ion batteries are also a suitable substitute to expensive Li-ion batteries. In these batteries, Zn-metal works as a negative electrode and exhibit outstanding features among the many mentioned electrochemical batteries owing to their high theoretical specific capacity of 820 mAh g⁻¹, and low diffusion profile of about 0.76 V compared to the standard electrode. Significant breakthroughs have been achieved toward this type of rechargeable batteries for cathode materials, such as manganese and vanadium oxide. Although a high-capacity has been achieved in these cathode materials but unfortunately they show lower potential voltage of less than 1.0 V. In order to overcome these challenges, Xinliang et al [121] have recently fabricated a zinc hybrid-ion battery cathode through a phase transition process, which can significantly enhances battery capacity, resulting in adequate capacity and cycling stability. They have demonstrated the higher potential of the V₂CȚₓ for zinc hybrid-ion battery, and provide an efficient approach to attain enhanced battery efficiency through the introduction of a phase transition appropriate to the electrode materials (see figure 3). This demonstrates that the Li⁺/Zn²⁺ insertion leads to the improvement of layer spacing of the V₂CȚₓ, which facilitates the further insertion and extraction of ions. To summarize, from the brief collection of the latest experimental results, it is clear that MXenes and functionalized of MXenes offer a promising performance when used as anode in Li and non-Li ion batteries. Theoretical considerations based on DFT are expected to provide guidance for the selection as well as the optimization of potential MXene-based anodes.

3.2. 2D MXenes as host materials for lithium–sulfur batteries

Recently, lithium–sulfur (Li–S) batteries have attracted widespread interest as a promising and upcoming non-toxic and eco-friendly alternative in electrochemical storage systems. Li–S batteries show significantly higher theoretical specific capacity (about 1675 mAh g⁻¹ for S-containing cathode and 3860 mAh g⁻¹ for metallic Li-anode) and energy density (2500 Wh kg⁻¹ taking into account full reaction to Li₂S₈) over those of conventional alkali metal-ion batteries [126–128]. These batteries mainly consist of a Li-metal anodes, an S-containing cathodes and a separator which is impregnated with organic electrolyte [129, 130]. Figures 4(a) and 6 depicts a schematic illustration of a standard Li–S battery, based on the conversion process: 16Li + S₈ ⇄ 8Li₂S. During the discharge process, the Li-anode releases Li⁺-ions and electrons (e⁻). Subsequently, these Li⁺-ions diffuse to the positive electrode via liquid electrolyte [131]. Simultaneously, the e⁻ switch over from external-circuit to sulfur-cathode, and S₈ gets reduced to long chain lithium poly-sulfides (LiₓS₈ with n≥4) according to the following reactions [132]: 2Li⁺ + S₈ + 2e⁻ → Li₂S₈, 3Li⁺S₈ + 2Li⁺ + 2e⁻ → 4Li₂S₈, Li₂S₈ + 2Li⁺ + 2e⁻ → 2Li₂S₄. Further Li₂S₄ reacts with Li to form short-chain LiₓS₄ (n = 2,1) in following reactions: Li₂S₄ + 2Li⁺ + 2e⁻ → 2Li₂S₂, Li₂S₂ + 2Li⁺ + 2e⁻ → Li₂S₄.

Despite above-mentioned advantages and the flexibility of Li–S batteries, their practical implementation in day-to-day life remains challenging due to many crucial issues related to the sulfur cathode, e.g. the shuttling effect of intermediate soluble LiₓS₄ with 3≤ n≤ 8), high volume change of sulfur and electrical
insulating nature of S and the short-chain polysulfides ($Li_2S_2$ and $Li_2S$) as illustrated in figure 4(b). A description of these critical issues are discussed briefly in the following sections:

1. **Shuttle effect**: This corresponds to the diffusion back-and-forth of $Li_2S_n$ polysulfides between the Li-metal anode and S-containing cathode. In other words, it is produced through the dissolution of $Li_2S_n$ in the liquid electrolyte (see figure 4(a)). During discharging and charging process, once the solid sulfur in S-containing cathode is reduced to long-chain $Li_2S_n$ ($n = 8, 6, 4$) polysulfides, which dissolve into the liquid-electrolyte and react with the Li-metal anode. In the process, they are electro-chemically transformed into short-chain $Li_2S$ and $Li_2S_2$ polysulfides, resulting the loss of the active materials. Subsequently, $Li_2S$ and $Li_2S_2$ re-diffuse to the S-containing cathode and form long-chain polysulfides during charging process, followed by re-diffusion of long-chain polysulfides again towards the anode side, provoking an irreversible loss of sulfur, insufficient Coulombic performance, auto-discharge processes and poor cycle stability [133].

2. **Large volume expansion of S**: Considerably higher crystalline density of sulfur (approximately $2.07 \text{ g cm}^{-3}$) compared to that of lithium polysulfides leads to a significant volume expansion of about ~80% during the lithiation process. The successive volume expansion/contraction throughout the discharging/charging cycles causes fragmentation of the active materials, leading to considerable structural instability of the electrode, quick capacity decay and safety issues [134].
3. **Insulating nature of S, Li$_2$S and Li$_2$S$_2$:** While Li–S batteries are in operation, Li$_2$S and Li$_2$S$_2$ are susceptible to coating the sulfur and hindering its further utilization. Therefore, a significant quantity of conductive carbon additive is required to ensure both the electron transport and the electrochemical reaction which results in poor gravimetric-capacity [135].

Significant progress has been undertaken toward designing of modern and innovative cathode materials to overcome all the aforementioned limitations, in particular 'Shuttle effect of soluble LiPSs' [136]. A typical advancement during early investigations was the implementation of porous conductive carbon as cathode of Li–S batteries [137–139]. Nevertheless, the introduction of porous carbon based cathode materials and LiPSs are not sufficient to hinder the migration and diffusion of soluble LiPSs. This leads to low cycling-stability over the long term charge/discharge process. It has been recently revealed by studying a wide category of materials, based on graphene oxides [140, 141], metal-oxides such as TiO$_2$ and MnO$_2$ [142, 143], and metal–organic frameworks (MOFs) [144, 145]. The crucial and important factor to overcome is the LiPSs migration and to achieve a long cell life, which consists strong chemical interactions over time between the host materials and the dissolved LiPSs. However, several of these materials do not possess the characteristics required for effective cathode, namely good mechanical stability and excellent electronic conductivity. In this context, MXenes can potentially fulfill a crucial role owing to their capability of achieving high-electronic conductivity as well as a significant surface area characteristics, which can enhance the electron diffusion between electrodes and improve the chemical interaction of the sulfur cathode with LiPSs. This has led to widespread interest with a growing number of publications in recent years as shown in figure 4(c).

DFT based first principles calculations have yielded a relevant criteria for the theoretical strength of LiPSs/MXene interaction based on binding energies, which is the difference between the total energies of the...
optimized MXene+LiPSs system and summation of MXenes system without LiPSs and isolated LiPSs. Zhao et al have demonstrated a promising host material for trapping soluble S-containing polysulfides in oxygen functionalized titanium carbide-based MXenes, namely Ti$_2$CO$_2$ and Ti$_3$C$_2$O$_2$, which comes from the attraction between the positively charged Li-ions in Li$_2$S$_n$ polysulfides and negatively charged oxygen-atoms. This leads to relatively high binding energies ranging from 1 to 2 eV (see table 1) [146]. Chung et al have investigated the impact of different non-uniform surface including the substitutents, vacancy, and S-trapped sites of fluorine and oxygen functionalized Ti$_2$C for anchoring characteristics of S-containing species (Li$_2$S$_n$) [147, 148]. Through an energetic analysis, they have confirmed that Ti$_2$CF$_2$ successfully suppresses the shuttling of LiPSs, while the neutralization of soluble long-chain polysulfides to insoluble elemental sulfur on Ti$_2$CO$_2$ eliminates the shuttling.

