# Commission on Crystallography of Materials

## RECENT PROGRESS ON THE RESEARCH OF MATERIALS SCIENCE

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### Abstract:

The great progress in material science has largely changed people's life. Searching materials with exotic functions using different methods are frontiers of materials science. This paper will review the recent achievements in this area, including new methods developed for the crystal structure prediction and the results got based on these methods; the high pressure synthesis of new emergent materials; the metallic hydrogen and related compounds; two dimensional metal carbides, nitrides and their application on the energy storage.

### Introduction:

The making use of functional materials is the necessary motive of the developing human society. From the Bronze Age to Iron Age and finally to the modern life, the materials of bronze, iron and silicon all played important roles. They promoted the people's ability to conquer nature. For this reason nowadays the material science has become a very flourishing area. Compared to the previous work, the research route had greatly changed. Searching for new functional materials is not solo focusing on changing the combination of elements. The new concept "material design" had been introduced, which means using the theoretical method to predict new structure to guide the experiment. The methods for material fabrication are also changed from conventional to unconventional, such as extreme condition of high pressure, which can be used to synthesize the new materials which can't exist at ambient pressure. Meanwhile the material state are also expanded from three dimensional to low dimensional. The most important result is the two dimensional materials Graphene [1], which has unusual electronic, mechanical and optical properties. In present paper, we will give a brief summary about the recent progress on the crystal structure prediction, the high pressure synthesis of emergent materials, metallic hydrogen and related compounds, and newly found two dimensional metal carbides and nitrides.

### Results:

### Progress on the crystal structure prediction:

Crystal structure prediction is believed to be predictable for a long time. There are two difficulties have to be overcome before the successes of the crystal structure prediction: 1) Ranking problem: as the energy differences between different polymorphs are often very small, it's very difficult to get a reliable calculation on the relative structure. 2) Search problem: the number of possible arrangements of atoms in space is very large: for a unit cell with N atoms, the number of possible structures is C ~ exp(ad), where *d* is the number of degrees of freedom and *a* is some system-specific constant. If the positions of all N atoms are uncorrelated, then d = 3N + 3, resulting in a very high-dimensional problem.

Though most of the above problems had been resolved, the structure relaxation and energy evaluations are still very difficult and too expensive at the *ab* initio level. Thanks for the development of machine learning forcefield (MLF) method, people can train the *ab* initio energies, stress and forces on the atoms for a number of configurations. For example, Oganov *et al.* [2] combined the MFL and the USPEX and successfully found $\alpha$-boron, $\gamma$-boron and several versions of tetragonal T52-boron, even the extremely complex and disordered $\beta$-boron (Fig. 1a). In addition to these known phases, they predicted a new low

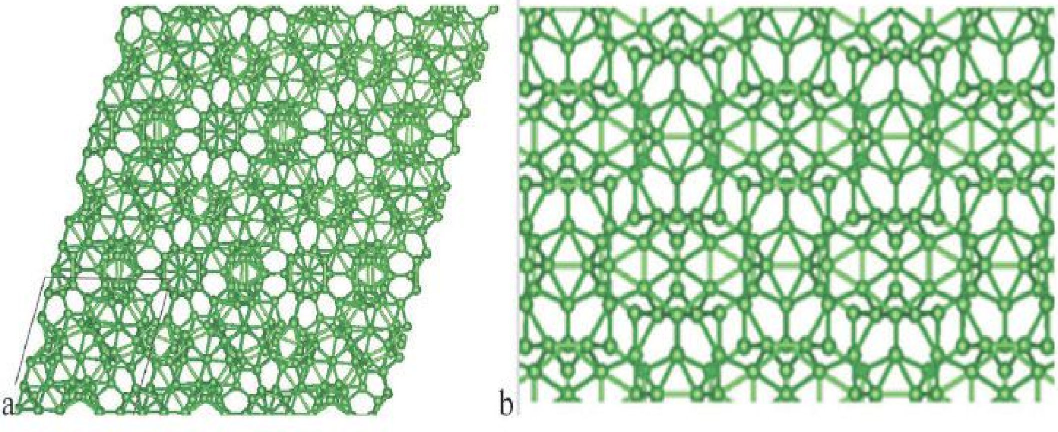


**Figure 1** (a) $\beta$-boron approximant with 106 atoms per cell. (b) *I*m3 structure.

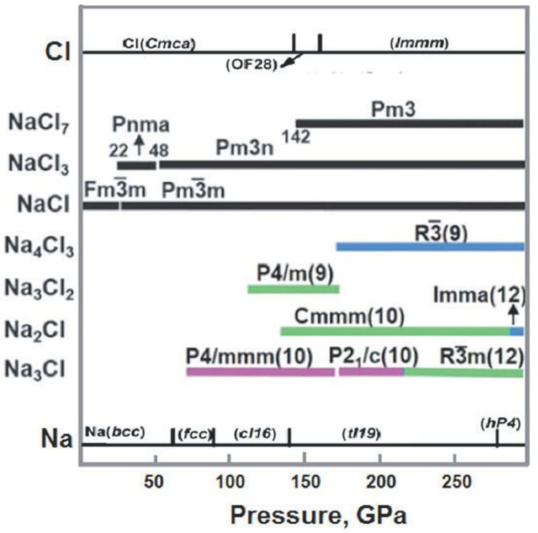


**Figure 2.** Pressure-composition phase diagram of the Na–Cl system.

energy cubic $Im3$ phase (with 54 atoms per cell, Fig. 1b), which is only 29 meV per atom higher in energy than a-boron and energetically degenerate with the experimentally known T52-boron. Moreover use of a MLF has allowed a speedup of 100–1000 times.

