



## **WO<sub>3</sub>-based materials for energy conversion and storage devices**

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### **Abstract:**

Tungsten trioxide (WO<sub>3</sub>) is a versatile transition metal oxide with significant applications in energy conversion and storage devices due to its unique physical, chemical, and electronic properties. Advanced materials with various compositions and morphologies have been developed in order to improve its properties for targeted applications. In this paper, properties and challenges of WO<sub>3</sub>-based materials for Li-ion batteries and photoelectrochemical cells are presented.

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**Keywords:** tungsten oxide, Li-ion batteries, photoelectrochemical cells

## **1. INTRODUCTION**

Tungsten oxide-based materials have gained significant attention for their versatile applications in energy conversion and storage devices. These materials exhibit unique properties that make them suitable for use in photocatalysis, water splitting, solar energy conversion, and electrochromic devices [1]. The dimensionality of WO<sub>3</sub> structures plays a crucial role in influencing their physicochemical properties and performance in solar energy conversion applications [2].

WO<sub>3</sub>-based nanomaterials have been extensively studied for their potential in supercapacitors, lithium-ion batteries, and electrochromic devices, with recent developments focusing on bifunctional and multifunctional devices [3]. Despite their promising features, pristine WO<sub>3</sub> suffers from low specific surface area and energy density. To address these limitations, researchers have explored various WO<sub>3</sub> composites, including WO<sub>3</sub>/carbon, WO<sub>3</sub>/polymers, and WO<sub>3</sub>/metal oxides, to enhance their performance in energy storage applications [4].

## 2. WO<sub>3</sub>-BASED MATERIALS IN Li-ION BATTERIES

Tungsten trioxide (WO<sub>3</sub>) has garnered significant attention as a potential anode material for lithium-ion batteries (LIBs) due to its favorable electrochemical properties and high theoretical capacity. As a transition metal oxide, WO<sub>3</sub> exhibits unique characteristics that can enhance the performance of LIBs, including its ability to undergo lithium intercalation and conversion reactions.

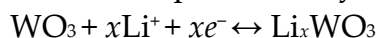
WO<sub>3</sub> exists in several polymorphic forms, with monoclinic and hexagonal structures being the most studied for battery applications. The most common phase for WO<sub>3</sub>, characterized by a well-defined structure that allows effective lithium ion intercalation. Known for its high ionic conductivity and large interstitial sites, facilitating ion migration, hexagonal WO<sub>3</sub> exhibits a particular tunnel structure. The intercalation of alkaline cations such as Li<sup>+</sup>, Na<sup>+</sup>, and K<sup>+</sup> in hexagonal tungsten oxide leads to the formation of hexagonal M<sub>x</sub>WO<sub>3</sub> tungsten bronzes, which makes it a good candidate for LIB anode [5].

The morphology of WO<sub>3</sub> nanostructures—such as nanowires, nanorods, and microflowers—plays a crucial role in determining their electrochemical performance. For instance, WO<sub>3</sub> microflowers have shown superior cycling stability compared to nanowires due to their larger surface area and more favorable lithium ion diffusion paths [6,7].

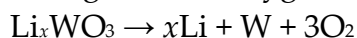
Nanowire structures provide a high surface area-to-volume ratio, facilitating faster lithium ion diffusion. They typically exhibit initial discharge capacities around 664.3 mAh/g but may suffer from lower cycle stability due to structural degradation during cycling.

In the meantime, microflower structures offer better cycle stability; these structures can achieve initial discharge capacities of up to 718.8 mAh/g. Their unique morphology provides structural integrity during charge/discharge cycles [6].

The electrochemical reactions occurring in  $\text{WO}_3$  during lithium insertion can be represented by the following equations:



This equation illustrates the intercalation of lithium ions into the  $\text{WO}_3$  lattice. Upon further cycling, the conversion of lithium-doped  $\text{WO}_3$  back to metallic tungsten and oxygen occurs, according to the following equation:



Recent studies have highlighted a unique self-recovery phenomenon in reduced  $\text{WO}_3$  (R- $\text{WO}_3$ ), where the capacity significantly recovers after an initial drop during cycling. This can be attributed to the activation of oxygen vacancies that enhance electrochemical reactivity [8].

