

## Supporting information

### Highly Efficient Visible-Light Photocatalysts: $\text{Bi}_2\text{O}_3@\text{TiO}_2$ Derived from Ti-MOFs for Eriochrome Black T Degradation: A Joint Experimental and Computational Study

Jing Meng <sup>1,†</sup>, Asmaa G. Ashry <sup>2,†</sup>, Ahmed S. Abou-Elyazed <sup>2,3,\*</sup>, Zhe Zhang <sup>1</sup>, Xiaolin Li <sup>3,\*</sup>, Tamer Z. Sharara <sup>4</sup> and Safinaz H. El-Demerdash <sup>2</sup>

<sup>1</sup> School of Civil Engineering, Nantong Institute of Technology, Nantong 226002, China;

mengjing@ntit.edu.cn (J.M.); 20239078@ntit.edu.cn (Z.Z.)

<sup>2</sup> Chemistry Department, Faculty of Science, Menoufia University, Shebin El-Kom 32511, Egypt;

asmaaashry137@yahoo.com (A.G.A.); hamdysafinaz@yahoo.com (S.H.E.-D.)

<sup>3</sup> Institute of Intelligent Manufacturing Technology, Shenzhen Polytechnic University, Shenzhen

518055, China

<sup>4</sup> EPRI Nanotechnology Center, Egyptian Petroleum Research Institute, Nasr City, Cairo 11727,

Egypt; tamerzakisharara@yahoo.com

\* Correspondence: ahmedphysical90@gmail.com (A.S.A.-E.); lixiaolin0427@szpu.edu.cn (X.L.)

† These authors contributed equally to this work.

## Reusability test

### Reusability without regeneration

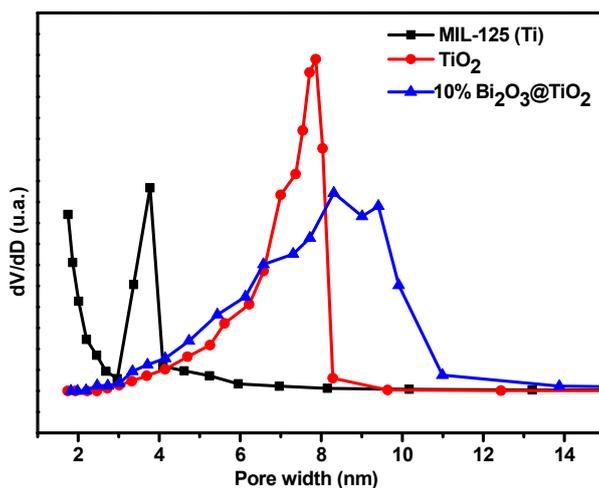
The recycle experiment was made without regeneration of the photocatalyst for 4 cycles (after each cycle the photocatalyst was obtained by centrifugation and then added to another 50 ml of 50 mg L<sup>-1</sup> EBT dye solution.

### Reusability with regeneration

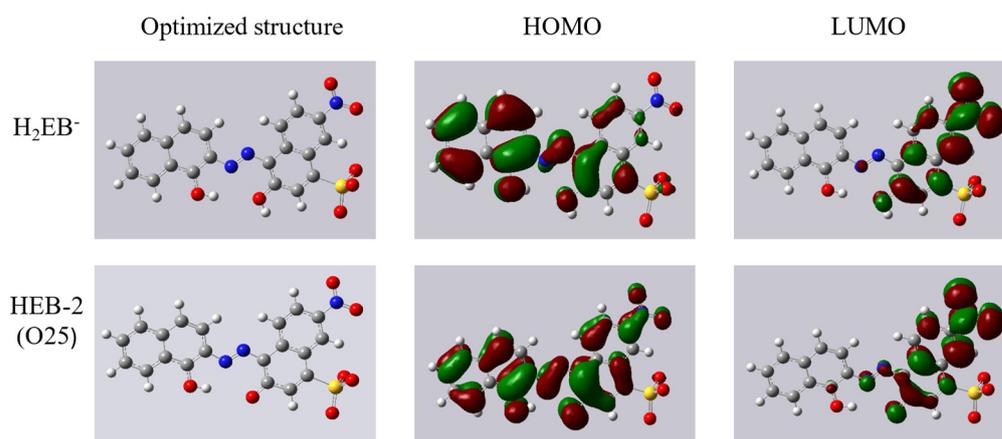
the recycle experiment was made with regeneration of the photocatalyst for 4 cycles (after each cycle the photocatalyst was obtained by centrifugation, washed several times through sonication with water and ethanol and then dried in vacuum oven over night at 60°C.

