

LDFT computational method

Calculation of the as-prepared composite photocatalysts were carried out by using Gaussian 09 program (see ***Supporting Information***) at the density functional B3LYP level using the LANL2DZ basis set for both geometry optimization and frequency calculation. After initial calculation the separated TiO₂ and LMS moieties, the structures of promising TiO₂-LMS combinations were also calculated using the B3LYP density functional with the LANL2DZ basis set. The minimum energy was calculated by using DFT-D3 method to obtain the optimum binding site.

Capture tests of hydroxyl radical ($\cdot\text{OH}$)

The formation of hydroxyl radical ($\cdot\text{OH}$) of as-prepared materials was detected by a photoluminescence method using terephthalic acid (TA) as a probe molecule. Fifty milligrams of as-prepared sample was dispersed in the aqueous solution (250 mL) containing twenty milligrams TA and twenty milligrams NaOH. Xenon long-arc lamp irradiation was used as visible-light source. Four milliliter of reaction solution was collected every 15 min for analysis, and then the filtered sample was used for PL measurement at an F-4500 fluorescence spectrophotometer with the excitation wavelength of 321 nm. The scan speed was $240\text{ nm}\cdot\text{min}^{-1}$, PMT voltage was 700 V, and the width of excitation and emission slit were set to be both 5 nm.

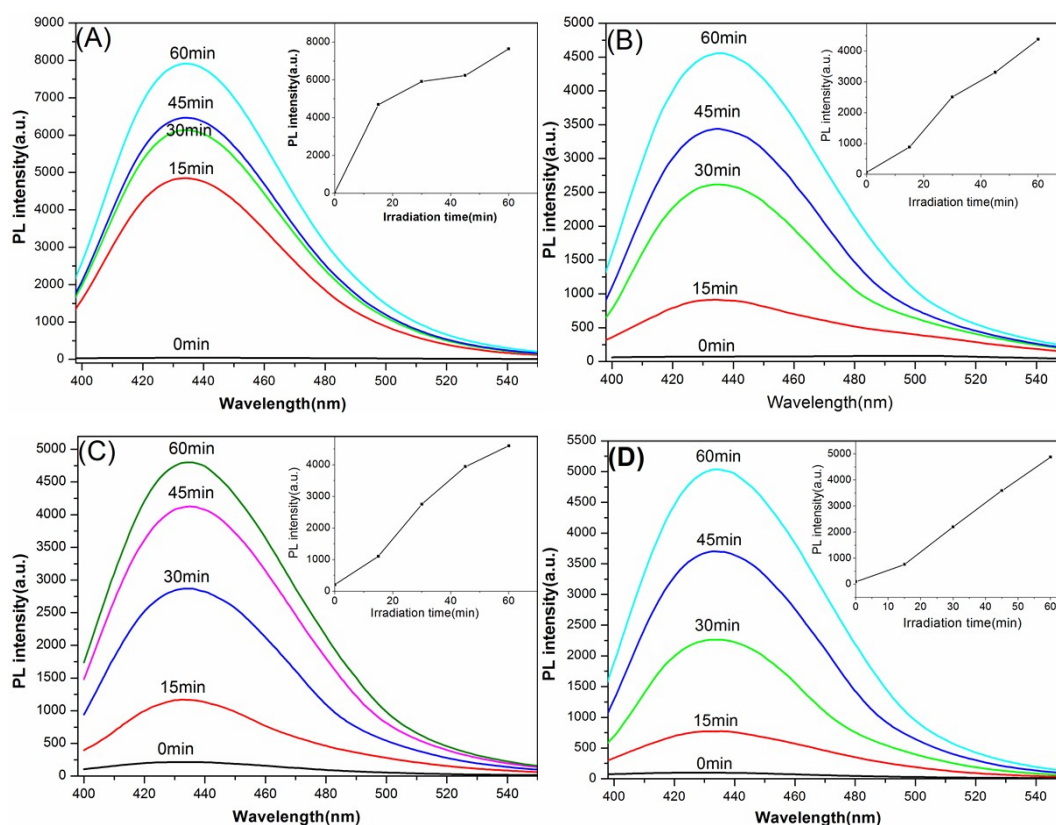


Figure S1. PL spectra change of terephthalic acid in different time for $\cdot\text{OH}$ captured experiment of P25 (A) and $\text{TiO}_2/\text{MoS}_2$ (B), TiO_2/WS_2 (C) and $\text{TiO}_2/\text{SnS}_2$ (D). The insert images are the PL intensity changing with time.

The photoluminescence technique was served to examine the formation of hydroxyl radicals ($\cdot\text{OH}$) on the TiO_2/LMS surface. Hydroxyl radicals were analyzed by the conversion of terephthalic acid to 2-hydroxy terephthalic acid, which can be used as a hydroxyl radical molecular sensing probes for hydroxyl radical detection in photocatalytic reaction. Figure S1 shows the PL spectrum changes during visible light irradiation of P25, $\text{TiO}_2/\text{MoS}_2$, TiO_2/WS_2 and SnS_2 , respectively. The fluorescence intensities at about 426 nm exhibit a gradually increasing tendency against the irradiation time, which is caused by chemical reactions between terephthalic acid

and $\cdot\text{OH}$. The insert plots of TiO_2/LMS show that these PL intensities increase almost linearly against the irradiation time as compared P25, suggesting that $\text{TiO}_2/\text{MoS}_2$, TiO_2/WS_2 and $\text{TiO}_2/\text{SnS}_2$ composites possessed better photostability. Further, the PL intensity of P25 in unit time was higher than that of TiO_2/LMS , indicating the production rate of $\cdot\text{OH}$ on P25 faster than that on TiO_2/LMS . However, the results of photocatalytic experiment showed that the photocatalytic activity was far less than that of TiO_2/LMS , which speculated that $\cdot\text{OH}$ was not the main active species in the photocatalytic process.