

Efficient TiO₂/SubPc photocatalyst for degradation of organic dyes under visible light

Ya-Fei Wang ^a, Bing-Bing Zhang ^a, Zhuo Li ^{a,b*}, Bing Wang ^a, Lin-Yu Jiao ^{a,b}, Chen Wang ^{a,b},

Lin Yang ^a, Hai-Xia Ma ^a, Ling-Yan Pang ^d, Xiao-Xun Ma ^{a,b,c*}

Table S1. Crystallographic data of H₁₂SubPcB-OPhCHO

Complex	H ₁₂ SubPcB-OPhCHO
formula	C ₃₁ H ₁₇ BN ₆ O ₂
formula weight	516.32
<i>T</i> /K	296(2)
crystal system	Monoclinic
space group	<i>P</i> 2 ₁ / <i>n</i>
<i>a</i> /Å	15.606(3)
<i>b</i> /Å	9.991(2)
<i>c</i> /Å	16.737(4)
<i>α</i> /°	90.00
<i>β</i> /°	111.846(4)
<i>γ</i> /°	90.00
<i>V</i> /Å ³	2422.3(9)
<i>Z</i>	4
<i>D</i> /g·cm ⁻³	1.416
<i>F</i> (000)	1064
<i>μ</i> /mm ⁻¹	0.092
data/restraints/Parameters	4446/0/362
<i>R</i> ₁ ^a [<i>I</i> > 2σ(<i>I</i>)]	0.0664
<i>wR</i> ₂ ^a [<i>I</i> > 2σ(<i>I</i>)]	0.1367

R_I^a (all data)	0.1503
wR_2^a (all data)	0.1716
Largest diff peak/hole ($e \cdot \text{\AA}^{-3}$)	0.228,-0.260

$$^aR_1 = \frac{\sum ||F_o| - |F_c||}{\sum |F_o|}; wR_2 = [\frac{\sum w(F_o^2 - F_c^2)^2}{\sum w(F_o^2)^2}]^{1/2}$$

Table S2. Selected bond length (\AA) data for SubPc2

Bond	Bond length	Bond	Bond length
B(1)-O(1)	1.460(5)	C(3)-H(3)	0.9300
B(1)-N(5)	1.482(5)	C(4)-C(5)	1.393(6)
B(1)-N(1)	1.490(5)	C(4)-H(4)	0.9300
B(1)-N(3)	1.497(5)	C(8)-N(2)	1.339(4)
C(1)-N(6)	1.342(5)	C(8)-N(1)	1.361(4)
C(1)-N(1)	1.358(4)	C(9)-N(2)	1.352(4)
C(1)-C(2)	1.462(5)	C(9)-C(10)	1.444(5)
C(2)-C(3)	1.389(5)	C(10)-C(15)	1.419(5)

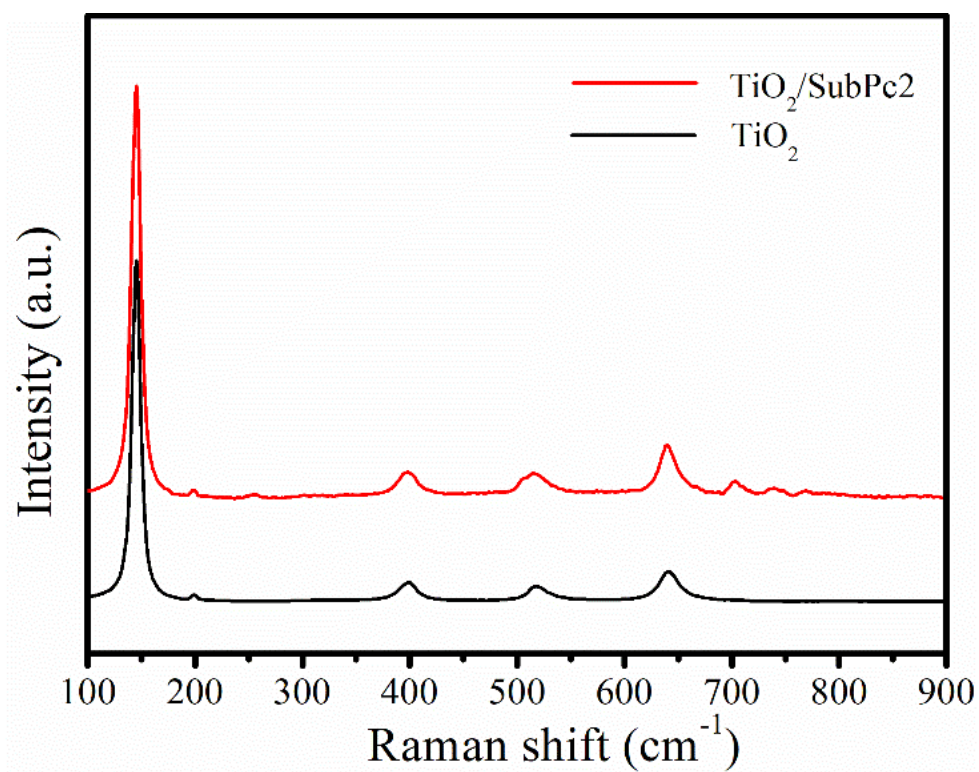


Fig. S1. Raman spectra of TiO₂ and TiO₂/SubPc₂ (25:1).

