Research on the Applications of Novel Two-Dimensional Materials in Energy Storage and Energy Conversion

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Abstract. The current energy structure dominated by fossil energy is not only difficult to support the continuous growth of global energy demand but also threatens ecological security due to carbon emissions, and the intermittent and regional defects of renewable energy that need to make breakthroughs in efficient energy storage and conversion technology. Faced with the dual challenges of the structural crisis of the traditional energy system and climate change, the new generation of energy technology with new two-dimensional materials as the core is becoming a key breakthrough to solve the dilemma. Two-dimensional materials show revolutionary potential in the energy field due to their properties such as atomic thickness, controllable electronic structure, and highly active surface. In terms of energy storage, through layer number regulation and heterogeneous structure construction, its conductivity, light absorption efficiency, and ion diffusion rate can be accurately optimized, which can provide an ideal ion transport channel for the energy storage system to alleviate the volume expansion problem. In terms of energy conversion, two-dimensional materials improve catalytic efficiency through the quantum confinement effect. Despite the challenges of preparation processes, environmental stability, and industry suitability, by incorporating artificial intelligence in the development process, upgrading preparation processes, and interdisciplinary collaborative innovation, two-dimensional materials are driving the leapfrog development from nanoscience to engineering applications, which is expected to reshape the energy technology landscape and accelerate the achievement of global carbon neutrality goals.

Keywords: Two-dimensional materials, batteries, supercapacitors, solar energy conversion, thermoelectric conversion.

1. Introduction

The traditional energy system is facing a structural crisis. Since this century, energy consumption has continued to rise at an average annual growth rate of 1.5%, and the total amount has reached 600 exajoules in 2022, of which fossil energy accounts for 82% [1]. This energy mix emits about 33 billion tons of carbon dioxide into the atmosphere every year, significantly exacerbating the surface greenhouse effect. According to the International Energy Agency, maintaining the current energy pattern will lead to a global temperature rise of more than 2.5 degrees Celsius in 2050, far exceeding the 1.5 degrees Celsius safe threshold set by the Paris Agreement [2]. The non-renewable nature of fossil energy and the environmental crisis caused by it have highlighted the urgency of developing an efficient, clean, and sustainable energy system.

In this context, the energy revolution is accelerating the reshaping of human civilization. Although the United Nations proposed to achieve the goal of 36% renewable energy by 2030, the inherent intermittency and geographical limitations of clean energy such as wind, water, and light have spawned a rigid demand for energy storage technology. Current mainstream technologies such as lithium-ion batteries face energy density bottlenecks and capacity attenuation caused by electrode expansion, and perovskite solar cells are subject to stability defects and toxicity risks. These technical shortboards are essentially due to the limitations of the intrinsic properties of materials, and the innovative research and development of breaking through the existing material system has become a key breakthrough to promote the upgrading of energy storage and conversion technology and achieve the goal of carbon neutrality.

In this context, the discovery of two-dimensional materials opens entirely new possibilities for energy technology breakthroughs. Two-dimensional materials refer to materials where electrons can move freely in only two dimensions, from 1 to 100 nanometers, such as nanofilms, superlattices, and quantum Wells. Since graphene was successfully stripped in 2004, the two-dimensional material family has expanded to include transition metal disulfide compounds, MXenes, black phosphorus, and more than 5000 members [3]. Because of their unique physical and chemical properties, two-dimensional materials show great potential in energy technology breakthroughs. Their core advantages are embodied in three aspects, respectively the uniqueness of the structure, the adjustability of performance, and the composite ability. First, the atomic-level thickness of the two-dimensional material, from 0.3 to 2 nanometers, and the planar expansion properties give the very high specific surface area sufficient active sites for ion adsorption and catalytic reactions. Second, material properties can be precisely designed through layer control, construction of the heterostructure, or chemical modification. Third, two-dimensional materials can be flexibly assembled into thin films, aerogels, or three-dimensional network structures, enabling cross-scale performance optimization from nanoscale to macroscopic devices.

