

# **Boosting Visible-light-driven Photocatalytic Antibacterial Performance of MoS<sub>2</sub> Nanosheets by poly (3-(4-methyl-3'-thiophenoxy) propyltrimethylammonium chloride (PThM) modification**

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## **1: Reagent**

The chemicals used in the experiment are as follows: Thiophene was purchased from Hengshengji Technology Co., Ltd (China). N-methyl formamide (NMF) was furnished from Sigma-Aldrich (China). Ferric chloride (FeCl<sub>3</sub>) was offered from Proudén Biotechnology Co., Ltd (China). N-butyl lithium was supplied from Aladdin Industrial Corporation (USA). 3-Bromo-4-methylthiophene was purchased from Aladdin Reagent Co., Ltd (China). Toluene was provided by Anhui Tuoyan Scientific Instrument Co., Ltd (China). MgSO<sub>4</sub> was purchased from Hefei Economic and Technological Development Zone Maijia Experimental Supplies Business Department (China). THF was offered by Hefei Shangcheng Experimental Supplies Co., Ltd (China). CHCl<sub>3</sub> was purchased from Hefei Meifeng Chemical Instrument Co., Ltd (China). The silica gel was purchased from Hefei Hengshengji Technology Co., Ltd (China). n-hexane was purchased from Hefei Shangcheng Experimental Supplies Co., Ltd (China). Others were offered from Macklin Reagent Co., Ltd (China).

## **2: Characterization**

Transmission electron microscopy (TEM; JEM-2100, Hitachi) and scanning electron microscopy (SEM; S-4800, Hitachi) equipped with energy-dispersive spectrometer (EDS) were used to observe the morphology and elements of the products. The crystal phases of materials were analyzed by X-ray photoelectron spectroscopy (XPS; Thermo fisher scientific, Waltham, MA, USA). A Nicolet Nexus 870 machine was used to measure the Fourier Transform Infrared (FT-IR) spectrum. The X-ray diffraction (XRD; XD3, PERSEE) of MoS<sub>2</sub>, PTh/MoS<sub>2</sub> and PThM/MoS<sub>2</sub> were used to characterize crystallinity of materials in the 2 $\theta$  range of 5-70°. X-ray photoelectron spectrometer (XPS) was also used to study the chemical elements. The UV-vis diffuse reflectance spectroscopy (DRS) mode was tested on the UV-3600 spectrometer. The electrochemical workstation (CHI760E) in a general three-electrode experimental cell can performed electrochemical impedance spectroscopy (EIS) and photocurrent tests. The ultra-high resolution confocal microscope (Leica TCS SP8X, Germany) with 535 nm excitation showed the fluorescence images of Escherichia coli.

## **3. About bacteria**

The bacteria used in the experiment were E. coli, which was purchased from the China Industrial Microbial Culture Collection and Management Center. Usually the strains are stored in the refrigerator at -20 °C. When using, took appropriate amount of bacteria in liquid culture medium and put it in shaker to grow.

## **4. Quantitative evaluation of antibacterial effects**

Whether modification of polythiophene and cationic conjugated polythiophene can improve the antibacterial performance of MoS<sub>2</sub> was quantitatively determined by plate coating method. After co-processing the material with bacteria, spread it on the