With the development of the crystal structure prediction method, lots of new phenomena and supersizing new compounds had been predicted and many of them had been confirmed in experiment. A typical result is the unexpected stable phase of Na-Cl series compounds. As we all know at ambient pressure, the only stable phase for Na-Cl is salt. However, people found at pressures amenable to experiment, new compounds emerge as stable – $Na_3Cl$, $Na_2Cl$, $Na_3Cl_2$, $Na_4Cl_4$, $NaC_{13}$, and $NaC_{17}$ [3, 4], see Fig. 2. For two compounds, $Na_3Cl$ and $NaCl_3$, experimental synthesis was attempted and led to their successful synthesis [3]. Most of these newly predicted sodium chlorides are metallic, despite the large electronegativity difference that they would expect to dictate ionic bonding and make $Na^+Cl^-$ the only allowed compound.

To resolve the very high-dimensional problem, Collins *et al.* developed a method called FUSE [5]. In this method the structures assembles are not from atoms, but from atomic pairs or triples – in ionic crystals cations are expected to be surrounded by anions, rather than by other cations – hence, the pairs can be cation–anion. This simple trick allows rather complex systems to be studied, and Collins *et al.* have reported a successful exploration of the challenging quasiternary $SrO–TiO_2–Y_2O_3$ system (Fig. 3).

## Progress on the discovery of new emergent materials:

Emergent phenomena occur in many body systems of condensed matter, showing exotic properties with phase evolution that will not happen in an individual particle [6]. Emergent materials are compounds showing emergent phenomena [7]. This session will present three examples using high pressure in terms of self-oxidation, inner compression and pure doping to discover new emergent materials. All of these results in this session based on our group's recent works.

First one is the high Tc cuprate superconductor. High Tc superconductor materials is the most important strong correlated materials. The typical features of these series compounds is the CuO2-plane that supporting the superconducting current and the charge reservoir layer where the doping occurred. Usually the layer immediately outside the CuO2 plane is called the apical oxygen layer. As there is a direct connection between the apical oxygen and the CuO2 plane, truing the apical oxygen will be a great effect on the

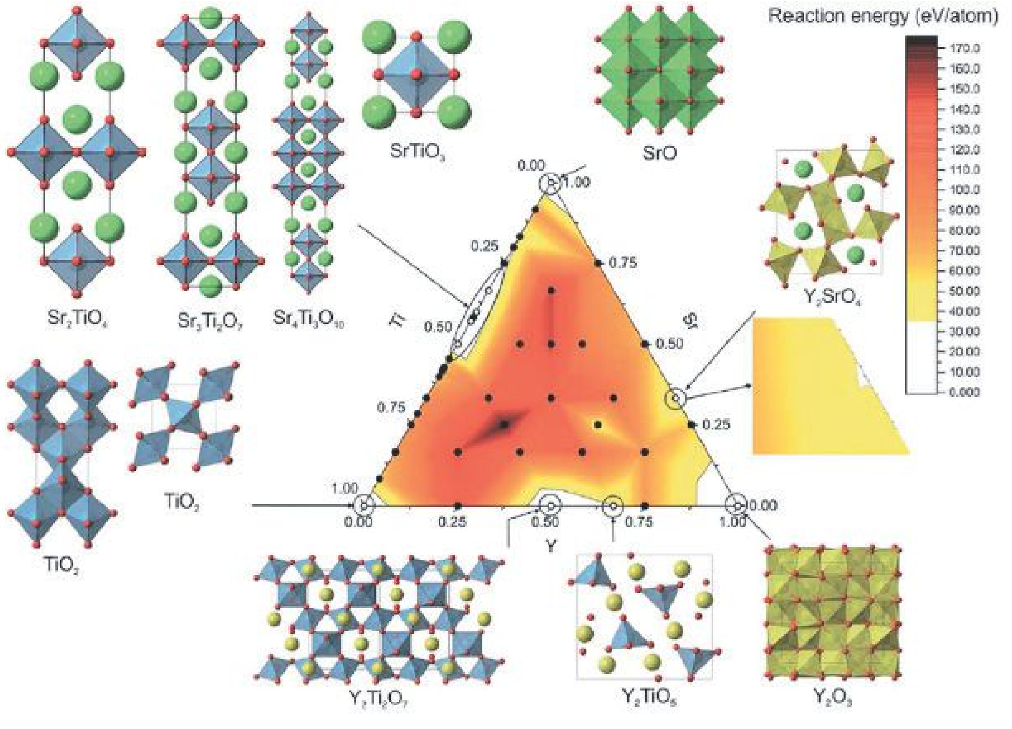


**Figure 3.** Results of the FUSE method for the $SrO–TiO_2–Y_2O_3$ system, showing numerous correctly predicted ground states.