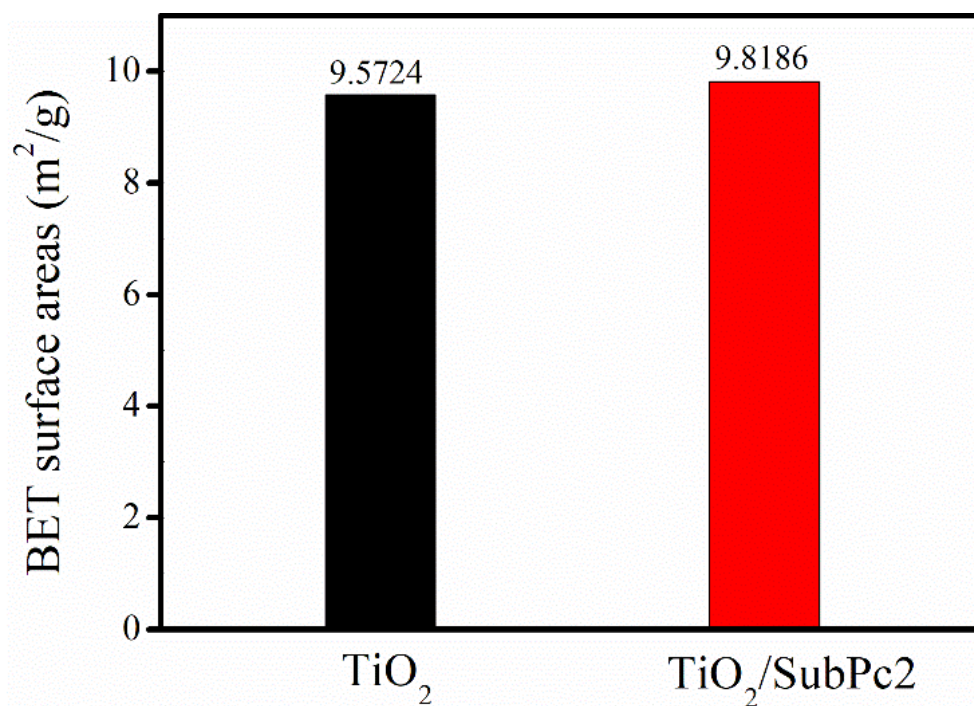


Fig. S2. The BET surface area of TiO₂ and TiO₂/SubPc₂ (25:1).

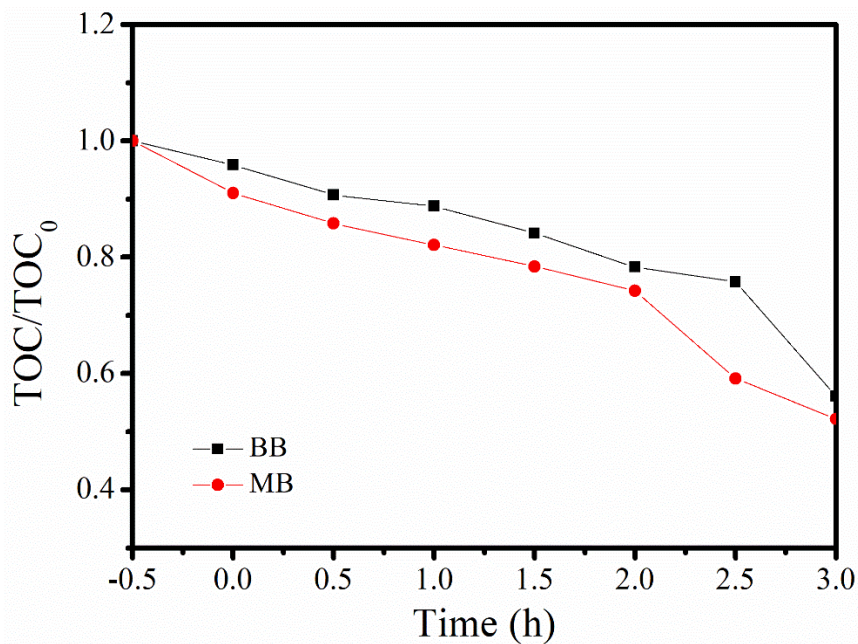


Fig. S3. TOC evolution during BB and MB photodegradation on $\text{TiO}_2/\text{SubPc}_2$ (25:1) photocatalytic.

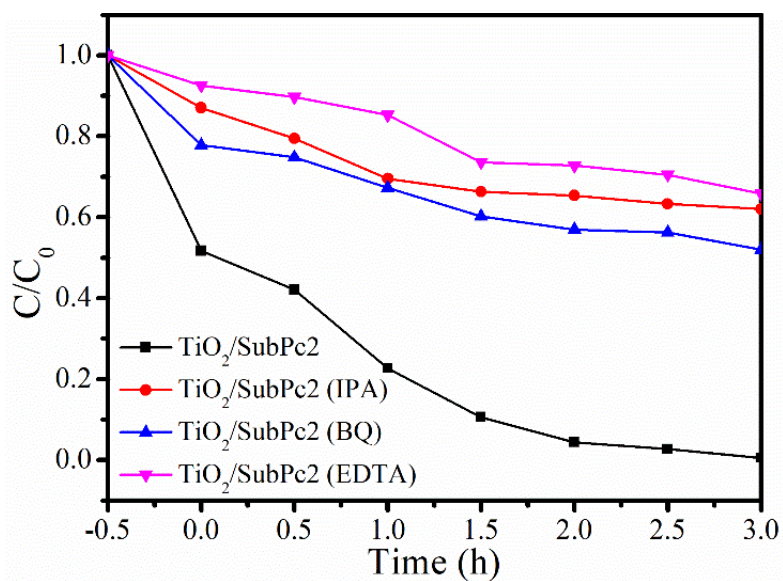


Fig. S4. Effects of different scavengers on BB photodegradation using $\text{TiO}_2/\text{SubPc}_2$ (25:1) photocatalyst under visible light irradiation.

The CCDC number of the SubPc2 is 2026629.

Published in NEW JOURNAL OF CHEMISTRY