

Supporting Information For

MoO₃ and Cu_{0.33}MoO₃ Nanorods for Unprecedented UV/Visible Light Photocatalysis

Imran Shakir, Muhammad Shahid, and D.J. Kang*

BK 21 Physics Research Division, Department of Energy Science, Institute of Basic Science, SKKU Advanced
Institute of Basic Science, SKKU Advanced Institute of Nanotechnology, Sungkyunkwan University, Suwon 440-746,
Korea

Synthesis of Nanorods

All chemicals (MoO_2 99.99%, $\text{Cu}(\text{NO}_3)_2 \cdot x\text{H}_2\text{O}$, hydrochloric acid 95%, Toluidine Blue O (85% dye content)) used in this study were purchased from Sigma Aldrich and used as received. In the synthesis of MoO_3 nanorods, 3 mmol of MoO_2 are dissolved in $\text{HCl}/\text{H}_2\text{O}_2 = 1:5$ v/v stirred magnetically for 30 min at pH (1-2), and for the synthesis of Cu doped MoO_3 nanorods, 0.5mmol of $\text{Cu}(\text{NO}_3)_2 \cdot x\text{H}_2\text{O}$ is mixed with the above solution. The final yellowish solution is transferred into a Teflon-lined stainless steel autoclave (25 ml capacity), kept at 180 °C for 12 hrs and cooled naturally to room temperature. The precipitates were filtered, washed several times with distilled water and ethanol, and dried on a hot plate at 100 °C for 12 hrs, resulting in high quality MoO_3 and Cu-doped MoO_3 nanorods.

Diffuse reflectance absorption spectra

Before the photocatalytic activity characterization, it is important to study the optical absorption of the as-prepared MoO_3 and $\text{Cu}_{0.33}\text{MoO}_3$ nanorods because the UV-vis absorption edge is relevant to the energy band of semiconductor catalyst [1]. The optical absorption spectra of the as-prepared samples are shown in Fig. (S1). Compared with MoO_3 , there was strong photoabsorption in the visible region for the Cu-doped MoO_3 photocatalyst. The red shift of the absorption edge implied a decrease in the band gap energy. It was clear that doping led to a modification of the electronic structure around the conduction band edge of MoO_3 , thus resulted in the band gap narrowing [2].

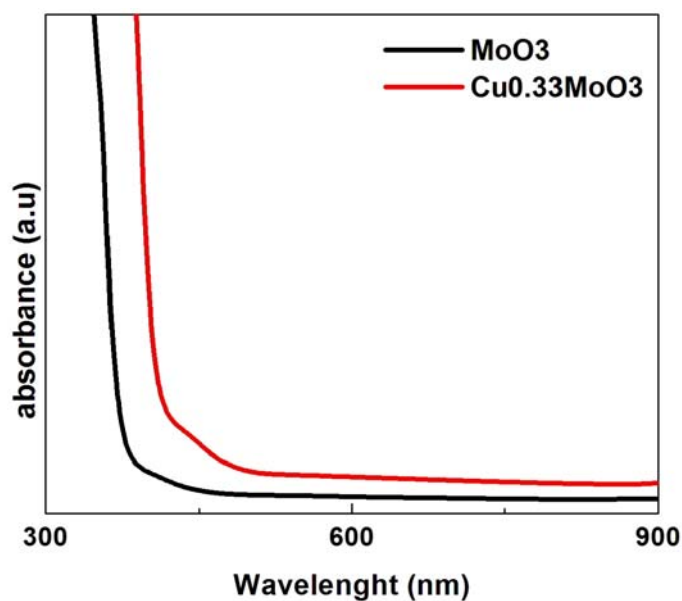


Fig. S(1). Diffuse reflectance absorption spectra of MoO_3 and $\text{Cu}_{0.33}\text{MoO}_3$