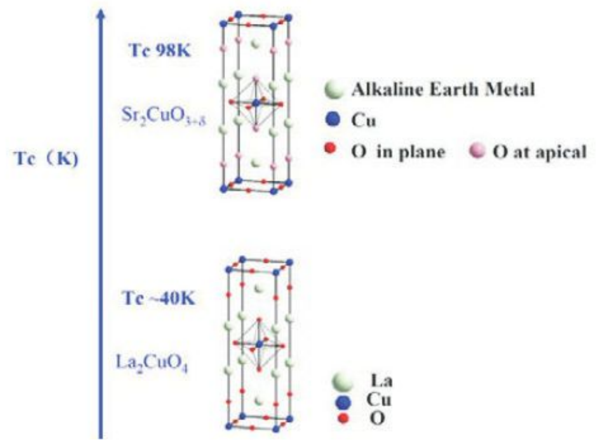


**Figure 4.** The superconductivity transition temperature of $Sr_2CuO_{3+\delta}$ isostructural to $La_2CuO_4$ can be enhanced by apical oxygen.

superconductivity. However most of the high Tc superconductors contain the apical oxygen with fully occupation. Using the method called self-oxidation, which means the oxidizer serves as both oxygen source and component of the new compound, the hole doped $Sr_2CuO_{3+ä}$ superconductor was synthesized under high pressure and high temperature [8]. This compound crystallized into an oxygen deficient $La_2CuO_4$ structure with partially occupied apical site, as shown in the Fig. 4. The apical oxygen service as a hole dopant and the carrier density is determined by the amount of extra oxygen d located at apical site. The experiment results indicated that the Tc changed from 60 K of $Sr_2CuO_{3.2}$ to 75 K for $Sr_2CuO_{3.4}$ and then 58 K for $Sr_2CuO_{3.6}$ by changing the nominal composition of oxygen content. Moreover, the Tc can be enhanced to 90 K for $Sr_2CuO_{3.4}$ after annealing at 200 C at ambient pressure.

The other example is 111-type iron-based superconductor. As we all know, the superconductivity in iron-based superconductors is usually generated by depressing the spin-density wave by ionic substitution or external pressure. We utilized the method of inner compression, which means introducing the element with small atomic radius to induce the chemical pressure to modify the materials properties of iron-based superconductor and found the 111-type iron based superconductor LiFeAs [9]. This crystal structure is shown in Fig. 5. The Fe atoms are in forth-fold coordination, forming a FeAs4 tetrahedron. The nearest neighbor Fe-Fe distance in LiFeAs is 2.66 Å, which is about 6.5% less than that in LaFeAsO with d = 2.853 Å [10]. Unlike the 1111 and 122 iron type, in which the superconductivity is induced by the chemical doping, the superconductivity of LiFeAs is generated by inner pressure in parent compound. This make the 111 system to show the following advantages of (1) precluding the disorder caused by chemical doping (2) free of charge polarization at surface, which is good for the characterization of electronic properties using the ARPES and STM. (3) Simply composition that allows to easier focus on the intrinsic aspects of iron based superconductor.

The last one is the ruthenate $BaRuO_3$. Ruthenates, which has a strong spin orbital coupling, has attracted much attention since they exhibit exotic superconductivity, non- Fermi liquid behavior and quantum phenomena. The A site atomic size for $ABO_3$ composition cause the dramatic change in physical properties without change the valence state of Ru ions. However most of research focus on the perovskite ruthenates having the Ru-O bond under compression (Tolerance factor >1). It's still a challenge to explore the compound with Ru-O in a stretched state (Tolerance factor <1) due to the difficulty in synthesis. We had successfully fabricated $BaRuO_3$ itinerate ferromagnetic as a cubic perovskite at high pressure by a pure doping method [11], which means doping is achieved by a pressure induced change in chemical bonding that in turn gives to magnetic exchange interaction. $BaRuO_3$ adopts a series of structures depending how it is synthesizing (Fig. 6a). In this series structure the tolerance factor (>1) is accommodated by the formation of hexagonal polytypes consisted of face share (F) or corner shared (C) RuO6 octahedra connections. These sequence will greatly change the Ru-Ru bond properties and finally lead to the evolution of magnetic properties, as shown in Fig. 6b.