Existing experimental studies show that the introduction of two-dimensional materials can improve the performance of energy devices. For example, in the field of energy storage, the power density of MXenes-based supercapacitors exceeds 10 kW/kg, which is 5 times that of commercial activated carbon materials. In the area of energy conversion, the MoS_2/g-C_3N_4 hetero-photocatalyzed hydrogen production rate was 12.3 mmol/g/h, which was an 8-fold improvement over the pure g-C_3N_4 [4]. These breakthroughs signal that two-dimensional materials are becoming a central driver of innovation in energy technology.

2. Novel Two-Dimensional Materials

Two-dimensional materials are a new class of nanomaterials with atomic-level thickness, as shown in Fig.1, whose core feature is that only a single or several layers of atoms form a planar crystal structure, the thickness is usually less than 1 nanometer, and the transverse size can be extended to the order of micron or even millimeter. Due to quantum confinement effects and highly exposed surface atoms, these materials exhibit physical and chemical behaviors that differ from traditional three-dimensional block materials, making them revolutionary material systems in the fields of energy, electronics, and catalysis.

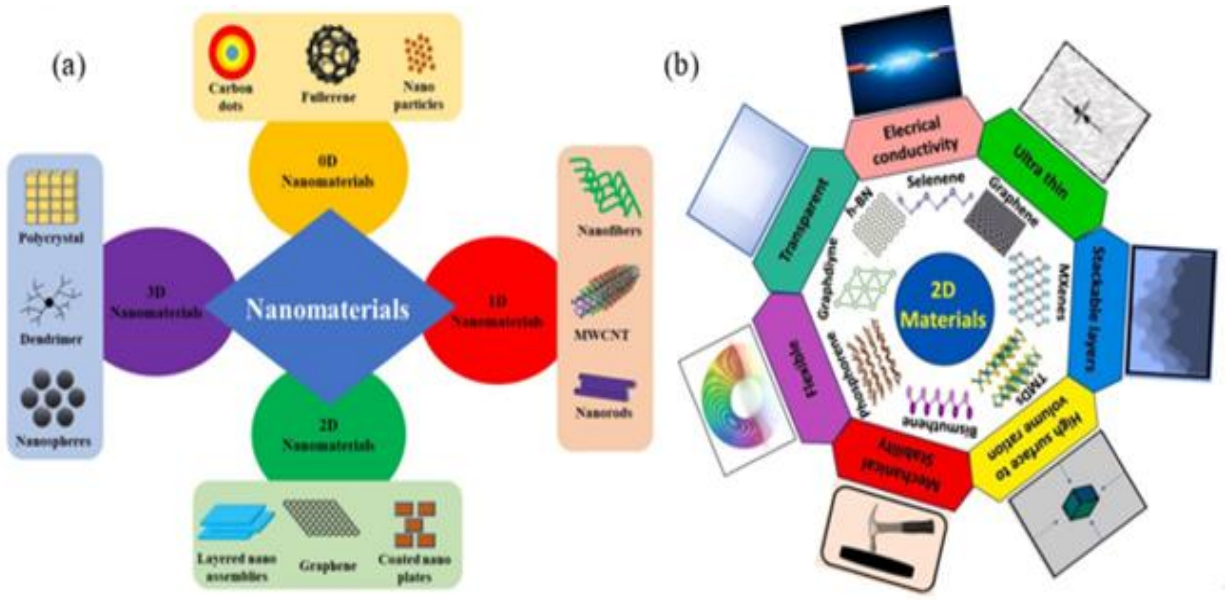

Fig 1. (a) The classification of nanomaterials,
(b) New two-dimensional materials and their properties [5, 6].

First, carbon-based two-dimensional materials are typically represented by graphene, whose single-layer structure consists of carbon atoms formed by sp^2 hybridization into a honeycomb lattice. The electron mobility of graphene reaches 200000 $cm^2/(V \cdot s)$, about 100 times that of copper. At the same time, graphene has a theoretical specific surface area of 2630 m^2/g, providing an ideal charge-storage interface for lithium-ion batteries and supercapacitors [7]. In addition, in the field of carbon-based two-dimensional materials, new carbon-based materials such as graphdiyne and g-C_3N_4 have been derived in recent years, further expanding their application scenarios in fields such as photocatalysis.

