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# Electronic structure, optical, photocatalytic and charge storage performance of $WO_3$ nanostructures

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ABSTRACT

In this paper, we report the fabrication of $WO_3$ nanostructures via hydrothermal route. This is the first report on pristine $WO_3$ nanoparticles being synthesized in a relatively short timed (4h) hydrothermal reaction. The obtained material was characterized in detail by a number of techniques: X-ray powder diffraction, scanning electron microscopy (SEM), optical studies, and Fourier transform analysis. From the observed results, these $WO_3$ nanoparticles exhibit a diameter approximately between 3 and 30 nm. Density functional theory calculations confirm the electronic band gap of 3.4 eV in accordance to experimental band gap obtained from optical absorption spectra. Cyclic voltammetry of the prepared $WO_3$ nanoparticles reveal the exhibition of remarkable electrochemical activity. In addition, the $WO_3$ particles were exposed to phenol and it was observed that 90.8% of phenol was degraded during the reaction time of 1.5 h. According to The International Commission on Illumination (CIE) the synthesized material shows blue emission and is suitable for blue LEDs.

## 1. Introduction

Recent advancements in novel transition metal oxides nanostructures have captivated much attention due to the counter effects of proportion, morphology, and crystallinity on their various properties such as, optical, magnetic and electric [1–4]. Tungsten oxide is one of the largely investigated materials among them, due to its good photocatalytic, electrochromic, electric and photochromic properties. This material is regarded as one of the significant, suitable and favorable element in a broad spectrum of applications such as, display and field emission appliances, gas sensors, and photocatalysis, etc. Tungsten oxide a semiconductor having wide band-gap employs multiple applications. $WO_3$ is widely considered for its distinctive optical, electrical, and structural properties [5–12]. It is an indirect bandgap semiconductor, suitable for catching the visible range of the solar spectrum [13,14] and useful in electrochemical appliances, such as storage lithium ion cells, based on its abundant natural insinuate reactivity. Nanosizing such elements have concerned wonderful attention as this leads to the reduction of size, material, cost, space and miniaturization induces the quantum confinement effects leading to unique physical, chemical, and optical properties. Many synthetic methodologies have been dedicated to the development of nano-scaled tungsten oxide until now. Song et al. obtained $WO_3$ nanobelts and nanowires by a hydrothermal method using cetyltrimethylammonium bromide and $K_2SO_4$ [15,16]. The electrolytic synthesis of nanoporous tungsten oxide films was proposed by Baeck et al. using a solution comprising a tungsten-peroxo complex as the inorganic precursor and sodium dodecyl sulphate (SDS) as the structure-directing agent. Electrochromic and photocatalytic characteristics were improved in these materials. Rapid adsorption process was also used to synthesize larger surface area, porous, nanoparticulate tungsten oxide, which had increased photoactivity and current density for hydrogen intercalation [17,18]. A simple solvothermal technique using tungsten hexachloride ($WCl_6$) as a precursor and cyclohexanol as a solvent was used to generate bunched tungsten oxide nanowires with controllable shape. The gas sensor characteristics of manufactured $WO_3$ based sensors were previously described employing a static intelligent gas sensing analysis platform. Due to their excellent catalytic performance, electrochemical durability, and low price, these compounds have been identified as one of the most promising alternatives for electrocatalytic hydrogen evolution processes (HER). Because of its high surface area to volume ratio, the electrocatalytic performance of $WO_3$ has been substantially improved in recent

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