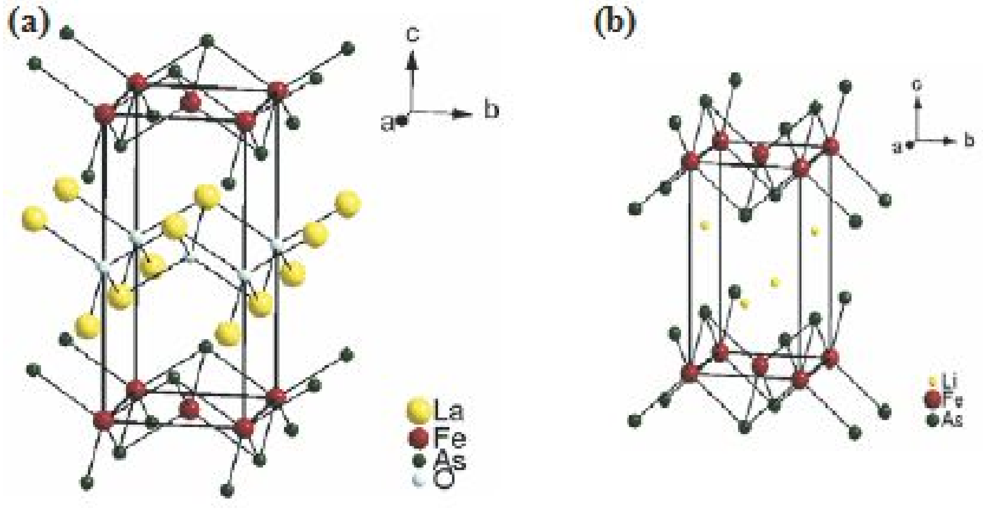
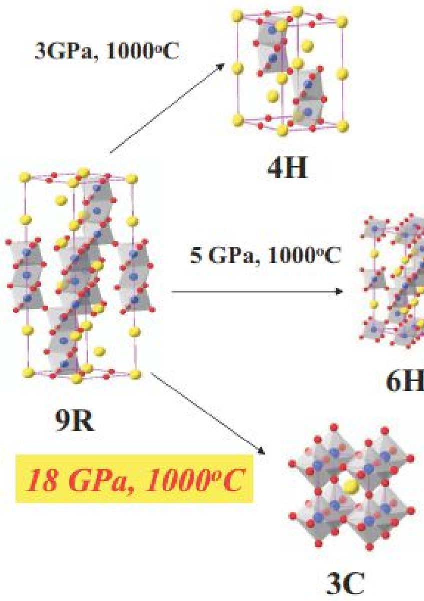


**Figure 5.** The crystal structures of (1) 1111-type LaFeAsO (b) 111-type LiFeAs superconductors.

a)



b)

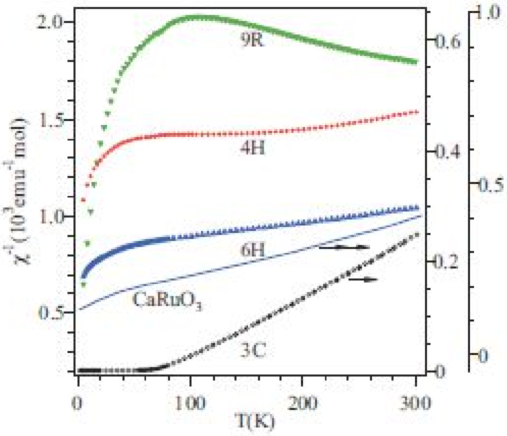


**Figure 6.** (a) The 9R, 4H, 6H and 3C phases of $BaRuO_3$ synthesized as a function of pressure. (b) Temperature dependence of the inverse magnetic susceptibility of 9R, 4H, and 3C phases of $BaRuO_3$

## Progress on the metallic hydrogen and related compounds:

The metallic hydrogen has long been regarded as the Holy Grail of the high pressure physics since Wigner and Huntington [12] predicted that if solid molecular hydrogen was sufficiently compressed in the T=0 K limit, molecules would dissociate to form atomic metallic hydrogen, followed by the prediction [13] that the high temperature superconductivity for metallic hydrogen. In this session, we will review the recent progress on the metallic hydrogen and the hydrogen-rich materials.

Though the theorists had drawn great prospect for the metallic hydrogen, to realize it is still a huge challenge in experiment, especially for reaching to the high pressure up to several megabars. In 2017, Silvera et al. [14] reported that realization of metallic hydrogen using the specific designed diamond anvil cell with a pressure up to 495 GPa