Liang et al reported Ti$_2$CT$_x$ as a sulfur host materials of the cathode, which enhances the performance of Li–S batteries [122, 123]. It has been noticed on the basis of the ion-electron pairs nature of S-atoms [149] that the polysulfides are able to act as soft bases, which means that the MXene host without terminal groups may strongly interact with the polysulphides via the Ti–S coordination (see figure 4(d)) [122]. Furthermore, recent findings by Nazar’s group provide insights into the formation of Ti–S bonds with the formation of a great quantity of thiosulfate-polynionate molecules on the surfaces of host-materials upon the contact with polysulphides [143]. Figure 4(e) illustrates the interaction between OH-decorated MXene and Li$_2$S$_n$ species which can be described in a two-step process [123]: I) the Li$_2$S$_n$ species are initially chemisorbed on the MXene surface, undergo redox reactions with the OH-termimtions and form thiosulphate groups, II) the titanium atoms easily accept extra Li$_2$S$_n$ polysulfides in the electrolyte which forms Ti-S bonds through acid-Lewis base interactions.

Min Fang et al described the effect of many-body dispersion (MBD) in on the binding energies of polysulfides on Ti$_2$CF$_2$ as host materials, and further discussed the anchoring mechanism of Li$_2$S$_n$ polysulfide reduction [124]. They found by comparing the Li$_2$S$_n$ polysulfides, that Li$_2$S$_4$ tends to adsorb vertically on Ti$_2$CF$_2$ with the both Li-atoms binding with Ti$_2$CF$_2$ due to strong Li–F interaction (see figure 4(f)). MBD method predicts the lower binding energies over 20% compared to vdW$^{surf}$ method in the case of long chain polysulfides with the ratio for many-body effect range between 16.8% and 33.3% during the delithiation of Li$_2$S$_n$ polysulfides. Based on experimental approach, Tang et al also reported that Ti$_3$C$_2$T$_x$ with nanoscale S uniformly decorated on the surface have the enhanced performance of very Ti$_3$C$_2$T$_x$ (see table 2) [151, 152]. A recent computational study by Wang et al investigated the feasibility of S functionalization of MXenes to create a sulfur rich cathode. This showed that vanadium carbide with S-functionalization (V$_2$C$_x$S$_y$) presents a enhanced binding energy (see table 1 and figure 4(g)). This suppresses the shuttling of soluble polysulfides by preventing the decomposition of the Li$_2$S$_n$ polysulfides [125]. Unlike the standard conductive hosts for S-cathodes, MXenes have the potential to effectively trap Li$_2$S$_n$ LiPSs during the discharge/charge for Li–S batteries. MXenes with functionalization can additionally enhance the binding capacity of Li$_2$S$_n$ polysulfides, which suppress the shuttle effect of soluble polysulfides in Li–S batteries.

| Host Materials | Li$_2$S | Li$_2$S$_2$ | Li$_2$S$_4$ | Li$_2$S$_6$ | Li$_2$S$_8$ | S$_n$ | Reference |
|----------------|--------|-----------|-----------|-----------|-----------|------|-----------|
| Ti$_2$C        | 5.82   | 8.87      | 15.41     | 22.71     | 29.73     | –    | [150]     |
| Ti$_2$C$_2$    | 5.68   | 8.78      | 15.21     | 21.96     | 29.54     | –    | [150]     |
| Ti$_2$N        | 6.09   | 9.16      | 15.85     | 22.47     | 29.18     | –    | [150]     |
| Ti$_2$N$_2$    | 6.13   | 9.21      | 15.59     | 22.62     | 29.33     | –    | [150]     |
| V$_2$C         | 6.42   | 9.61      | 12.19     | 19.69     | 15.27     | 19.52| [125]     |
| V$_2$C(O)$_2$  | 4.42   | 3.80      | 2.91      | 2.48      | 3.06      | 1.07 | [125]     |
| V$_2$C(S)$_2$  | 2.16   | 1.89      | 1.31      | 1.05      | 1.10      | 0.69 | [125]     |
| Ti$_3$C(OH)$_2$| –      | –         | 3.43      | 4.49      | 4.90      | –    | [150]     |
| Ti$_2$CO$_2$   | –      | –         | 2.58      | 1.53      | 1.72      | –    | [124]     |
| TiS$_2$        | 3.02   | 3.12      | 1.92      | 1.47      | 1.71      | 0.95 | [146]     |
| Ti$_2$CF$_2$   | –      | –         | 1.59      | 1.51      | 1.30      | –    | [124]     |
| Ti$_2$CF$_2$   | 2.36   | 2.14      | 1.61      | 1.28      | 4.51      | –    | [124]     |
| Ti$_2$CF$_2$   | –      | –         | 1.02      | 0.42      | 0.34      | –    | [146]     |
| Ti$_2$CO$_2$   | –      | –         | 1.11      | 1.03      | 1.15      | –    | [148]     |
| Ti$_2$CO$_2$   | –      | –         | 0.85      | 0.43      | 1.15      | –    | [146]     |
Table 2. Electrochemical characteristics summary of experimental advances MXene as cathode host for Li–S battery, e.g., current rate (C), cycle number, reversible capacity (mAhg$^{-1}$) and electrochemical mechanism.

| Hosts materials                  | Rate (C) | Cycle number | RC (mAhg$^{-1}$) | Electrochemical mechanism        | Reference |
|----------------------------------|----------|--------------|-----------------|----------------------------------|-----------|
| S@Ti$_2$C$_2$T$_x$               | 0.2      | 800          | 724             | Double mechanism                 | [151]     |
| Ti$_2$C-S                        | 0.5      | 400          | 960             | Chemical adsorption              | [150]     |
| Ti$_3$C$_2$T$_x$/S               | 1        | 1000         | 689.7           | Chemical adsorption              | [153]     |
| Li$_2$S/Ti$_3$C$_2$T$_x$         | 0.1      | 100          | 525             | Chemical adsorption              | [154]     |
| Ti$_3$C$_2$T$_x$/rGO/S           | 1        | 500          | 596             | Chemical adsorption              | [155]     |
| Ti$_3$C$_2$T$_x$/ MoS$_2$-C-S    | 0.5      | 300          | 799.3           | Electrocatalysis                 | [152]     |
| S@TiO$_2$/Ti$_2$C                | 2        | 200          | 464             | Chemical adsorption              | [156]     |
| Ti$_3$C$_2$T$_x$/CNT             | 0.5      | 1200         | 1240            | Double mechanism                 | [123]     |
| Ti$_3$C$_2$T$_x$/graphene/Li$_2$S| 0.2      | 100          | 710             | Dual chemisorption               | [157]     |
| Ti$_3$C$_2$T$_x$/MnO$_2$         | 0.2      | 500          | 1140            | Electrostatic self-assembly      | [158]     |
| Mo$_2$C/C                        | 1        | 600          | 1050            | Chemical adsorption              | [159]     |
| Mo$_2$C/CNFs                     | 0.1      | 50           | 1017            | physical/chemical adsorption     | [160]     |
| W$_2$C NPs/CNFs                  | 1        | 500          | 1200            | Dual chemisorption               | [161]     |
| W$_2$C/N/P- rGO                  | 1        | 400          | 914             | Chemical adsorption              | [162]     |