Second, transition metal chalcogenides mainly include MoS_2 and WSe_2. The material is formed by two layers of sulfur atoms, including sulfur, selenium, and tellurium, sandwiched between a layer of transition metal atoms, whose electronic properties change significantly with the number of layers. The monolayer MoS2 is a direct bandgap semiconductor, while the multilayer structure transforms into an indirect bandgap [8]. For example, the light absorption coefficient of single-layer MoS2 can reach more than 10 times that of silicon materials, which provides a new idea for the efficient conversion of solar energy [9].

Third, the two-dimensional phosphate-based materials are mainly black phosphate-based materials, whose folded layer structure gives them anisotropic electron transport properties. The band gap of this kind of material can be continuously adjusted in the infrared to visible range, making it an ideal candidate for multispectral optoelectronic devices. In addition, the discovery of equivalent allotropes of blue phosphorus and purple phosphorus has further enriched possibilities for the new applications of phosphate-based materials.

In addition to the above-mentioned several two-dimensional materials, in recent years, more new two-dimensional material systems are also emerging. For example, boron nitride is an ideal dielectric layer in electronic devices because of its atomically flat surface and excellent insulation. As shown in Fig.2, such as Ti_2T_x, are formulated through selective etching of the MAX phase precursor system and are abundant in -OH, -F, and other functional groups to be prominent in ion-intercalation energy storage [10]. Other Xenes, such as silene and germanene, have attracted much attention in quantum devices. Through mechanical stripping, chemical vapor deposition, liquid phase stripping, and other preparation technologies, these new materials have realized the leap from laboratory research to industrial application.

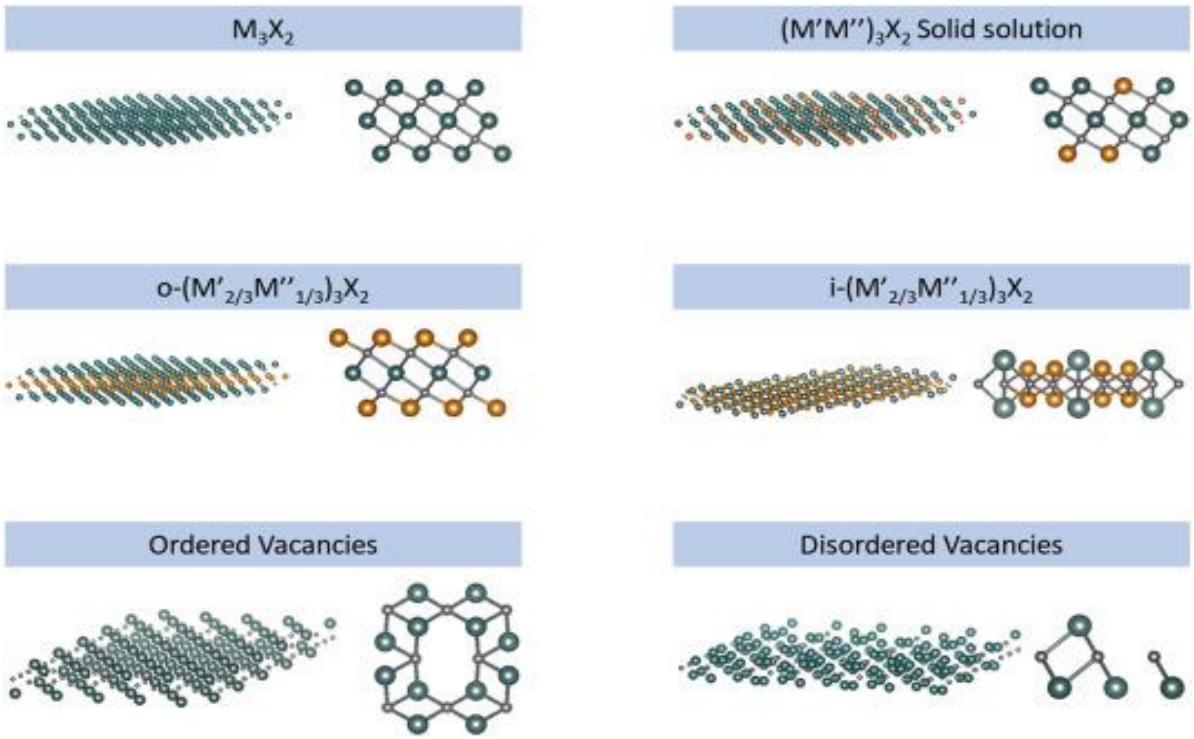

Fig 2. Different structures of MXene [11].