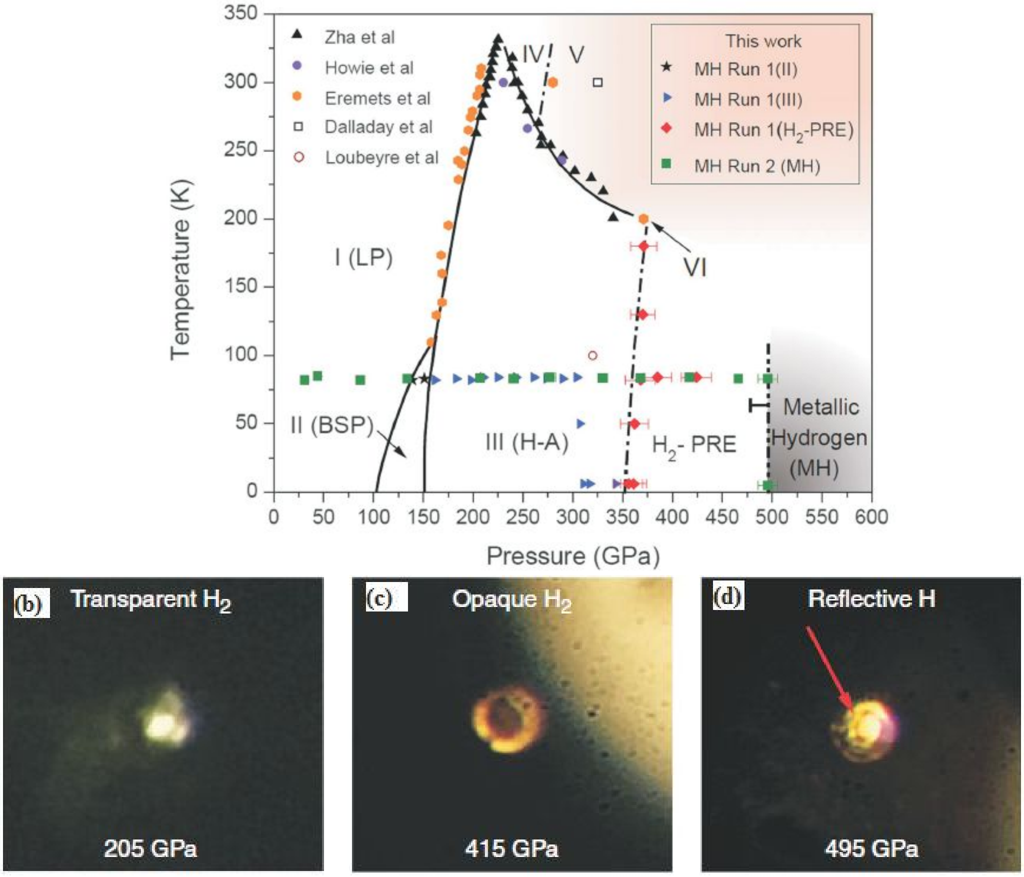


**Figure 7.** (a) The T-P phase diagram of hydrogen based on the current experiment. (b-d) Photographs of hydrogen at different stages of compression, the reflection in Fig. d showed the formation of metallic hydrogen.

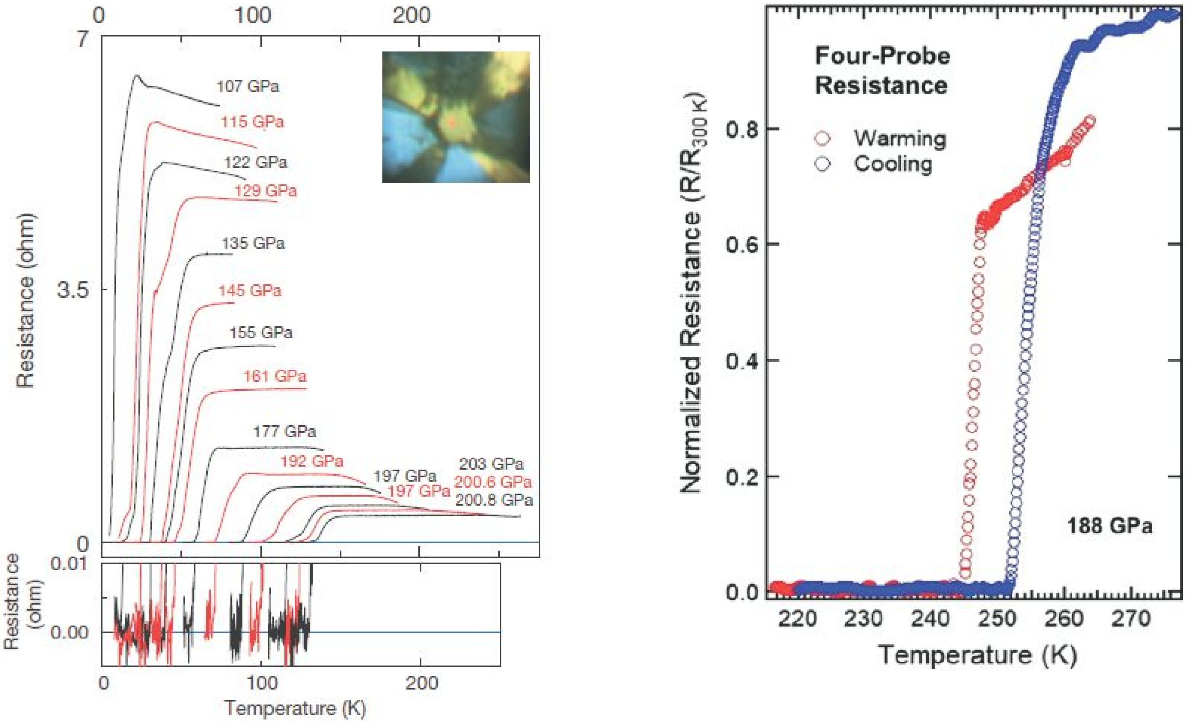


**Figure 8.** (a) Temperature dependence of the resistance of sulfur hydride measured at different pressures, and the pressure dependence of Tc. (b) Normalized electrical resistance of the $LaH_{10+x}$ sample.