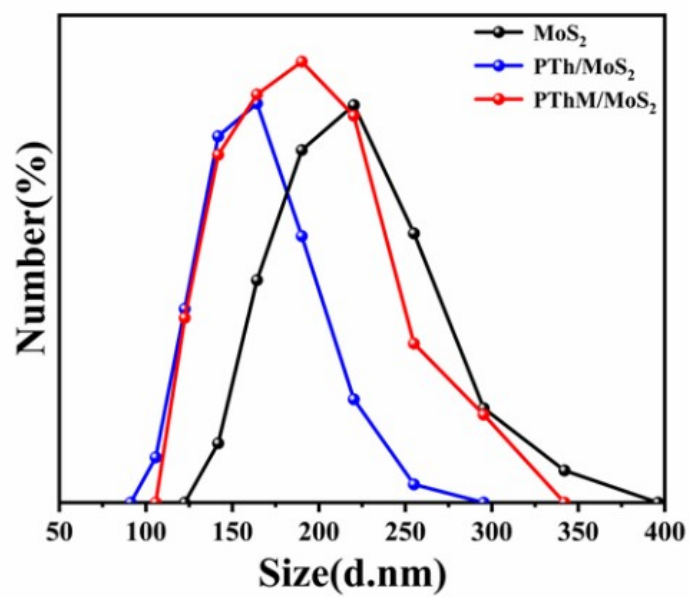
agar panel and cultivated it in a biological incubator. Biological incubator can provide good environmental conditions for the growth of cells. By counting the number of bacteria on the petri dish, conclusions can be drawn (repeated experiments are required to avoid chance of experimental results).

## **5. Optical properties**

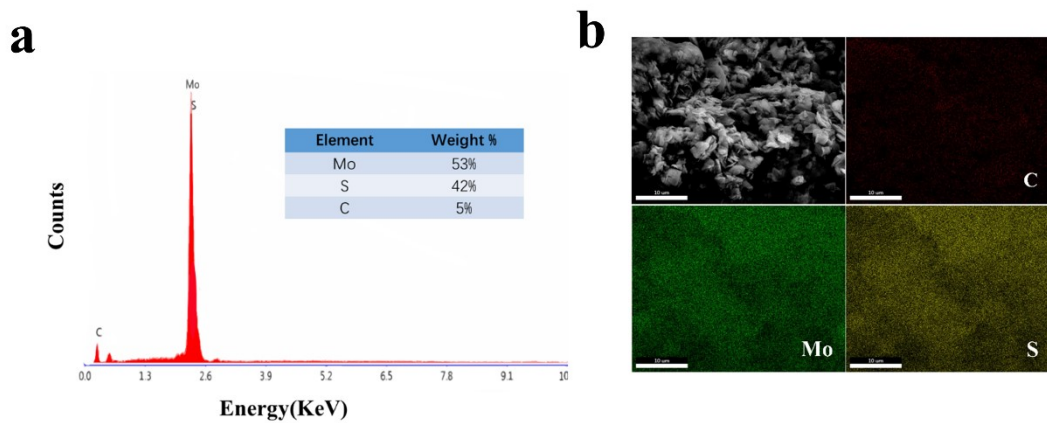
The electrochemical station was used to study the photocurrent and photoimpedance properties of PTh/MoS<sub>2</sub> and PThM/MoS<sub>2</sub>. Specifically: the powder was ground, smeared, dried, and fixed on conductive glass. Using a three-electrode system, under the irradiation of a xenon lamp, the photocurrent and photoimpedance tests were carried out in 0.1 sodium sulfate and impedance solution, respectively.

