

# A type-II MoS<sub>2</sub>/ZnO heterostructure with enhanced photocatalytic activity

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## ABSTRACT

ZnO and MoS<sub>2</sub>/ZnO composite were synthesized by co-precipitation method and their structural and optical properties were studied using XRD, Raman, and photoluminescence spectroscopy. The MoS<sub>2</sub>/ZnO composite has shown 40% enhancement in photocatalytic degradation of an organic dye as compared to ZnO. The contribution of active species such as superoxide (<sup>•</sup>O<sub>2</sub>), hydroxyl radical (<sup>•</sup>OH), and hole (h<sup>+</sup>) in the photocatalytic process were tested and their role was ordered as follows: <sup>•</sup>O<sub>2</sub> > <sup>•</sup>OH > h<sup>+</sup>. In total, the enhancement in photocatalytic performance of composite was correlated to specific surface area, association of all active species, and the synergistic effect between MoS<sub>2</sub> and ZnO.

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## 1. Introduction

After the discovery of graphene, research on non-graphene 2D materials such as hexagonal boron nitride, phosphorene, and transition metal dichalcogenides (TMDCs), has attracted immense interest. Among TMDCs, molybdenum disulfide (MoS<sub>2</sub>) has been explored intensively due to its unique electrical, optical and chemical properties [1–3]. The indirect to direct band gap transition and large surface area with abundant edge active sites witnessed in few-layer MoS<sub>2</sub> are strategic for photocatalytic, and photovoltaic applications nevertheless of its high electron-hole recombination rate [4,5]. On other-hand, oxide semiconductor like zinc oxide (ZnO) and titanium oxide (TiO<sub>2</sub>) were extensively investigated for photocatalytic application due to high stability, low cost and eco-friendly nature [6–8]. Among them, ZnO is more desirable for photocatalytic and photovoltaic applications owing to its direct band gap, high exciton binding energy, and high charge mobility. However, the poor charge transferability and high electron-hole recombination rate of ZnO limits its efficiency. The drawbacks resulted from the intrinsic properties of MoS<sub>2</sub> and ZnO can be resolved by forming a heterostructure MoS<sub>2</sub>/ZnO with the appropriate interface and bandgap engineering. Thereon, the

heterostructures of MoS<sub>2</sub> with WS<sub>2</sub>, ZnO, TiO<sub>2</sub>, GaN, and graphene were studied intensively for various applications. [11–13].

Here, we report the synthesis of MoS<sub>2</sub>/ZnO composite (MZO) with a type-II heterostructure that features spatial separation of valence band (VB) and conduction band (CB). Such, spatial distribution of VB and CB offers more reactive sites for photocatalytic application, i.e., redox reactions can take place at both MoS<sub>2</sub> and ZnO sites. The contribution of reactive species such as superoxide (<sup>•</sup>O<sub>2</sub>), hydroxyl radical (<sup>•</sup>OH), and hole (h<sup>+</sup>) involved in the photocatalytic performance was also explored.

## 2. Experimental section

The synthesis of MoS<sub>2</sub>/ZnO composite (MZO) via hydrothermal method, laser irradiation have reported previous with an equimolar or large weight ratio of MoS<sub>2</sub> in ZnO. Here, we report the synthesis of MZO via co-precipitation method with a very low weight ratio of MoS<sub>2</sub>, i.e., 1:1000 ratio of MoS<sub>2</sub>:Zn. Further, we eliminated the involvement of heavy organic solvents for exfoliation on MoS<sub>2</sub>. The zinc acetate and exfoliated MoS<sub>2</sub> were used as precursors for the nanocomposite synthesis. Detailed methods are presented in Supplementary information. The photocatalytic performance of the samples was gauged by the degradation of aqueous methylene blue (MB) dye (10 mg/L) under UV light. The scavenger test was done by adding benzoquinone (BQ), isopropanol (IPA) and ethylenediaminetetraacetic acid (EDTA) as scavengers for <sup>•</sup>O<sub>2</sub>, <sup>•</sup>OH, and h<sup>+</sup> respectively.

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