4. Van der waals heteroctruture for energy storage

4.1. Types of heterostructures

The standard method to improve the performances of electrochemical properties of 2D layered materials, including MXenes, is by hybridization with complementary materials into multifunctional heterostructures or composites, including 0D–2D, 1D–2D, 2D–2D, and lateral-2D structures constructed from low-dimensional ingredient nanostructures. In this section, we will review the emerging applications of 2D heterostructures that enhances the performance in the field of electrochemical storage. The numerous nanostructures with different dimensionalities, such as quantum dots (QDs)/nanoparticles (0D), nanotube/nanorods (1D), and 2D nanosheets, have been established to hybridize with 2D MXene nanosheets to form heterostructures as presented in figure 5. These hybridizations can substantially improve the overall electronic conductivity, especially for the heterostructures hybridized with a conductive matrix, such as carbon-nanotubes (CNTs), different nanoparticles, and conductive polymers, etc [77]. The expansion of volume during the insertion process can also be effectively tuned by the designed porous and hollow hybrid structures and it shows better performance for electrochemical energy storage including lithium ions battery (LIB) and other batteries [54, 77, 163–167].

Two main categories of heterostructures corresponding to the wide range of applications are vertically stacked heterostructure (see in figure 5(c)) and horizontal in-plane (lateral) heterostructure (see in figure 5(d)). The vertically stacked heterostructures are those in which two or more 2DMs have interfacial contact, and it may be either due to strong (i.e. covalent) or weak (i.e. vdW) interactions. The sequence of stacking is significant because it may change the physical and chemical properties, modulated by different stacking orders. Also, the horizontal or lateral heterointerfaces have at least two different 2DMs joined together at the edge results in strong bonding between the edge atoms. The 2D hybrid heterostructures have demonstrated their competency by outperforming potential devices made from mono-layered 2DMs. This improvement is attributed to synergistic effects caused by close interaction between different materials, which may result in considerable changes in physical and chemical properties that ultimately allow us to modulate or activate useful features for various applications.
2D heterostructures are generally synthesized by using a single 2D nanomaterial as a substrate, then adding secondary layers via either a ‘top-down’ or ‘bottom-up’ approach. The solid-based techniques [169–171] have shown special importance for energy storage and conversion. Large, high quality nanosheets cannot be made via chemical vapor deposition (CVD) [172, 173], however the technique can synthesize relatively small nanosheets for 2D heterostructures for energy storage and conversion. The energy-related applications are sensitive to surface [174], porosity [175] and electrolyte exposed active edge sites [19, 54, 176–180]. The 2D hybrid heterostructures can help to overcome the limitations of single 2DMs, distinct from the various supercapacitor and the battery performance improvements achieved recently. The Ragone plot (i.e. energy density vs. power density) of batteries offer low power density and high energy density, whereas supercapacitors have vice-versa. Jiang et al [168] synthesized a novel 2D hybrid nanosheet superstructure consisting of the alternative atomic interface contact/interaction between single-layer MoS2 and single-layer carbon nanosheet with very limited interface contact as shown in figure 5(e). It was reported that the optimized MoS2/m-C hybrid superstructure solves most of the key challenges for MoS2-base anode materials for LIBs, such as poor electrical conductivity of MoS2 along the perpendicular direction, accommodating the volume expansion upon lithiation, overcoming the aggregation and restacking of MoS2.
Figure 6. Overview of 2D MXene hybrid materials for batteries. (a), (b) Schematic illustration of the configuration of anode/cathode for rechargeable metal-ion batteries (X/Y represents the anode/cathode material, respectively). (c), (d) Schematic illustration of a hybrid anode/cathode of lithium–sulfur batteries.

layered material, providing the largest interface contact for Li-ion storage and also for mitigating the polysulfide shutting [168]. A MoS$_2$/m-C nanosheet superstructure has been demonstrated as an anode materials for Li-ion storage in which it exhibits a high reversible specific capacity of 1183 mAh g$^{-1}$ at current density of 200 mAg$^{-1}$, shown in figure 5(f). From the DFT investigations, the MoS$_2$/m-C hybrid superstructure interface provided the most energetically favored process for high Li-ion storage and demonstrating the explicit synergetic effect between MoS$_2$ and single-layer of carbon nanosheet as shown in figure 5(g). Besides this, other MoS$_2$-based hybrid superstructures displayed good battery performances [181–184]. In the next section, we will discuss some recent advances about 2D hybrid heterostructures for batteries to recount their promising potential in this field.

4.2. Lithium ions batteries

Generally, conventional LIBs use graphite as the anode. The limitations of graphite such as low specific capacity 372 mAh g$^{-1}$ and poor rate capability motivate researchers to focus on the new smart 2DMs such as graphene and other mono elemental, TMDs, MXenes etc. The single layer of graphene appeared to have a moderate capacity, unavailable voltage platform, and low Coulombic efficiency. The single layer of MXene also shows relatively low specific capacity as compared to their hybrid heterostructures [19, 21, 23]. As discussed in earlier sections, most of the MXenes are potential candidates who have displayed high electrical conductivity, fast molecular and ion transport, low operating voltages, and high storage capacities [19, 185]. The cyclic voltammogram measurements of single layer of Ti$_3$C$_2$ nanosheet show charge and discharge capacities of 264.5 and 123.6 mAh g$^{-1}$ in the first cycle at 1 C, with a Coulomb nine efficiency of 47% [186]. Whereas r-GO/Ti$_3$C$_2$ heterostructures show the discharge capacity of 930 mAh g$^{-1}$, while its charge capacity is 500 mAh g$^{-1}$, with Coulombic efficiency more than 95% [187]. This significant improvement of r-GO/Ti$_3$C$_2$ over monolayer has also been reported by other groups [164, 188–192]. Recently, r-GO/Ti$_2$CT films significantly enhanced electrochemical performance with an improved reversible capacity of $\approx$700 mAh g$^{-1}$ at 0.1 Ag$^{-1}$ with high Coulombic efficiency, excellent cycling stability and rate performance [187]. Moreover, the MoS$_2$@Ti$_3$C$_2$ nanocomposites give a reversible discharge capacity of 131.6 mAh g$^{-1}$ and corresponding a current density of 1000 mAh g$^{-1}$ for 200 cycles with excellent cycling stability, which is significantly higher than that of its pure Ti$_3$C$_2$ (58 mAh g$^{-1}$) and MoS$_2$ (3.6 mAh g$^{-1}$) [193]. Additionally, Ti$_3$C$_2$/CNTs heterostructure also show very high discharge and charge capacities of 642.5 and 403.5 mAh g$^{-1}$, respectively [194]. The Ti$_3$C$_2$/CNTs heterostructure not showed only high reversible capacity, but has long cyclic stability and excellent rate capability [194].