The performance of  $\text{WO}_3$ -based materials is often assessed through various electrochemical tests, including cyclic voltammetry (CV) and charge-discharge cycling tests. Key performance metrics include initial capacity (the first cycle discharge capacity often serves as an indicator of material viability), cycling stability (the ability to retain capacity over numerous cycles is critical for practical applications), and rate capability (the ability to deliver current at varying densities without significant capacity loss is essential for high-performance batteries) [9].

### **3. TUNGSTEN TRIOXIDE MATERIALS FOR PHOTOELECTROCHEMICAL APPLICATIONS**

Photoelectrochemical cells (PEC) are devices that combine the water electrolysis and solar energy harvest, with the anode made from an semiconducting light-absorbing material.

Tungsten trioxide ( $\text{WO}_3$ ) has emerged as a promising material for photoelectrochemical (PEC) applications, particularly in water splitting for hydrogen production. Its unique properties, such as suitable band gap, stability, and electron transport capabilities, make it an attractive candidate for use as a photoanode.

WO<sub>3</sub> has a band gap ranging from 2.5 eV to 2.9 eV, which allows it to absorb visible light effectively. This is advantageous compared to other common semiconductors like TiO<sub>2</sub>, which has a higher band gap (~3.2 eV) and thus absorbs less visible light [10]. Furthermore, WO<sub>3</sub> exhibits superior electron transport properties with an electron mobility of approximately 12 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>, significantly higher than that of TiO<sub>2</sub> (~0.3 cm<sup>2</sup> V<sup>-1</sup> s<sup>-1</sup>). This high mobility facilitates better charge carrier transport, which is crucial for efficient PEC performance.

However, the performance of WO<sub>3</sub> can be significantly improved through the controlled growth of nanostructures. Thus, dense grown WO<sub>3</sub> nanoplates have shown enhanced photocurrent densities due to their large surface area and efficient charge transport kinetics. Moreover, integrating WO<sub>3</sub> with other semiconductor materials or using co-catalysts (e.g., CoOx, RuO<sub>2</sub>) can enhance its oxidation kinetics and reduce charge recombination rates at the semiconductor/electrolyte interface. This approach has been shown to improve the overall efficiency of water splitting reactions [11]. The WO<sub>3</sub>/CdS composite has demonstrated superior photocatalytic activity compared to the pure components. Previous studies have shown that the hydrogen production rate can be significantly enhanced, achieving rates as high as 2852.5 μmol g<sup>-1</sup> h<sup>-1</sup> under optimal conditions (5.5 times that of pure CdS) [12]. The synergistic effect between WO<sub>3</sub> and CdS allows for more effective utilization of visible light, leading to improved overall performance in hydrogen evolution.

Despite its advantages, WO<sub>3</sub> faces several challenges in PEC applications. Among them, charge transfer at the WO<sub>3</sub>/electrolyte interface can be slow, leading to high overpotentials during water splitting processes. Stability issues have been observed under operational conditions, particularly with crystalline-to-amorphous phase transformations that can occur during prolonged exposure to light or heat [11].

#### 4. CONCLUSION

The crystalline structure and morphology of WO<sub>3</sub> nanostructures significantly influences their electrochemical performance in lithium-ion batteries. The arrangement of atoms within different phases affects lithium ion intercalation efficiency, electrical conductivity, structural stability during cycling, and overall battery longevity.

Moreover, structures such as microflowers and nanorods provide enhanced surface area, facilitate lithium ion diffusion, and improve cycling stability compared to traditional bulk materials or less optimized forms like nanowires. Understanding these relationships allows researchers to design more effective anode materials for future energy storage applications, ultimately improving the efficiency and longevity of lithium-ion batteries. Continued exploration into optimizing these nanostructures will be essential for advancing battery technologies.

WO<sub>3</sub> presents significant potential for photoelectrochemical applications, particularly in water splitting for hydrogen production. Its favorable band gap, excellent electron transport properties, and chemical stability make it a strong candidate for photoanodes. However, challenges related to charge transfer efficiency and phase stability must be addressed through ongoing research and development efforts. Future advancements may involve optimizing nanostructures and exploring heterojunction configurations to enhance the overall efficiency of WO<sub>3</sub>-based photoelectrochemical systems.

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