

Optoelectronic Properties and Applications of MXene Quantum Dots

Mingen Yang *

School of Artificial Intelligence and Low-Altitude Technology, South China Agricultural University, Guangzhou, China

* Corresponding Author Email: 202434510229@stu.scau.edu.cn

Abstract. MXene quantum dots (MQDs), as an emerging class of zero-dimensional nanomaterials, possess the quantum confinement effect, tunable bandgap structure, and excellent optoelectronic properties. It shows broad application prospects in fields such as sensing detection, biomedicine, optoelectronic devices, and energy and environment. This article systematically reviews the crystal structure, surface functional group characteristics, and size effect of MQDs. The mainstream preparation methods, such as hydrothermal/solvent thermal treatment, were introduced. The optical properties, such as ultraviolet-visible light absorption, tunable fluorescence emission, and nonlinear optical response, as well as key photovoltaic performances such as photoelectric conversion, photothermal effect, and carrier transport, were systematically investigated. The paper mainly elaborates on the application progress of MQDs in fields such as fluorescence sensing, biological imaging and diagnosis, photodetectors, photocatalysis, and energy storage. This article analyzes the prominent challenges currently faced by MXene quantum dots and looks forward to their future directions, which can provide a systematic reference for the basic research and engineering application of MQDs.

Keywords: MXene quantum dots; photoelectronic properties; optoelectronic devices.

1. Introduction

Over the years, two-dimensional nanomaterials such as graphene, transition metal dichalcogenides, and MXenes have become research hotspots in the fields of materials science and optoelectronics [1, 2]. MXene quantum dots (MQDs) based on MXene materials have advantages of high electrical conductivity, large specific surface area, and adjustable surface functional groups. This breakthrough in structure and performance endows MQDs with unique advantages in optoelectronic-related fields such as fluorescent sensing, bioimaging, photodetection, and photocatalysis.

At present, the preparation methods of MQDs mainly include the hydrothermal/solvent thermal method, the ultrasonic exfoliation method, the chemical cutting method, and the electrochemical exfoliation method, etc. In terms of performance research, MQDs exhibit outstanding optical absorption, tunable fluorescence emission, nonlinear optical response, and efficient photoelectric conversion capabilities. However, issues such as the luminescence quantum yield, structural stability, and size uniformity still need to be further addressed. Some related application research is also moving from the laboratory to the practical scene. This paper focuses on the structural features, preparation methods, photoelectric properties, and the typical applications of MQDs. The research progress of MQDs in the fields of sensing detection, biomedicine, optoelectronic devices, and energy environment is the key point elaborated in this article. This paper also summarizes the current situation and challenges in this field, providing a reference for subsequent related research.

2. Structure and Fundamental Properties of MQDs

When MXene materials are further exfoliated and cut, we can obtain zero-dimensional MQDs with lateral dimensions less than 10 nm. The typical composition of MQDs is $M_{n+1}X_nT_x$, where M is a transition metal element, X is carbon or nitrogen element, and T_x represents the surface-bound functional groups, mainly including -OH, -O, -F, etc [2]. The quantum confinement effect of MQDs is remarkable. Both electrons and holes are spatially confined in three dimensions, and the band gap

can be adjusted, thereby generating observable fluorescence emission. Compared with two-dimensional MXene nanosheets, MQDs retain high conductivity and also have a smaller size and a larger specific surface area. Its surface active sites are rich, which is conducive to the separation of photogenerated carriers and surface reactions. Moreover, the surface of MQDs is rich in polar functional groups, has good water solubility, and is easy to disperse. It can also be further controlled to regulate the band structure and the luminescent properties through surface modification. These structural features jointly determine the excellent optical absorption, fluorescence emission, photoelectric response, and photocatalytic performance of MQDs, making them a highly promising new type of photoelectric functional material [3].

3. Preparation Method of MQDs

The preparation of MQDs is a crucial step that determines their size distribution, surface state, and photoelectric properties. The commonly used preparation methods include hydrothermal and solvent thermal methods, ultrasonic exfoliation method, chemical cutting method, and electrochemical exfoliation method [1]. The hydrothermal/solvent-based method disperses MXene nanosheets in a solvent and achieves the disintegration, etching, and reorganization of the layers under high-temperature and high-pressure conditions. This method is relatively simple to operate and has a high yield. The resulting quantum dots have good crystallinity and are easy to enhance the luminescence efficiency through doping and surface modification. It is currently the mainstream method for laboratory-based production [4]. Other mainstream methods include the ultrasonic peeling method, the chemical cutting method, the electrochemical peeling method, etc. Overall, the hydrothermal/solvent-based method is the most widely used due to its optimal comprehensive performance. But the future development is inclined towards the development of more environmentally friendly, controllable, and scalable production techniques.

4. The Photoelectric Properties of MQDs

MQDs possess both excellent optical properties and photoelectric conversion capabilities, which enable them to show broad application prospects in fields such as optoelectronic devices, bioimaging, and energy and environment.