**Table S1.** Acid properties of TiO<sub>2</sub> and 10% Bi<sub>2</sub>O<sub>3</sub>@TiO<sub>2</sub>.

Peak No.	Peak temp. (°C)	Amount of active sites (mmol)	Amount of active sites/adsorbent (mmol/g)	Peak temp. (°C)	Amount of active sites (mmol)	Amount of active sites/adsorbent (mmol/g)
	<b>TiO<sub>2</sub></b>			<b>10% Bi<sub>2</sub>O<sub>3</sub>@TiO<sub>2</sub></b>		
1	54.1	0.001	0.015	178.3	0.001	0.011
2	294.9	0.003	0.057	240.1	0.002	0.029
3	399.4	0.001	0.019	367.4	0.003	0.051
4	-	-	-	549.8	0.004	0.076



**Figure S1.** pore size distribution of various samples.

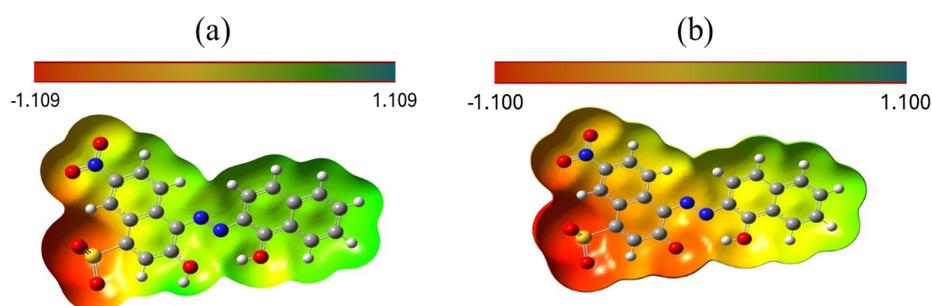


**Figure S2.** The optimized structures, FMO amplitudes (The LUMO and HOMO electron densities) for neutral EBT and protonated forms calculated by DFT/B3LYP/6-311++G(d,p) level.

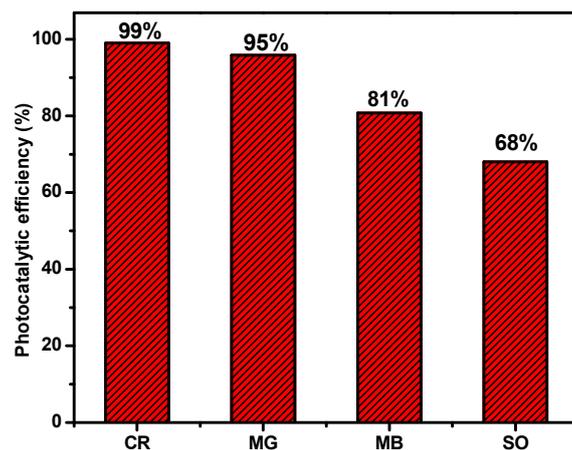
**Table S2.** Mulliken atomic charges of the B3LYP/6-311++G(d,p) optimized neutral and protonated EB in an aqueous medium.