(See Fig. 7). In their experiment they made a great deal improvements for the diamond anvil cell, for example the using of CVD grown synthetic diamonds and the culet flat is the 100 crystal direction, annealing the diamond anvils for a few days near their metastability temperature in an ultrahigh vacuum to remove putative residual stress, and coating the gaskets with gold. However, there are still great debates on this result, one important thing is the pressure was determined by the linear extrapolation of the P vs. the screw rotation or load curve, but not determined directly from the evolutions of some physical property. Moreover, the only one piece “metallic hydrogen” disappeared due to the misoperation, and the fabrication can’t be repeated currently. So additional experimental measurements are still required to verify this claim.

As it’s still a hard wok to realize the metallic hydrogen, H-rich materials have been considered as an alternative, because they can metallize at much lower pressures than are accessible to experiments [15]. Followed this principle, theorists predicted that the superconductivity can be realized in the sulfur hydride system [16, 17]. Inspired by these results, Eremtes *et al.* successfully observed a pressure induced superconductivity in $H_3S$ with Tc around 203 K at a pressure up of 200 GPa (Fig. 8 a) [18]. This result had broken the record in the high temperature superconductors with Tc around 163 K, and provided a new route to search new superconductor. More importantly, the recently result indicated the superconductivity transition temperature up to 260 K (Fig. 8b) had been observed in $LaH_{10}$ with pressure around 180-200 GPa [19], which almost approached to the room temperature. We noticed the theoretical prediction played an important role in these process, not only the observation of superconductivity in $H_3S$, but also for that in $LaH_{10}$ [20, 21]. Honestly speaking, the above phenomenon can only be observed at an extreme condition, how to quench them to ambient pressure and make them to be applicable are still need further hard work.

## Progress on the 2D metal carbides and nitrides:

The family of 2D transition metal carbides, carbonitrides and nitrides (usually referred to as MXenes) has expanded rapidly since the discovery of $Ti_3C_2$ in 2011[22]. Currently there are about 20 different MXenes have been synthesized and showing the great potential for application. In this session we will give a brief review about the crystal structures, samples fabrication and their applications in energy storage.

The general formula of MXenes is $M_{n+1}X_nT_x$ ($n = 1$–3). M represents an early transition metal (such as Sc, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo), X is carbon and/ or nitrogen and $Tx$ represents the surface terminations (hydroxyl, oxygen or fluorine) [23]. Fig. 9 illustrate the structures of $M_2X$, $M_3X_2$ and $M_4X_3$. Similar to their MAX precursors, M atoms in MXenes are arranged in a close-packed structure and X atoms fill the octahedral interstitial sites. The overall crystal of MXenes is a hexagonal close-packed structure. However, the ordering of M atoms changes from $M_2X$ to $M_3X_2$ and $M_4X_3$ [Fig. 10]. In $M_2X$, M atoms follow ABABAB ordering (hexagonal close-packed stacking), whereas in $M_3C_2$ and $M_4C_3$, M atoms have ABCABC ordering (face-centered cubic stacking). This wide chemical and structural variety makes MXenes competitive with other 2D materials.

Usually MXenes can be fabricated by selective etching of certain atomic layers from their layered precursors, such as MAX phases. Because the M–A bond is metallic, it was impossible to separate the $M_{n+1}X_n$ layers and make MXenes by mechanical shearing method. However M–A