Through component design, constructions of the heterostructures, and defect engineering, different types of new two-dimensional materials form a complete material system covering conductors, semiconductors, and insulators, consequently providing more freedom for customized development of energy devices. As a result, the diversity and pluralism make two-dimensional materials a key breakthrough to developing the bottleneck of traditional energy technology.

3. Applications in Energy Storage

Two-dimensional materials show disruptive potential in batteries and supercapacitors due to their high specific surface area, fast ion diffusion channels, and controllable electronic structures. This chapter systematically analyzes the innovative application mechanism of two-dimensional materials from the three dimensions of lithium and sodium ion batteries, new battery systems, and supercapacitors. The new two-dimensional materials can be divided into carbon-based two-dimensional materials, transition metal chalcogenides, and phosphate-based two-dimensional materials according to their chemical composition and structural characteristics.

In recent years, two-dimensional black phosphorus has become a research hotspot in the field of energy storage due to its unique structure and excellent physicochemical properties. In the following study, the researchers systematically describe the preparation technology of two-dimensional black phosphorus, its inherent properties, environmental stability regulation strategies, and its application in lithium-ion batteries, and discuss the key challenges and technological breakthroughs for future development. In terms of structure, the folded layered structure of two-dimensional black phosphorus endows it with remarkable anisotropy, showing outstanding mechanical, electrical, and electrochemical properties.

As shown in Fig.3, the crystal structure of the black phosphorus layer phosphorus atoms is arranged in an orthogonal lattice. Although its mechanical properties are lower than Young's modulus of graphene, it has excellent mechanical flexibility and can withstand large strains of more than 10%, so it can be applied to flexible electronic devices. Secondly, from the perspective of electrical properties, the energy gap of two-dimensional black phosphorus is adjustable with the number of layers, and it has both semiconductor characteristics and high carrier mobility. The theoretical value can reach 1000 $cm^2/(V \cdot s)$, which is superior to transition metal chalcogenides [12]. Finally, from the perspective of electrochemical performance, the theoretical specific capacity of two-dimensional black phosphorus is seven times that of graphite, and each phosphorus atom can be combined with three lithium to form Li_3P. In addition, two-dimensional black phosphorus has the characteristics of rapid ion diffusion and low-volume expansion, which is suitable for use in lithium-ion batteries [13].