In the field of optical properties, the MQDs exhibit distinct characteristic absorption peaks in the ultraviolet to visible light range. Its typical absorption peaks are located in the range of 260-350 nm. The quantum confinement effect intensifies, and the absorption peaks will show a significant blue shift as the size of the quantum dots decreases. The range of the absorption spectrum can be effectively regulated by adjusting the size, elemental composition, and surface groups of the quantum dots. Its photoluminescence performance mainly emits in the blue light region. The emission range can be extended to green light, yellow light, and even white light through doping, compounding, and surface modification. The fluorescence emission depends on the excitation wavelength. Its intrinsic quantum yield is relatively low and usually less than 5%. However, the quantum yield can be increased to more than 20% through adding elements such as nitrogen and phosphorus, or by modifying with ligands such as glutathione [4]. In addition, MQDs also have excellent nonlinear optical responses, including two-photon absorption and saturable absorption. They can generate two-photon fluorescence when excited by near-infrared light. Then they are able to perform deep-tissue penetration imaging [5].

In terms of photoelectric performance, MQDs can efficiently generate electron-hole pairs under light irradiation. The large number of active sites and edge structures on their surface contributes to suppressing carrier recombination, while the parent structure with high conductivity can rapidly transport carriers. They improve the response speed and sensitivity of optoelectronic devices. Based on their obvious photoconductive effect, the conductivity of MQDs increases significantly under light illumination, and they show a fast and stable photoelectric response. They can be applied to

ultraviolet-visible photodetectors to fabricate flexible, transparent, and photosensitive devices that need high sensitivity. Meanwhile, they have strong light absorption capacity in visible and near-infrared regions, which can efficiently convert light energy into thermal energy, exhibiting excellent photothermal conversion performance that can be used for photothermal imaging and photothermal therapy [6]. Their tunable bandgap structure and high carrier separation efficiency also endow them with great potential in energy and environmental fields such as photocatalytic hydrogen production and CO₂ reduction.

5. Progress in Optoelectronic-Related Applications of MQDs

5.1. Fluorescent Sensing and Detection

The fluorescent properties of MQDs are highly sensitive to changes in the external environment, and they are prone to quenching or enhancement under the influence of factors such as metal ions, pH, and small molecules. This characteristic makes them ideal materials for constructing high-sensitivity fluorescent sensors. In terms of metal ion detection, researchers have utilized the selective response of MQDs to heavy metal ions such as Cu²⁺, Fe³⁺, and Hg²⁺, realizing rapid and visual detection of trace heavy metals in the water environment. For example, through surface functional modification, the detection limit of MQDs for Fe³⁺ can reach the nanomolar level, with excellent selectivity and anti-interference ability [7].

In the field of small biological molecule detection, fluorescent sensors based on MQDs have been successfully applied to the detection of substances such as H₂O₂, glucose, dopamine, and ascorbic acid. Their detection mechanism mainly relies on the changes in fluorescent signals caused by the specific interaction between target molecules and the functional groups on the surface of quantum dots. In addition, pH-sensitive MQD probes can real-time monitor the pH value of solutions through changes in fluorescent color, which has important value in the detection of cellular microenvironments and the monitoring of industrial processes.

The development of multi-functional integrated sensing platforms has further expanded the application scope of MQDs in recent years. The MQDs are applied to the fields of environment monitoring, food safety, and biological analysis. For example, combining with portable devices like smartphones to achieve on-site rapid detection. The MQDs have shown excellent practical features [6, 7].

5.2. Bioimaging and Theranostics

The application of MQDs in the biomedical field has become a prominent research focus over the past few years. They are used in building ideal multifunctional nanotheranostic platforms because of their low toxicity, favorable biocompatibility, superior optical properties, and multimodal therapeutic functions. In the realm of bioimaging, the fluorescence emission features of MQDs enable their utilization as fluorescent probes for cell labeling and in vivo imaging. Their two-photon fluorescence properties offer unique advantages for deep-tissue imaging. It can achieve high resolution and low background noise imaging of biological tissues [5]. Compared to traditional organic fluorophores and semiconductor quantum dots, MQDs exhibit better photostability and biosafety, which makes them very suitable for long-term tracking and observation.

In terms of disease treatment, the photothermal conversion capability of MQDs offers a new strategy for tumor photothermal therapy. The research conducted by Jun Yao et al. has verified that, through relatively mild laser irradiation, MXene quantum dots, such as Ti₃C₂, can generate local high temperatures at the tumor site. The local high temperatures will induce the ablation of tumor cells, achieving non-invasive and targeted tumor treatment. Furthermore, researchers are also exploring the application of MQDs in photodynamic therapy and other areas [8]. Additionally, studies by Laura S. Pires et al. have highlighted the important potential of MQDs in drug delivery, wound healing, and biosensing. It paves the way for the construction of multimodal synergistic therapeutic systems and provides a new technological pathway for disease diagnosis and treatment [9].