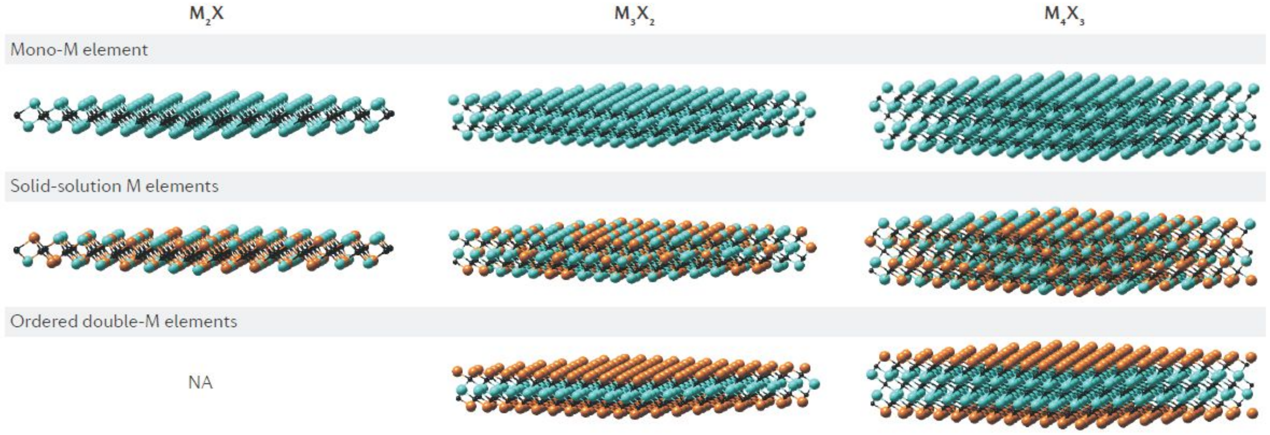


**Figure 9.** Crystal structure of $M_2X$, $M_3X_2$ and $M_4X_3$

bonds are more chemically active than the stronger M–X bonds, which makes selective etching of A-element layers possible; highly selective etching is the key condition for making MXenes. Aqueous fluoride-containing acidic solutions have been predominantly used to selectively etch the A-element layers from MAX phases to synthesize MXenes, either by using aqueous hydrofluoric acid (HF) [23] or by in situ formation of HF through the reaction of hydrochloric acid (HCl) and fluoride (LiF) [24]. Besides the fluoride-containing acidic solution etching, it is also possible to synthesize MXenes high-temperature etching [25] or bottom-up synthesis methods, such as chemical vapor deposition (CVD) [26].

Among most interesting physical properties of MXenes, energy storage has been the first and most studied application. Theoretical study indicated that MXenes are promising candidates for energy storage application [27]. Especially compounds such as $Ti_2C$, $Nb_2C$, $V_2C$ and $Sc_2C$, which show a very low formula weights. The electrodes of these compounds are expected to show higher gravimetric capacity. Currently a lithium-ion capacity of 750 mAh $g^{-1}$ has been achieved by optimization of the electrode architecture, hybridizing porous MXene flakes with carbon-nanotube [28].

MXenes can also accommodate ions of various sizes between 2D layers of $M_{n+1}X_nT_x$. This makes them suitable for non-lithium-ion batteries (NLiBs). Theoretical capacities for some oxygen-terminated MXenes in Na-, K-, Mg-, Ca- and Al-ion batteries [29] are shown in Fig. 11a. Owing to chemical and structural variability and surface chemistry