## **6. Mechanism test**

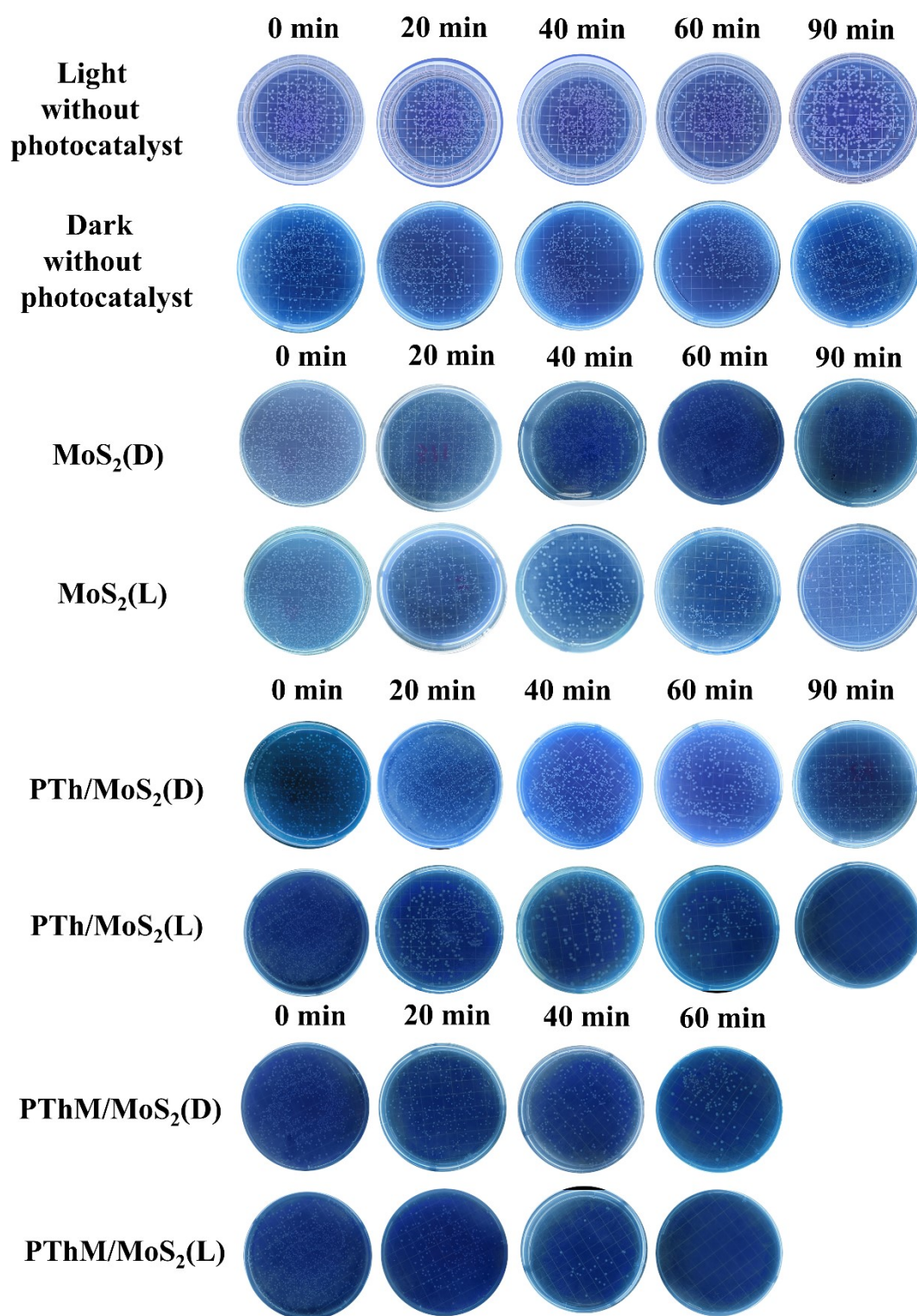
ESR experiment (qualitative) and capture agent (quantitative) explored the existence of reactive oxygen species. Free radical scavengers such as DMPO can specifically combine with short-lived superoxide and hydroxyl radicals to form longer-lived DMPO-O<sub>2</sub><sup>•-</sup>, DMPO-OH<sup>•</sup>. As long as DMPO was added in the photocatalytic reaction, it can capture superoxide free radicals and hydroxyl free radicals to generate the above two kinds of long-life free radical adjuncts. These two kinds of free radical adjuncts have different ESR spectra, which can be used to qualitatively judge what kind of free radicals were generated. In the capture agent experiment, the corresponding active oxygen capture agent was added on the basis of the light sterilization performance experiment, and by comparing the decline of antibacterial efficiency, it was quantitatively analyzed which active oxygen was leading the sterilization.



**Fig.S1.** Size distribution of MoS<sub>2</sub>, PTh/MoS<sub>2</sub> and PThM/MoS<sub>2</sub>.



**Fig.S2.** Energy dispersive spectrum analysis (a) and mapping (b) of PTh/MoS<sub>2</sub>.



**Fig.S3.** Different photocatalytic antibacterial treatment time obtained by planar coating method.