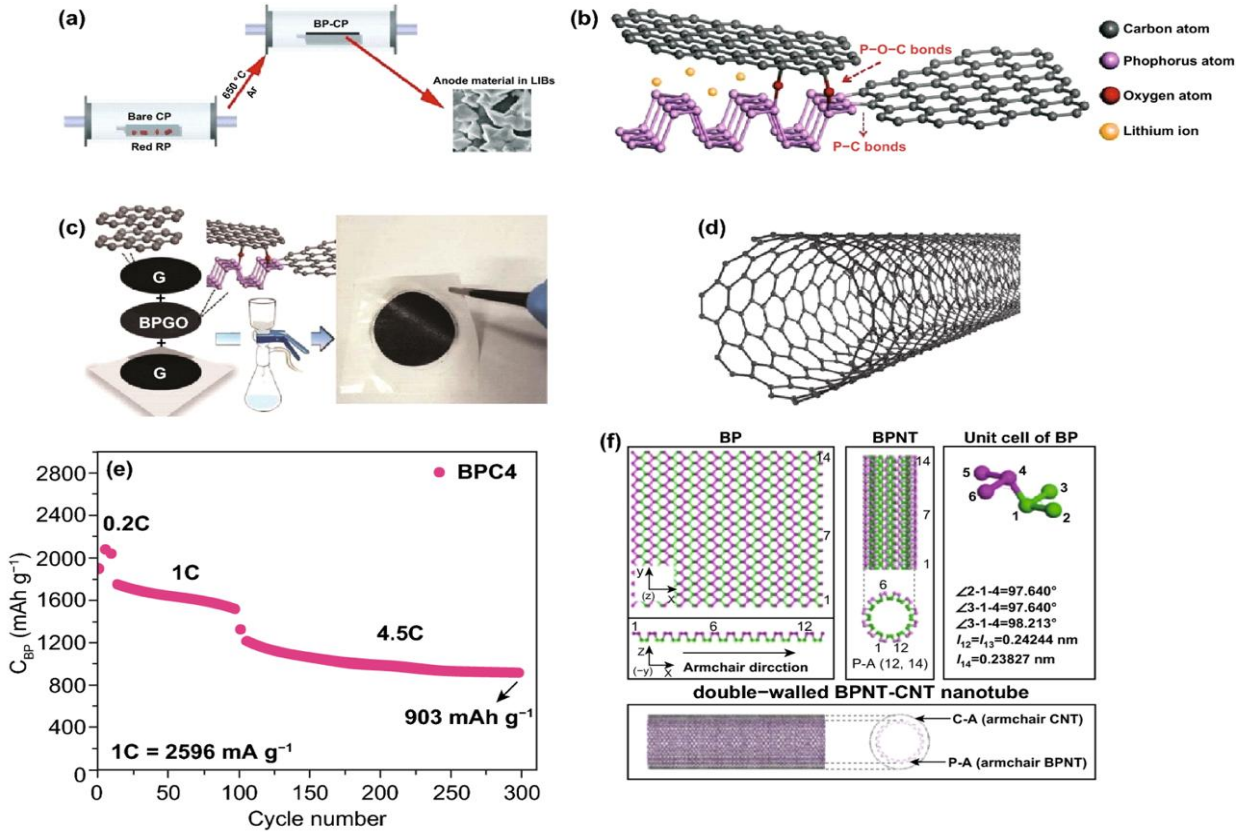

Fig 3. (a) The thermal-vaporization deposition process of BP-CP synthesis. (b) The chemical bonds of BPGO and (c) G-BPGO-G thin film preparation process. (d) Atomic structure of CNT. (e) High-rate cycle stability of BP-CNT at 1 C and 4.5 C. (f) The theoretical model of BPNT-CNT double-walled nanotube structure [14].

In summary, despite its challenges in terms of preparation, stability, and cyclic performance, two-dimensional black phosphorus materials show great potential in lithium-ion batteries due to their high specific capacity, fast ion transport, and tunable properties. Through material composite and structural optimization, the black phosphate-based anode is expected to promote the development of the next generation of high-energy-density batteries. Future research should focus on the combination of basic scientific breakthroughs and engineering technologies to achieve practical applications.

4. Challenges and Perspectives

In conclusion, emerging two-dimensional materials, including graphene and transition metal disulfides, show extraordinary potential in advanced energy technologies such as high-capacity lithium-ion batteries, flexible supercapacitors, photochemical water decomposition, and selective electrocatalytic reactions. Their atomic-level thickness, tunable electronic structure, and abundant surface-active sites differ fundamentally from bulk materials in terms of charge transfer dynamics and quantum confinement effects. However, before industrial deployment, key challenges spanning material synthesis, structural stability, and scalable manufacturing must be systematically addressed.

First, there are technical difficulties in the large-scale preparation of new two-dimensional materials. The existing preparation methods, such as chemical vapor deposition, mechanical stripping, and liquid stripping, are difficult to balance high quality and high yield. For example, chemical vapor deposition can prepare high-quality single-layer materials, but the yield is low, and the equipment cost is high. Although the liquid phase stripping method is suitable for mass production, it is easy to introduce impurities and structural defects.