Similarly, many researchers tried to improve the electrochemical performance, by forming free standing, flexible MXene/CNTs composite electrodes. Correspondingly, the specific capacity and resultant rate performance have been enhanced via improved ion accessibility. Nb$_x$CT$_x$ could be effectively synthesized in...
the presence of isopropylamine, as reported by Mashtalir and co-workers [17]. The free standing flexible Nb$_2$CT$_x$/CNT composite paper electrode gives an excellent cyclability, and Li-storage capacity of more than 400 mAh g$^{-1}$ at 0.5 C after 100 cycles and Coulombic efficiency is approximately 100% for anode materials. Especially in case of a full battery, when an Nb$_2$CT$_x$/CNT film used as an anode and a LiFePO$_4$ electrode as a cathode material then the charge and discharge capacity of 24 mAh g$^{-1}$ for Nb$_2$CT$_x$/CNT was reported for anode materials [195]. Apart from that, porous structure Ti$_3$C$_2$T$_x$/CNT films have been reported by Ren et al [190], in which significantly enhanced reversible storage capacity of lithium ions of $\approx$1250 mAh g$^{-1}$ at 0.1 C, good rate performance of 330 mAh g$^{-1}$ at 10 C, and excellent cycling stability was resulted. The free-standing and flexible Ti$_3$C$_2$T$_x$/CNT for Mg$_2^+$/Li$^+$ battery delivered a capacity of $\approx$100 mAh g$^{-1}$ at 0.1 C and $\approx$50 mAh g$^{-1}$ at 10 C. The capacity was maintained for >500 cycles at 80 mAh g$^{-1}$ at 1 C with Coulombic efficiency was very close to 100% [188]. The free-standing Mo$_2$CT$_x$/8 wt% CNT films, perform a stable reversible capacities of 250 and 76 mAh g$^{-1}$ at 5 and 10 Ag$^{-1}$ over 1000 cycles for Li-ions as an electrode material, respectively [38].

Recently, MXene/oxides composite have been also used as an anode material for rechargeable batteries. The TiO$_2$ is a good candidate as an anode material for storage devices due to the low cost, environmental friendliness, and availability [196]. Researchers follow mainly two approaches, selectively partial oxidation of MXene and introduction of external metal ion to interpose oxides into MXene [197–201]. Ahmed et al [197] reported, TiO$_2$/Ti$_2$C hybrid materials delivered discharge capacities of 389, 337 and 297 mAh g$^{-1}$ at current densities of 100, 500 and 1000 mAg$^{-1}$ at 50 cycles, respectively and it has excellent rate capability of 150 mAh g$^{-1}$ at 5000 mAg$^{-1}$. The Nb$_2$CT$_x$ containing external Nb$_2$O$_3$ nanoparticles (Nb$_2$CT$_x$@Nb$_2$O$_3$) were synthesized via CO$_2$ oxidation which gives a capacity of 208 mAh g$^{-1}$ at 0.25 C and the specific capacity of 94% with the Coulombic efficiency of 100% after 400 cycles [198]. As reported by Zhao et al [202], the hybrid structure Ti$_3$C$_2$T$_x$/NiCo$_2$O$_4$ used as an electrode achieved high reversible capacities of 1330, and 650 and 350 mAh g$^{-1}$ at 0.1, 5 and 10 C with stable over hundreds of cycles, respectively.

Furthermore, tin-based materials were used commonly as electrodes for LIBs due to the high capacities and environmental friendly [199–201]. According to Luo et al [200], the Sn$^{4+}$ ion decorated Ti$_3$C$_2$ nanocomposites (PVP-Sn(IV)@Ti$_3$C$_2$) by liquid-phase immersion methods, give a good reversible volumetric capacity of 1375 mAh cm$^{-3}$ (635 mAh g$^{-1}$) at 216.5 mA cm$^{-3}$ (100 mAg$^{-1}$) after 50 cycles with a high current density of 6495 mA cm$^{-3}$ (3 A g$^{-1}$) and these nanocomposites maintain after 100 cycles with a stable rate capacity of 504.5 mAh cm$^{-3}$ (233 mAh g$^{-1}$), which is considerably higher than that of a graphite electrode (i.e. 550 mA cm$^{-3}$). The Sn(IV) nanoparticle-modified Ti$_3$C$_2$ MXene (i.e. SnO$_2$-Ti$_3$C$_2$) hybrid structure synthesized via a hydrothermal method used as anode material for LIBs with excellent electrochemical performance. It shows the outstanding initial capacity of 1030.1 mAh g$^{-1}$ at 100 mAg$^{-1}$, and maintain 360 mAh g$^{-1}$ after 200 cycles [201].

Recently, Ti$_3$C$_2$ has been synthesized in the presence of NiCo-MOF (3D Ti$_3$C$_2$/NiCo-MOF composite structure). This significantly enhanced the electrochemical performance of Li-ion battery [222]. Ti$_3$C$_2$/NiCo-MOF composite structure was prepared by vacuum-assisted filtration technology as shown in figure 7(a). During the synthesis of this composite, when NiCo-MOF was added into Ti$_3$C$_2$ nanosheets solution via vacuum-assisted filtration, the porous structure was naturally constructed due to the interlayer hydrogen bonds between MXene and MOF nanostructure. The rate performance of Ti$_3$C$_2$/NiCo-MOF composite and bare Ti$_3$C$_2$ electrode at different current densities are presented in figure 7(b). It is evident that the bare Ti$_3$C$_2$ electrode displayed a charging capacity of 141 and 67 mAh g$^{-1}$ at the current density of 0.1 and 1 Ag$^{-1}$, respectively. It shows relatively low electrochemical performance for Li ion diffusion limited by compact stacking of multi-layer Ti$_3$C$_2$ structure [222]. On the other hand, the electrochemical performance of Ti$_3$C$_2$/NiCo-MOF composite structure is mainly depends on the loading of NiCo-MOF in the hybrid structure. The Ti$_3$C$_2$/NiCo-MOF-0.4 composite structure exhibits the highest capacity of in all the considered compositions of NiCo-MOF loading and corresponding discharge capacity of 402 and 256 at the current density of 0.1 and 1 Ag$^{-1}$, respectively. The capacity maintains its initial value even at lower current density of 0.1 Ag$^{-1}$, it means that the Ti$_3$C$_2$/NiCo-MOF-0.4 composite electrode displayed excellent rate performance for a Li-ion battery. Figure 7(c), shows a high discharge capacity of 504.5 mAh g$^{-1}$ at the first cycle. The Ti$_3$C$_2$/NiCo-MOF-0.4 composite electrode displayed a relatively high capacity of 240 mAh g$^{-1}$ with the Coulombic efficiency of 85.7% after 400 cycles, claims excellent long cycling life as well as at a high rate. Another reported work by Meng et al [222], the Ti$_3$C$_2$T$_x$-based composite (figure 7(d)) anode in LIBs exhibits higher capacity and better rate performance than pristine Ti$_3$C$_2$T$_x$ nanostructure. Figure 7(e) manifests the specific capacity at different current density with various concentration of Si nanoparticles. During the rolling process to in-situ produces Ti$_3$C$_2$T$_x$/Si composite material with 10% silicon nanoparticles.
displayed the best overall enhancement among capacity, rate capability and cyclic stability for Ti$_3$C$_2$Tx scrolls.