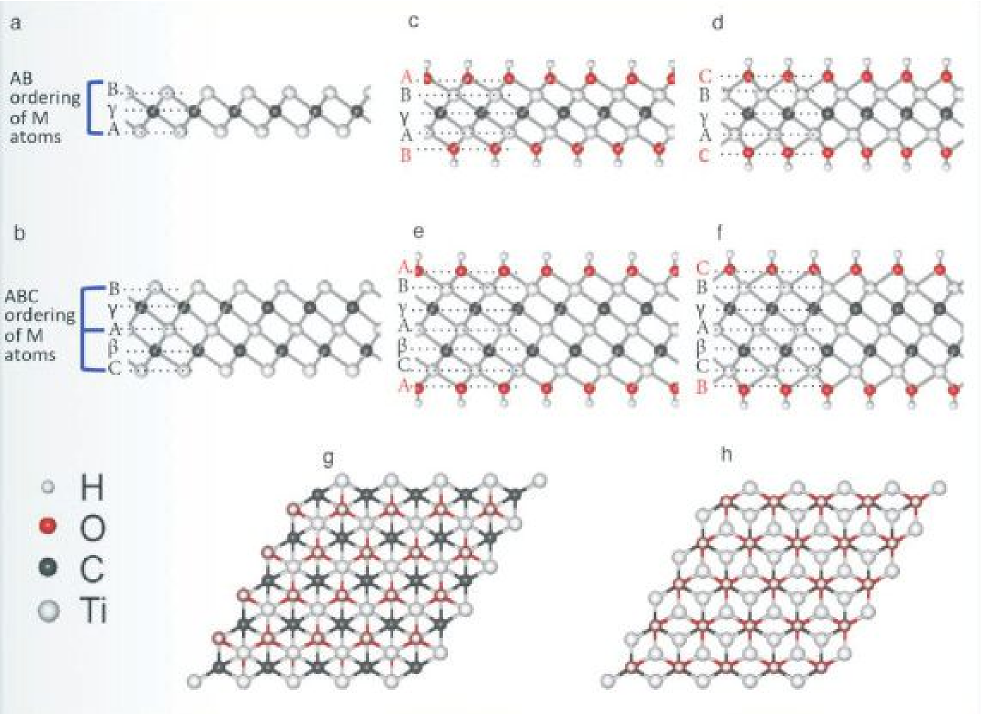


**Figure 10** MXene crystal structures showing atomic ordering of M, X and T elements.

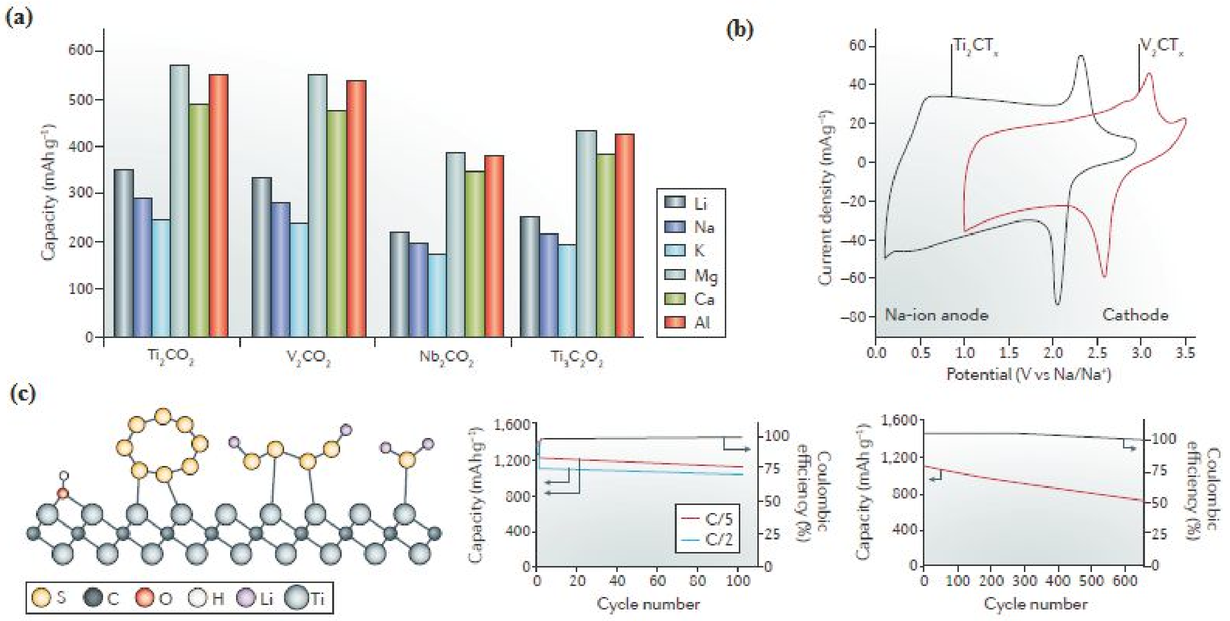


**Figure 11.** (a) Theoretical capacities of lithium and non-lithium ions on oxygen?terminated MXene nanosheets. (b) Cyclic voltammetry profiles of $Ti_2C$ and $V_2C$ in a sodium-ion electrolyte. (c) Performance of $Ti_2C$–S composite in Li–S batteries.

tunability, different MXenes can provide a range of working potentials, which makes some of them suitable as either anodes [30] or cathodes [31] (Fig. 11b). For example, $Ti_2CT_x$ or $Ti_3C_2T_x$ have been used as conductive sulfur hosts in Li–S batteries, resulting in dramatically improved cyclability and stability owing to the strong interaction of polysulfide species with MXene functional groups [32, 33] (Fig. 11c).

## Conclusions:

In this paper, we reviewed the recent progress on the materials science on the structure prediction, the high pressure synthesis of new emergent materials, the metallic hydrogen and related compounds, two dimensional metal carbides and nitrides. We can see clear the new concepts and new methods are powerful in changing the researching situation in material science. The final purpose is people can give a reliable prediction on any type of functional materials they expected and fabricate them in experiment successfully. To realize this dream, there are still many questions need to be addressed in the future.

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## Commission on High Pressure

# TOWARD THE DENSER, HOTTER, FASTER AND BRIGHTER FUTURE: CHALLENGES AND OPPORTUNITIES OF HIGH PRESSURE CRYSTALLOGRAPHY

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## Abstract

Reflection upon the past makes us not only wonder how the ideas of high pressure research sprang from the minds of creative visionaries and have been evolving over the past decades, but also to think about the direction the discipline is heading today. Like in most experimental sciences, this movement is shaped predominantly by emerging techniques and instrumentation. Coupling diamond anvil cells with laser heating made it possible to generate extreme pressures and temperatures in static experiments, effectively mimicking the thermodynamic conditions of planetary interiors. Double-stage and toroidal diamond anvils pushed the limits to about one terapascal (TPa) - ten million times the atmospheric pressure. Even higher, unimaginable pressures of several TPa are achieved in dynamic compression studies, which have paved the way to a better understanding of the physics and chemistry in the depths of giant exoplanets, and also allowed us to probe fundamental properties of matter at extremes, often extending our comprehension beyond textbook knowledge. On the other hand, extremely short and bright pulses from X-ray free-electron lasers are capable of generating and investigating formerly unobserved states of matter, such as the so-called warm dense matter, representing the missing link between solid and plasma. The scientific impact of the recent cutting-edge developments on selected topics in the field of Earth’s science and physics will be briefly mentioned in this report. The IUCr Commission on High Pressure (CHP) is engaged in a wide variety of activities directed at the community, including organizing annual workshops with a training session for early-stage researchers. The workshops have successfully introduced noteworthy new topics and innovative approaches, which will lead to a brighter future in this field.

The earliest *in situ* high-pressure diffraction studies date back to 1930s [1], but the major breakthrough came in 1958 with the advent of a diamond anvil cell (DAC) [2]. This small but mighty device revolutionized the world of extreme conditions research, not only boosting the achievable pressure limit but also permitting a number of experimental spectroscopic and diffraction techniques to effectively probe the sample. Soon the DAC began to evolve from its early prototype, continually striving to push the boundaries of pressure. In 1976, Ho-Kwang Mao and Peter M. Bell from Carnegie Institution of Washington ob-