In addition, the uniformity of layer number, transverse dimension control, and surface functional modification of two-dimensional materials still need to be broken through. Secondly, the new two-

dimensional material lacks stability. It is prone to structural degradation in extreme environments including high temperature, high pressure, and strong acid or alkaline electrolyte. For example, black phosphorus is easily oxidized in air, resulting in a significant decrease in cycle life. In photocatalysis, the surface-active sites of two-dimensional materials are easily deactivated by photo corrosion, which limits their long-term stability.

Third, emerging two-dimensional materials face similar cost-related challenges to other novel material systems. In the case of MoS_2, its large-scale synthesis requires the use of precious metal catalysts, while the subsequent stripping and purification process requires significant energy consumption. In addition, traditional electrode fabrication methods, such as slurry coating technology, exhibit inherent limitations in effectively utilizing the inherent performance advantages of two-dimensional nanomaterials.

Despite the challenges, the application of new two-dimensional materials in the field of energy is promising, and the number of research will not be small. With the increasingly urgent demand for global energy transformation, breakthroughs in the fields of efficient energy storage, conversion, and clean energy transformation of two-dimensional materials will profoundly affect future technologies. Through interdisciplinary innovation, it is expected to achieve industrial breakthroughs in key technologies of new two-dimensional materials within 5 to 10 years, providing core material support for carbon neutrality goals.

Future two-dimensional materials research should focus on multi-field collaborative innovation. On the one hand, artificial intelligence drives the performance prediction of materials and accelerates the development of new material systems. On the other hand, a macro preparation method that is both controllable and economical is created to build an intelligent energy device. This technological evolution will not only give rise to new interdisciplinary directions but also trigger changes from material innovation to energy system restructuring, providing the material foundation and technical support for achieving global carbon neutrality.

5. Conclusion

As an important part of the evolution of energy technology, new two-dimensional materials with their atomic-level layered structure and unique surface interface characteristics are reshaping the theoretical framework and application boundaries of traditional energy storage and conversion technologies. By systematically reviewing the research progress in this field in recent years, it can be found that such materials have shown significant breakthrough potential in energy storage and conversion because of their unique combination of physical and chemical properties, including high specific surface area, controllable electronic structure, excellent electrical conductivity, mechanical stability, etc. The synergistic effect of these characteristics not only provides new ideas for breaking the performance limits of traditional energy materials but also gives birth to emerging technological directions such as flexible energy storage and optoelectronic-thermal coupling conversion.

In the field of energy storage, the layered structure of two-dimensional materials provides an ideal transport channel for the insertion and removal of ions, and the abundant active sites on its surface significantly improve the interface efficiency of electrochemical reactions. This strong correlation between microstructure and macro performance makes the design of energy storage systems shift from experience-oriented to rational control. At the same time, in the field of energy conversion, the ability of two-dimensional materials to accurately regulate light absorption, carrier separation, and surface catalysis processes opens a new path to solve the bottleneck problem of energy conversion efficiency. Its anisotropic electron transport characteristics and customizable surface chemical environment are also suitable for multi-field coupled energy conversion.

The core difficulty of the current research is that the performance advantages of two-dimensional materials at the micro-scale have not been fully translated into the actual performance of macro devices. This gap is not only due to the attenuation of material consistency during large-scale preparation but also due to the lack of understanding of basic scientific issues such as heterogeneous

interface charge transport and surface interface stability. Future breakthroughs need to be built on the deep integration of multi-scale research. For example, at the atomic level, it is necessary to deepen the understanding of electron transport, defect engineering, and other mechanisms. At the mesoscopic scale, it is necessary to explore the engineering path of material assembly and device integration. Finally, it is necessary to construct a sustainable technology system covering the whole chain of preparation, application, and recycling.

Finally, it is worth emphasizing that the study of two-dimensional materials has shifted from simple performance optimization to multi-objective collaborative design covering performance, cost, and sustainability. This shift requires researchers to look beyond the traditional perspective of materials science to find solutions at the intersection of energy chemistry, environmental science, systems engineering, and other disciplines. Only through the deep interaction between basic research and industrial applications can the popularization of two-dimensional materials be finally realized and lasting impetus be injected into the transformation of human society to a sustainable energy world.

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