The hybrid structures are valuable to improve the reversible limit of MXene-based materials for the classical Li-storage system. These are the result of the development of two electrochemical responses (i.e. conversion/alloying for MXene-based composites and adsorption-desorption for MXene network). The efficient and environmentally friendly route of intercalation of inorganic compounds with MXenes, such as the composites presented in table 3, should be adopted to further enhance the reversible capacity of the resultant batteries. Most of the MXene composites displayed significant improvement in gravimetric capacity, and it showed the maximum capacity higher than that of the typical graphite anodes [224], some even the excellent capacity of 2000 mAh g$^{-1}$ [203, 218, 219]. These composites also showed superior rate behavior and cycle lifetime. Furthermore, they exhibited quite strongly pseudo-capacitive cyclic voltammetry and charge-discharge profiles, which means that the significant portions of their capacities are delivered at
higher voltages for conventional Li-ion battery anodes [190, 202, 203, 217–220]. From the above
descriptions, it is clear that the rate capacity of MXenes is excellent and intrinsically connected to capacitive
behavior [225]. Therefore, future work needs to optimize composite materials that exhibit fast redox peaks
where MXenes contribute by providing conductive networks.

4.3. Non-lithium ions batteries
As described in earlier section, rechargeable batteries with non-lithium-ions such as Na⁺, K⁺, Mg²⁺, Ca²⁺,
and Al³⁺ have received much attention as emerging low-cost and high-energy density technologies for
large-scale renewable energy storage devices [19, 22, 23]. The hybrid structures i.e. MoS₂-intercalated
Ti₃C₂Tx composite produced using a hydrothermal route were presented to render an enhanced high specific
capacity of 250.9 mAhg⁻¹ over 100 cycles, and rate performance with a capacity of 162.7 mAhg⁻¹ at 1 Ag⁻¹
[245]. An isolated Ti₃C₂ system gives a specific capacity of 100 mAhg⁻¹ and a current density of 20 mAg⁻¹
after 100 cycles [118]. Xie et al [189] reported that the porous MXene Ti₃C₂/CNTs films gave a high
volumetric capacity of 345 mAhcm⁻³ at 100 mAg⁻¹ after 500 cycles and reversible capacity of 175 mAhg⁻¹
at 20 mAg⁻¹ after 100 cycles. Sb₂O₃/Ti₃C₂Tx hybrid structure sodium storage, delivered a rate performance
of 295 mAhg⁻¹ at 2 Ag⁻¹ and at 100 mAg⁻¹ after 100 cycles enhanced the cycling performance up to 472
mAhg⁻¹ [230]. Some fruitful and enlightening attempts have been carried out to check the performance for
Table 4. Overview of electrochemical characteristics such as current rate (CR), reversible capacity (RC), cycle number (CN) and rate capability (RCap.) from MXene and MXene-based composite for Na-ions batteries. Here, DMSO stands for dimethyl sulfoxide, NR-nanoribbons.

| Materials               | CR  | RC (mAh g⁻¹) | CN (mAh g⁻¹) | RCap. | Reference (mAh g⁻¹) |
|-------------------------|-----|--------------|--------------|-------|---------------------|
| Ti₃C₂Tx                  | 200 | 79           | 500          | —     | [115]               |
| Ti₃C₂Tx                  | 200 | 178          | 500          | 105   | [116]               |
| Ti₃C₂Tx                  | 100 | 101          | 500          | —     | [117]               |
| TiO₂/Ti₃C₂Tx             | 200 | 267          | 2000         | 100   | [115]               |
| Ti₃CNTx                  | 10  | 90           | 100          | 75    | [226]               |
| H₂Ti₃C₂Tx                | 50  | 68           | 200          | 47    | [61]                |
| S-doped-Ti₃C₂Tx          | 100 | 183          | 2000         | 121.3 | [227]               |
| TiO₂@Ti₃C₂Tx             | 30  | 220          | 5000         | 215   | [228]               |
| CoNiO₂/Ti₃C₂Tx           | 100 | 223          | 140          | 211   | [229]               |
| SnS/Ti₃C₂Tx              | 100 | 413          | 50           | 400   | [117]               |
| Sb₂O₅/Ti₃C₂Tx            | 200 | 450          | 100          | —     | [230]               |
| DMSO/Ti₃C₂Tx             | 100 | 120          | 500          | 100   | [231]               |
| Crumpled Ti₃C₂Tx NR      | 20  | 250          | 50           | 120   | [232]               |
| Alkalized Ti₃C₂Tx        | 20  | 167          | 500          | —     | [233]               |
| Mo₂CT₂ spheres           | 50  | 370          | 1000         | —     | [163]               |
| Ti₃C₂Tx spheres          | 50  | 330          | 1000         | —     | [163]               |
| V₂C₅Tx spheres           | 50  | 340          | 1000         | —     | [163]               |
| Ti₃C₂Tx spheres          | 20  | 154          | 100          | 75    | [226]               |

Table 5. Overview of theoretical electrochemical performances of MXenes and MXene-based composite as electrode active material for metal-ions batteries.

| Materials               | Applications | Capacity (mAh g⁻¹) | Reference |
|-------------------------|--------------|--------------------|-----------|
| Ti₃C₂Tx                 | LIBs         | 447.8              | [234]     |
| Ti₃C₂O₂/graphene        | LIBs         | 426                | [235]     |
| Ti₃C₂                     | SIBs         | 351.8              | [234]     |
| Y₂C                     | SIBs         | 564                | [236]     |
| Ti₃C₂                     | KIBs         | 191.8              | [234]     |
| Ti₃C₂O₂/graphene        | KIBs         | 209.5              | [237]     |
| V₂C₅O₂/graphene         | KIBs         | 207.2              | [237]     |
| Zr₂C₂O₂                  | KIBs         | 474                | [238]     |
| Zr₂C₂O₂                  | KIBs         | 326                | [238]     |
| Ti₃C₂O₂                  | LIBs         | 383                | [114]     |
| Ti₃C₂O₂                  | LIBs         | 268                | [114]     |
| V₂C₅O₂                  | LIBs         | 367                | [114]     |
| Nb₂C₅O₂                  | LIBs         | 233                | [114]     |
| Ti₃C₂                     | LIBs         | 320                | [114]     |
| Ti₃N₂                     | LIBs/SIBs/KIBs | 484/484/1242/ | [239]     |
| Ti₃N₂O₂                  | LIBs/SIBs/KIBs | 378/378/378/ | [239]     |
| Ti₃NF₃                  | LIBs/SIBs/KIBs | 2269/756/1134/ | [239]     |
| VS₂/Mo₂C₂O₄N₅          | SIBs         | 420.09             | [240]     |
| VS₂/Nb₂C₂O₄N₅          | SIBs         | 428.29             | [240]     |
| VS₂/Ti₃C₂O₄N₅          | SIBs         | 601.44             | [240]     |
| VS₂/V₂C₅O₂N₅          | SIBs         | 585.29             | [240]     |
| ScC₂O₂                  | LIBs/graphene | 229.85             | [241]     |
| ScC₂(COH)₂/graphene     | LIBs         | 227.87             | [241]     |
| Ti₃C₂O₂/graphene        | LIBs         | 234.39             | [241]     |
| Ti₃C₂(OH)₂/graphene     | LIBs         | 232.34             | [241]     |
| V₂C₅O₂/graphene         | LIBs         | 234.12             | [241]     |
| V₂(C(OH)₂)/graphene     | LIBs         | 232.07             | [241]     |
| Cr₂C₂O₂                  | LIBs/SIBs/KIBs | 331/276/1239/ | [242]     |
| Cr₂C₂O₂                  | LIBs/SIBs/KIBs | 545/470/796/ | [242]     |
| Mo₂C                     | LIBs/SIBs | 263/263            | [243]     |
| Zr₂C                     | LIBs         | 310                | [244]     |
| Zr₂C₃S₂                  | LIBs         | 259                | [244]     |

practical applications of the full battery mechanism. Ti₃C₂/CNTs used as an anode and Naₐ₄₄MnO₂ as a cathode powers a 2.5 V light-emitting diode for ≈25 min which expending an electrical energy of 41 µWh
During the full cell mechanism, $\text{Ti}_5\text{C}_2/\text{CNT-SA}$ electrode gives the charge and discharge capacities of 270 and 286 mAhcm$^{-3}$ respectively. The corresponding volumetric discharge capacity was retained as 242 mAhcm$^{-3}$ at the current density of 50 mA g$^{-1}$ after 60 cycles with a Coulombic efficiency of 99% [246]. $\text{Ti}_5\text{C}_2$ monolayer displayed fast migration of K-ion with specific capacity of 191.8 mAhg$^{-1}$ using DFT in theoretical investigations by Dequan et al [234].