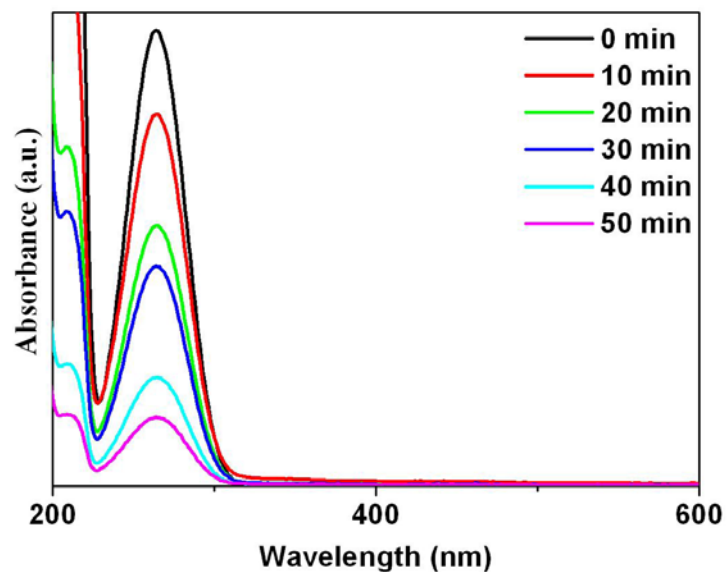
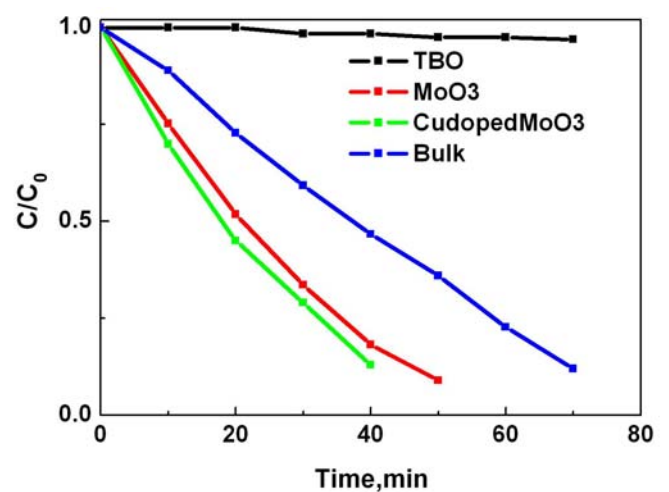
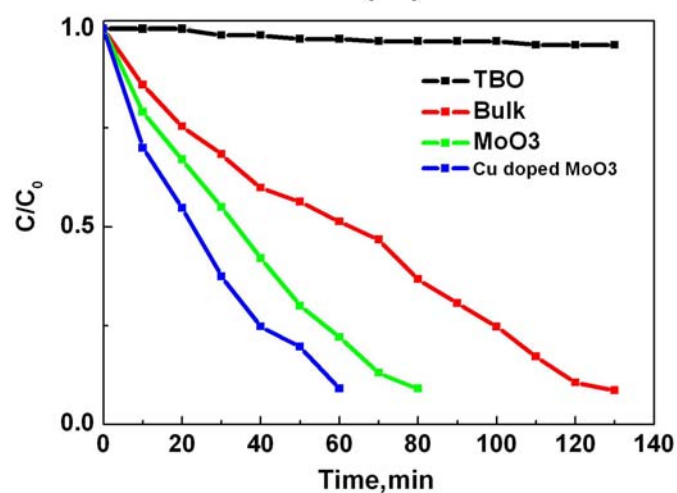


Fig S (2): Degradation profile of TBO on MoO₃ under UV irradiation.

In order to confirm the effect of doping concentration on photocatalytic activity, we reduced the concentration of Cu and observed that the kinetics of photo degradation of TBO is slower, as seen in Figure S3. We have seen that the variation in the Cu dopant in MoO_3 nanorods follows the same trend; the significant increase in the photocatalytic behavior occurred with maximum dopant concentration (3.3%).



(a)



(b)

Fig S (3). Photocatalytic study of MoO_3 , $\text{Cu}_{0.2}\text{MoO}_3$ nanorods, under UV (a) and visible light irradiation (b).

BET measurements

The specific surface area measurements were determined by Digisorb 2006 surface area, pore volume analyzer-Nova Quanta Chrome Corporation instrument using multipoint BET adsorption and it was presented in the supporting information. The surface area measurements showed that the surface area of the Cu doped MoO₃ nanorods is higher as compared to the bulk and pure MoO₃. This change in surface area after doping is indicative of the incorporation of copper within the structure of molybdenum oxide lattice and the accompanying structural rearrangement.

Sample	Specific surface area (m ² /g)	Total pore volume (cm ³ /g)	Average pore diameter (Å)
MoO ₃ nanorods	18	0.18	89.2
Cu _{0.33} MoO ₃ nanorods	24	0.17	203.9
MoO ₃ bulk	12	0.12	251.8

Table T1: Surface area, pore volume and average pore diameter of the different catalysts

Material	Dye	Degradation Time under UV light	Degradation Time under Visible light	Reference
TiO ₂ nanowires	Methyl Orange	180 min	Not available	[3]
Carbon doped TiO ₂	Rhodamine B	30 min	250 min	[4]
TiO ₂ nanorods	Phenol	360 min	Not available	[5]
TiO ₂ nanoparticles	Methylene blue	180 min	Not available	[6]
Carbon doped TiO ₂ nanorods	Toluene	Not available	180 min	[7]
S-doped TiO ₂	chlorobenzene	Not available	60 min	[8]
MoO ₃ nanorods	TBO/ chlorobenzene	50/80 min	80/160 min	Current work
CuMoO ₃ nanorods	TBO/ chlorobenzene	30/50 min	50/120 min	Current work

Table T2: Comparison of photocatalytic properties of TiO₂ and our samples.

Reference:

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