	Neutral EBT	H <sub>2</sub> EB <sup>-</sup>	HEB <sup>-2</sup> (O24)	HEB <sup>-2</sup> (O25)	EB <sup>-3</sup>
C9	0.205	0.089	-0.284	0.094	-0.253
C10	-0.171	-0.281	-0.185	-0.231	-0.251
C11	-0.145	-0.180	-0.054	-0.101	-0.351
C12	-0.221	-0.189	-0.351	-0.256	-0.238

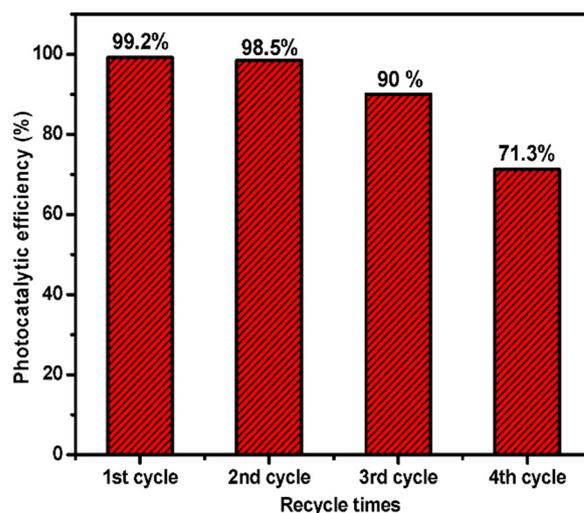
C14	-0.852	-1.048	-0.872	-0.844	-0.697
C19	-1.016	-0.388	-0.562	-0.538	-0.696
N21	-0.094	-0.033	0.060	0.001	0.117
N22	0.108	0.062	-0.046	-0.033	-0.189
N23	-0.0007	-0.083	-0.067	-0.102	-0.103
O24	-0.306	-0.310	-0.589	-0.326	-0.626
O25	-0.202	-0.200	-0.237	-0.534	-0.564
O26	-0.043	-0.080	-0.096	-0.121	-0.147
O27	-0.124	-0.108	-0.118	-0.147	-0.172
O28	-0.484	-0.417	-0.427	-0.434	-0.436
O29	-0.344	-0.417	-0.358	-0.430	-0.437
O30	-0.301	-0.346	-0.237	-0.354	-0.359
H5	0.217	0.206	0.199	0.193	0.172
H7	0.392	0.420	---	0.394	---
H8	0.348	0.346	0.341	---	---
H12	0.214	0.225	0.222	0.213	0.207
S1	0.748	0.707	0.741	0.760	0.806



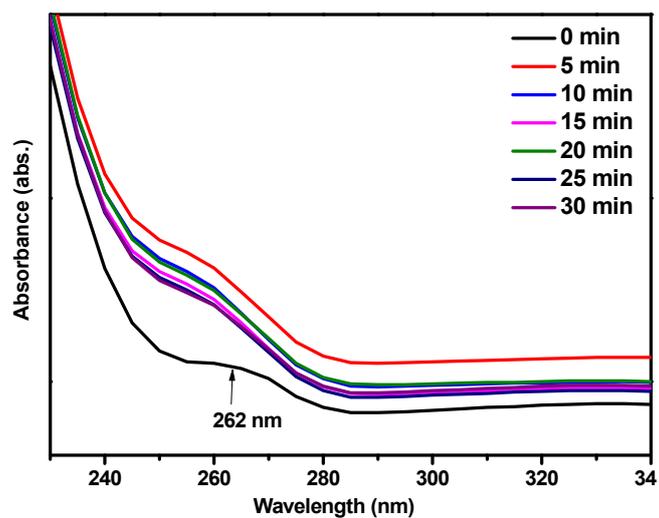
**Figure S3.** The contour representation of electrostatic potential regions of negative (positive) potential is red (green) for molecules; (a)  $\text{H}_2\text{EB}^-$  and (b)  $\text{HEB}^{-2}$  ( $\text{O}_{25}$ ) in the aqueous phase using the DFT/B3LYP/6-311++G(d,p) method.



**Figure S4.** The photocatalytic activity of 10% Bi<sub>2</sub>O<sub>3</sub>@TiO<sub>2</sub> towards different dyes at the studied optimum conditions.



**Figure S5.** The cycling runs of the degradation of EBT dye over 10% Bi<sub>2</sub>O<sub>3</sub>@TiO<sub>2</sub> after regeneration.



**Figure S6.** Decomposition of Lidocaine hydrochloride (0.05 g catalyst, 50 ppm 50 ml lidocaine hydrochloride solution, pH= 6, the irradiation time: 30 min) over 10% Bi<sub>2</sub>O<sub>3</sub>@TiO<sub>2</sub>.