While Zhao et al synthesized PDDC-N-rich porous carbon nanochips (NPCN)/$\text{Ti}_5\text{C}_2$ a hybrid structure which exhibited a good rate performance as shown in figure 8. The PDDC-NPCN/$\text{Ti}_5\text{C}_2$ hybrid structure is prepared in face-to-face manner by the electrostatic interaction between NPCN and multiple layers of $\text{Ti}_5\text{C}_2$ (see figure 8(a)). The PDDC-NPCN/$\text{Ti}_5\text{C}_2$ hybrid structure displayed a layered structure with large surface area and effectively utilize two components and more accessible active sites which can confirm the nearby contact between PDDC-NPCN and $\text{Ti}_5\text{C}_2$. The galvanostatic charge/discharge profiles of the PDDC-NPCN/$\text{Ti}_5\text{C}_2$ hybrid structure anode are measured at the current density of 0.1 Ag$^{-1}$ for initial first five cycles. The initial discharge capacity of 797.3 mAhg$^{-1}$ and charge capacities of 583.6 mAhg$^{-1}$ achieved as presented in figure 8(b). From figure 8(c), it is confirmed that the PDDC-NPCN/$\text{Ti}_5\text{C}_2$ hybrid structure anode exhibits superior rate performance at high current densities. Also, it shows high reversible capacity of 358 mAhg$^{-1}$ at the current density of 0.1 Ag$^{-1}$ even after 300 cycles while after 2000 cycles at the current density of 1.0 Ag$^{-1}$, it displayed a reversible capacity of 252 mAhg$^{-1}$ with a decay rate of only 0.03 per cycle (figure 8(d)). From XRD pattern, the diffraction peak (001) of $\text{Ti}_5\text{C}_2$ shifted to a lower angle and representing that the interlayer spacing expanded from 19.2 to 24.6 Å, which corresponds to the K$^+$ intercalation into the PDDC-NPCN/$\text{Ti}_5\text{C}_2$ composite anode. The hybrid structures provide a larger interlayer spacing which makes a 3D interconnected conductive framework to accelerate the ion/electron transfer rate. PDDC-NPCN/$\text{Ti}_5\text{C}_2$ composite also shows a high chemical stability due to its good tolerance toward volume change caused by phase change in fast charge and discharge process. Additionally, it was seen that the PDDC-NPCN/$\text{Ti}_5\text{C}_2$ composite material significantly reduces the K$^+$ binding strength, which accelerates reaction kinetics. PDDC-NPCN/$\text{Ti}_5\text{C}_2$ composite material exhibits high inter-layer spacing, providing significant capacity, excellent cycle performance, excellent speed performance, and exceptionally good speed capacity for K-ion battery. These theoretical and experimental results proposed a new strategy to prepare a high performance MXene-based composite material for K-ion battery anode.

To summarize, MXene heterostructures (MXenes composite) can accommodate metal ions due to their wide interlayer spacing, where graphite have lower spacing which does not prefer heavier ion intercalation [234, 235, 237, 238]. Although, in the case of full intercalations, the diffusion rates are limited, and in this case, an increase in the interlayer spacing of MXenes and their composites is needed. The performance of metal ions batteries are summarized in tables 4 and 5 in which $\text{Sb}_2\text{O}_3/\text{Ti}_5\text{C}_2\text{Ti}_x$ composite electrode displayed high performance by Guo and co-workers [230]. Overall the MXenes heterostructures (e.g. MXene combine with graphene or other layered materials) have lower diffusion barriers for alkali metals than MXene or isolated graphene [235, 237].

### 4.4. Lithium–sulfur battery

Li–S batteries have garnered much attention owing to the simple configurations, high energy density and capacity and more environmentally friendly as described in previous section. Hybrid structures and composites also enhance the properties of materials toward Li–S battery applications. As reported by Peng et al [250], hybrid structure TiC@G/S as cathode for Li–S battery shows without binder, separator, and current collector capacity of 670 mAhg$^{-1}$ at a current density of 0.2 C after 100 cycles with Coulombic efficiency of 95%. Generally, a typical cathode for Li–S battery is made by carbon/sulfur. According to Zhao et al [251], the multilayers of carbon/sulfur flakes derived from MXene $\text{Ti}_6\text{SC}$ displayed promising characteristics for Li–S battery. The fabricated Lamellar structured, flexible $\text{Ti}_5\text{C}_2$ MXene (graphene, BN) lithium film anode have low overpotential, exhibited high reversible capacity of 841 mAhg$^{-1}$ after 100 cycles. A lithium–sulfur full cell with $\text{Ti}_5\text{C}_2$-Li as anode and sulfur–carbon as cathode exhibited a high energy density and excellent cycle performances [252]. In another case, MXene nanosheets with hydroxyl group/CNTs composites were recently synthesized [123] and provided high polysulfide adsorption. This further enabled sulfur hosts with excellent long-term cycling performance, with reversible capacities of $\approx$450 mAhg$^{-1}$ at 0.5 C after 1200 cycles with a capacity retention of $\approx$95% [123]. 3D $\text{Ti}_5\text{C}_2\text{Ti}_x$/rGO/sulfur composites used as a cathode host material for Li–S battery prepared by using a liquid phase impregnation technique provided a high initial capacity of 1144.2 mAhg$^{-1}$ at 0.5 C with a high level of capacity retention of 878.4% after 300 cycles [253].