5.3. Photodetectors

With the rapid development of flexible electronics and wearable devices, there is an increasing need for new photodetector materials. MQDs have great potential in this field because of their high conductivity, broadband spectral response, and tunable bandgap. Thanks to the significant change in the photovoltaic conductivity of quantum dots under light irradiation, the photodetector based on MQDs can achieve highly sensitive and rapid response detection of ultraviolet and visible light signals. Contrasted with traditional silicon-based detectors, MQD-based photodetectors will possess prominent advantages, including bendability and stretchability. These features make them applicable for optical signal detection on curved and irregular surfaces, offering broad application prospects in wearable health monitoring, intelligent human-machine interaction, and flexible displays.

Researchers have continuously improved the performance metrics of photodetectors through optimizing the fabrication processes of MQDs, designing novel device structures, and developing composite material systems in recent years. For instance, compositing MQDs with two-dimensional materials like graphene and molybdenum disulfide (MoS_2) to construct heterojunction structures effectively improves carrier separation efficiency and device response speed. Additionally, fabricating MQD arrays via patterning techniques enables image sensing with high pixel density [1]. The material properties will continue to be optimized, and the device manufacturing techniques will also keep improving in the future. MQD-based photodetectors are expected to play an important role in intelligent sensing, machine vision, optical communications, and other fields.

5.4. Photocatalysis and Energy Devices

In the field of photocatalysis and energy, MQDs also show multifaceted application value. Their high electrical conductivity facilitates the rapid transport of photogenerated carriers. Their abundant surface active sites promote catalytic reactions and greatly improve photocatalytic efficiency. Detailed applications include photocatalytic water splitting for hydrogen production and photocatalytic CO_2 reduction for hydrocarbon fuel synthesis. Studies have shown that compositing MQDs with traditional photocatalysts such as TiO_2 and $\text{g-C}_3\text{N}_4$ will improve their performance. It will effectively suppress carrier recombination, broaden the spectral response range, and substantially enhance photocatalytic activity. Regarding energy storage and conversion devices, the high specific surface area and excellent conductivity of MQDs make them exhibit promising performance in supercapacitors, lithium-ion batteries, and sodium-ion batteries. They can function as electrode materials or conductive additives to strengthen the energy and power density, and cycling stability of these devices [10, 11]. Furthermore, MQDs have also been explored in solar cells and fuel cells. MQDs can improve charge transport characteristics and energy conversion efficiency by constructing heterojunctions or serving as interfacial modification layers, realizing the various applications of photoelectric materials in the energy sector [6].

6. Limitations and Future Directions

The large-scale application of MXene quantum dots still faces many problems that need to be solved urgently. Regarding preparation, there are deficiencies in controlling size uniformity, scalable production, and surface defect engineering. Green and controllable large-scale fabrication technologies are critically needed [1]. In terms of performance, the relatively low fluorescence quantum yield, poor long-term stability, and limited precision in bandgap modulation restrict their application. Concerning applications, the device integration level, adaptability to actual environments, and long-term biosafety still need further verification and assessment. Future work should focus on enhancing the stability of materials in oxygen-rich environments, improving mechanical properties, solving the problem of interlayer stacking, and optimizing their electrical conductivity. Researchers need to further deepen the structure-activity relationship research of MQDs to guide material design [1]. These efforts will promote the translation of MQDs from laboratory research to practical devices

and products and will help achieve key application breakthroughs in the fields of next-generation optoelectronic devices, intelligent sensing, precision medicine, and green energy conversion.

7. Conclusion

This paper systematically elaborates on the composition, structure, and unique physicochemical properties of MQDs. The technical characteristics of the mainstream preparation methods, such as hydrothermal and solvothermal techniques, have been summarized. This paper reveals key photoelectric properties such as characteristic UV-Vis absorption, tunable fluorescence emission, nonlinear optical response, and efficient photoelectric/photothermal conversion. The article focuses on reviewing research progress in fluorescence sensing, bioimaging and theranostics, photodetectors, photocatalysis, and energy devices. In summary, it enables highly sensitive detection of trace heavy metals and biological small molecules, can be used for cell labeling and two-photon imaging of deep tissues, can construct flexible and self-powered photoelectric detection devices, and performs exceptionally well in photocatalytic hydrogen production, CO₂ reduction, and energy storage systems such as supercapacitors and lithium-ion batteries. Currently, great progress has been made in the basic research and application exploration of MQDs. MQDs provide new pathways for the design of new photoelectric functional materials and key material support for high-performance optoelectronic devices, precision theranostics, and clean energy technologies. As an emerging material combining tunability, multifunctionality, and superior performance, MQDs have immense development potential. Continuous advancement in their fundamental research and application will powerfully promote technological innovation and industrial development in smart sensing, flexible electronics, precision medicine, and green energy.

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