Gao and co-workers [248] synthesized the $\text{TiO}_2$ QDs decorated on the surface of $\text{Ti}_5\text{C}_2\text{Ti}_x$ MXene (see figure 9(a)(I)) has a quite promising electrochemical performance as a sulfur host for achieving fast and stable Li–S batteries. The TiO$_2$ QDs/MXene hybrid structure exhibit superior performance suppressing the shuttling effect with polysulfides which gives excellent long-term cyclability and rate capability as presented
Figure 8. (a) Schematic representation of the fabrication of PDDC-NPCN/Ti$_3$C$_2$ hybrid structure, (b) initial galvanostatic charge/discharge profiles at the current density of 0.1 Ag$^{-1}$, (c) rate performance at different current densities and (d) long cycling performance at the current density of 1.0 and 2.0 Ag$^{-1}$ after 2000 cycles of the PDDC-NPCN/Ti$_3$C$_2$ hybrid structure anode for the potassium-ion storage performance. Reproduced from [247]. Copyright 2020, Royal Society of Chemistry.

in figure 9(a). Compared with a MXene/S cathode which displayed a lower discharging voltage (2.03–2.31 V), TiO$_2$ QDs/MXene delivered a slightly higher voltage (2.09–2.38 V) which described the reduction of elemental sulfur to higher-order polysulfides (Li$_2$S$_n$, 4 ≤ n ≤ 8). In contrast, the plateau at the lower voltage for these two cases is related to the reduction process of higher-order to lower-order lithium polysulfides [254]. The TiO$_2$ QDs/MXene hybrid structure exhibited higher capacities of 1158, 1037, 925, 812 and 663 mAhg$^{-1}$ at C/5, C/2, 1 C, 2 C and 5 C current densities, respectively, where 1 C = 1675 mAg$^{-1}$ as presented in figure 9(a)(III). Figure 9(a) (IV) displays the long-term cyclability of TiO$_2$ QDs/MXene composite, which shows the high capacity of 680 mAhg$^{-1}$ at 2 C after 500 cycles with sulfur loading of 1.5 mg cm$^{-2}$ and this value is significantly twice that of MXene/S cathodes. The Coulombic efficiency of TiO$_2$ in QDs/MXene composite cathodes reaches nearly 100% in the whole cycling process. More importantly, superior electrochemical performance could be available at higher sulfur loading of 5.5 mg cm$^{-2}$. Another reported work on Ti$_3$C$_2$T$_x$/MnO$_2$ composites delivered a high initial capacity of 1140 mAhg$^{-1}$ at 0.2 C after 500 cycles [158]. Table 2 displayed the summarized lists of cathode materials for Li–S batteries.

Another fascinating work by Lv et al. [249], the highly conductive Mo$_2$CT$_x$/CNT composites has been synthesized via a ball milling procedure (figure 9(b)(I)). The Mo$_2$CT$_x$/CNT composite electrode exhibited superior electrochemical performance in the terms of good rate capability, high capacity and high initial reversible capacity of 1314, 1068 and 959 mAhg$^{-1}$ at different sulfur loading of 1.8, 3.5 and 5.6 mg cm$^{-2}$, respectively (figure 9(b)(II)). Furthermore, the rate capacities of Mo$_2$CT$_x$/CNT/S electrode and their comparison with Mo$_2$CT$_x$/S at various current densities of 0.1 to 5 C are displayed in figure 9(b)(III). The charging-discharging profile for Mo$_2$CT$_x$/CNT/S and Mo$_2$CT$_x$/S composites is displayed in figure 9(b)(IV). The Mo$_2$CT$_x$/CNT composites exhibited the reversible capacities of 954 at 1 C after 100 cycles with ≈100% Coulombic efficiency which shows excellent electrochemical performance. MXenes and MXenes composites can capture the soluble LiPSs though a strong transition metal and sulfur interaction to suppress the shuttling effect. Also, functionalized MXenes surface displays strong chemisorption to LiPSs and thus
significantly reduces the active material loss and provide high capacities after long-term cycling. Based on the summarized lists of composites materials in all the tables, heterostructures proved to be promising candidates for energy storage applications.

5. Summary and outlook

Three types of MXenes, namely 2D metal carbides, 2D metal nitrides, and 2D metal carbonitrides with different surface functional group such as oxygen (–O), hydroxyl (OH) and/or fluorine (–F) were fabricated in last decade by selective etching and exfoliation of MAX phases. High surface charge and hydrophilicity of the MXenes lead to stable water-based colloidal arrangements that do not require surfactants for adjustment. This makes MXene synthesis and processing cheap and straightforward, which further encourages researchers to investigate their potential applications. To date, the continuous increase in the interest of electrochemical energy storage devices require further investigation and development of enhanced electrode materials, which can increase the loading of ions and molecules with high capacity and faster kinetics. From this viewpoint, a new smart 2D electrode material Ti3C2 MXene was reported and investigated in 2011. Furthermore, many other 2D MXenes exhibit attractive electronic, optical, photonic, photocatalyst, and thermoelectric properties. Apart from this, it has superior attributes for electrochemical such as high strength, high melting point, high electrical and thermal conductivity, oxidation resistance, hydrophilic nature, compositional variability, and large surface area. Therefore, MXenes have evolved as an alternative for advanced electrode materials. The MXene layers have large interlayer spacing, which is advantageous for different sized cations, to be easily intercalated into the layers. The combination of superior electrical
conductivity and mechanical strength and their functionalized surface by oxide and/or hydroxide, including uncovered redox-active transition metal atom, make MXenes alluring for the utilization as battery electrodes. MXenes exhibit high capacity and stability for Li- batteries. Besides lithium, there are several cations such as sodium (Na), potassium (K), magnesium (Mg), that intercalated in the MXenes layers and served as promising candidates for energy devices applications. The intercalation of the larger size of some cations has not been explored because there can be a propensity for large interlayer cations to lead to low conductivity, hence, it will influence the charge transfer and diffusion kinetics of the ions.

The present review summarizes the structural and electronic properties of bulk MAX phases and then their 2D counterparts MXenes along with the synthesis methods of precursors and exfoliation of nanoflakes. The applications of MXenes and MXenes composites/hybrid structures have been discussed in detail for and alkali-ion and Li–S batteries. The outstanding features makes MXenes outlier from other 2DMs families and make them promising candidates for high-performance electrodes. In particular, MXenes and its composites have many advantages for Li–S batteries, such as the unique layered structure of MXenes with the appropriate surface area for sulfur/sulfides, which provides excellent mechanical strength to resist the stress induced by large volume expansion of sulfur. The metallic conductivity facilitates the electron transport kinetics through the electrolyte/electrode interface, improves electrode polarization, and assists high rate responses even at a high sulfur loading. MXenes have been used both as sulfur hosts and modified spacers and the electrochemical performance of Li–S batteries based on MXene can improve mainly through the materials and design of the cell. It can be achieved by increasing active sites of interaction to strengthen immobilizing Li2Sn, introducing spacers to suppress the restacking of nanosheet and building 3D structures to improve sulfur loading, and so on. Surface chemistry plays a essential role in accomplishing electrodes with a superior affinity for LiPSs species. The functionalization of MXenes reduces the strong form of metal–sulfur bonds for LiPS’s species, and further enhances the Li-ion diffusivity on the surface, leading to excellent electrochemical performance. Furthermore, advantages of MXenes and its composites have been discussed for restacking, stability, high electrical conductivity, and fast electron/ion transfer, which open new research windows in the fields of energy conversion and storage applications. However, some of the MXenes composites with the conducting polymers are yet to be investigated. These possible MXenes hybrid structures may contribute to the field of potential applications in the next generations of battery electrodes. There are wide open challenges for controlled synthesis MXenes and MXenes composites for practical applications. New synthesis methods is needed for controlled synthesis of functionalized MXenes, as of current methods lead to random functionalization with more than one functional groups [255]. Rapid oxidation of MXene is a well known problem to be taken care of before its utilization in any commercial products such as energy production, conversion and storage applications.

Acknowledgments

DS and RA thanks Olle Engkvists Stiftelse (198-0390), Carl Tryggers Stiftelse for Vetenskaplig Forskning (CTS:18:4) and Swedish Research Council (VR-2016-06014) for financial support. VS acknowledges the SSF grant (ITM17-0324) for financial support. NK and AA acknowledge the PPR2 project: (MISTERSFC-CNRST) for financial support. SNIC and HPC2N are acknowledged for providing the computing facilities.

Authors contribution

DS, VS and NK have equally contributed in this review article. AA and RA has helped to improve the scientific content of the review article. RA has conceptualized, supervised, facilitate resources and funding for this work.

ORCID iDs

Deobrat Singh  https://orcid.org/0000-0001-7246-8743
Vivekanand Shukla  https://orcid.org/0000-0001-7724-6357
Nabil Khossossi  https://orcid.org/0000-0002-3914-4162
Rajeev Ahuja  https://orcid.org/0000-0003-1231-9994

References

[1] Zhu Y, Murali S, Cai W, Li X, Suk J W, Potts J R and Ruoff R S 2010 Adv. Mater. 22 3906–24
[208] Zhang C, Kim S, Ghidui M and Zhao M 2016 Adv. Funct. Mater. 26 4143
[209] Huang J, Meng R, Zu L, Wang Z, Feng N, Yang Z, Yu Y and Yang J 2018 Nano Energy 46 20–8
[210] Wang J, Dong S, Li H, Chen Z, Jiang S, Wu L and Zhang X 2018 J. Electroanal. Chem. 810 27–33
[211] Wang Y et al 2018 J. Mater. Chem. A 6 11189–97
[212] Chen C et al 2018 Angewandte Chemie Int. Edn 57 1846–1850
[213] Wu X, Wang Z, Yu M, Xi L and Qiu J 2017 Adv. Mater. 29 1607017
[214] Shen C, Wang L, Zhou A, Wang B, Wang X, Lian W, Hu Q, Qin G and Liu X 2018 Nanomaterials 8 80
[215] Ma Z, Zhou X, Deng W, Lei D and Liu Z 2018 ACS Appl. Mater. Interfaces 10 3634–43
[216] Kong F, He X, Liu Q, Qi X, Sun D, Zheng Y, Wang B and Bai Y 2018 Electrochem. Commun. 97 16–21
[217] Zhang Y et al 2019 ACS Nano 13 2167–75
[218] Zhang C, Park S H, Seral-Ascaso A, Barwich S, McEvoy N, Coleman J S, Gogotsi Y and Nicolosi V 2019 Nat. Commun. 10 1–9
[219] Tian Y, An Y and Feng J 2019 ACS Appl. Mater. Interfaces 11 10004–11
[220] Zhang L, Wang K and Zou B 2019 ChemSusChem 12 1612–30
[221] Li H, Lu M, Han W, Li H, Wu Y, Zhang W, Wang J and Zhang B 2019 J. Energy Chem. 38 50–4
[222] Meng J, Zhang F, Zhang L, Liu L, Chen J, Yang B and Yan X 2020 J. Energy Chem. 46 256–63
[223] Liu Y, He Y, Virgoun F, Plachy T, Saha P and Cheng Q 2020 Nanomaterials 10 695
[224] Pourali Z, Sovizi M and Yasfian M 2018 J. Alloys Compd. 738 130–7
[225] Zhan C, Naguib M, Lukatskaya M, Kent P R, Gogotsi Y and Jiang D e 2018 J. Phys. Chem. Lett. 9 1223–8
[226] Naguib M, Adams R A, Zhao Y, Zemlyanov D, Varma A, Nanda J and Pol V G 2017 Chem. Commun. 53 6883–6
[227] Li J, Yan D, Hou S, Li J, Lu T, Yao Y and Pan L 2018 J. Mater. Chem. A 6 1234–43
[228] Guo X, Zhang J, Song J, Wu W, Liu H and Wang G 2018 Energy Storage Mater. 14 306–13
[229] Tao M, Zhang Y, Zhan R, Guo B, Xu Q and Xu M 2018 Mater. Lett. 230 173–6
[230] Guo X, Xie X, Choi S, Zhao Y, Liu H, Wang C, Zhang S and Wang G 2017 J. Mater. Chem. A 5 12445–52
[231] Lv G, Wang J, Shi Z and Fan L 2018 Mater. Lett. 219 45–50
[232] Natu V, Clites M, Pomerantseva E and Barsoum M W 2018 Mater. Res. Lett. 6 230–5
[233] Guo Y G 2019 Nanostructures and Nanomaterials for Batteries: Principles and Applications (Berlin: Springer)
[234] Er D, Li J, Naguib M, Gogotsi Y and Shenoy V B 2014 ACS Appl. Mater. Interfaces 6 11173–9
[235] Du Y T, Kan X, Yang F, Gan L Y and Schwingschlägl U 2018 ACS Appl. Mater. Interfaces 10 32867–73
[236] Hou J, Tu K and Chen Z 2016 J. Phys. Chem. A 120 18473–8
[237] Demirgöz I, Peeters F M, Gulerseren O, Çakar D and Sevik C 2019 J. Phys. Chem. Lett. 10 727–34
[238] Meng Q, Ma J, Zhang Y, Li Z, Hu A, Kai J J and Fan J 2018 J. Mater. Chem. A 6 13652–60
[239] Wang D, Gao Y, Liu Y, Jin D, Gogotsi Y, Meng X, Du F, Chen G and Wei Y 2017 J. Phys. Chem. 121 13025–34
[240] Tang C, Min Y, Chen C, Xu W and Xu L 2019 Nano Lett. 19 5577–86
[241] Aierken Y, Sevik C, Gulerseren O, Peeters F M and Çakar D 2017 J. Mater. Chem. A 6 2337–45
[242] Li F, Cabrera C R, Wang J and Chen Z 2016 RSC Adv. 6 81591–6
[243] Çakar D, Sevik C, Gulerseren O and Peeters F M 2016 J. Mater. Chem. A 4 6029–35
[244] Zhi J, Chronoeas A, Eppinger J and Schwingschlägl U 2016 App. Mater. Today 5 19–24
[245] Wu Y, Nie P, Jiang J, Ding B, Dou H and Zhang X 2017 ChemElectroChem 4 1560–5
[246] Dall’Agneys Y, Taberna P L, Gogotsi Y and Simon P 2015 J. Phys. Chem. Lett. 6 2305–9
[247] Zhao R, Di H, Hui X, Zhao D, Wang R, Wang C and Yin L 2020 Energy Environ. Sci. 13 246–57
[248] Gao X T, Xie X, Zhu X D, Sun K N, Xie X M, Liu Y T, Yu J Y and Ding B 2018 Small 14 1804433
[249] Lv L, Guo C F, Sun W and Wang Y 2019 Small 15 1804388
[250] Peng H J, Zhang G, Chen X, Zhang Z W, Xu W T, Huang J Q and Zhang Q 2016 Angewandte Chemie Int. Edn. 55 12990–5
[251] Zhao M Q et al 2015 Angewandte Chemie Int. Edn. 54 4810–14
[252] Li B, Zhang D, Liu Y, Li S and Yang S 2017 Nano Energy 39 654–61
[253] Bao W, Xie X, Xu J, Guo X, Song J, Wu W, Su D and Wang G 2017 Chem. Eur. J. 23 12613–19
[254] Bao W, Liu L, Wang C, Choi S, Wang D and Wang G 2018 Adv. Energy Mater. 8 1702485
[255] Chaudhari N K, Jin H, Kim B, San Baek D, Joo S H and Lee K 2018 J. Mater. Chem. A 6 1865–1865