

Supporting information

Highly Efficient Visible-Light Photocatalysts: Bi₂O₃@TiO₂ Derived from Ti-MOFs for Eriochrome Black T Degradation: A Joint Experimental and Computational Study

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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⁻¹ 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 TiO₂ and 10% Bi₂O₃@TiO₂.

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)
	TiO₂				10% Bi₂O₃@TiO₂	
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

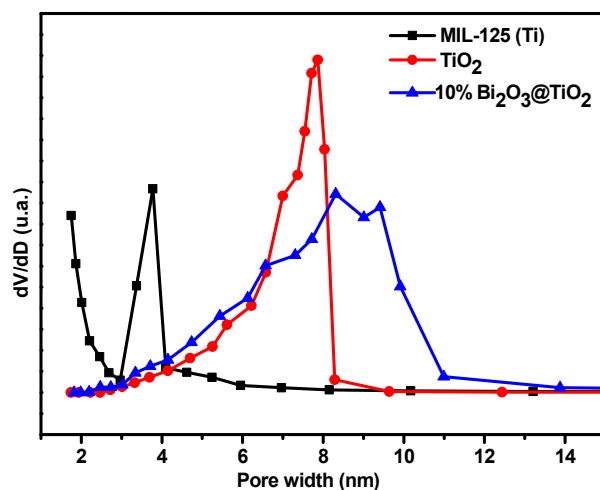


Figure S1. pore size distribution of various samples.

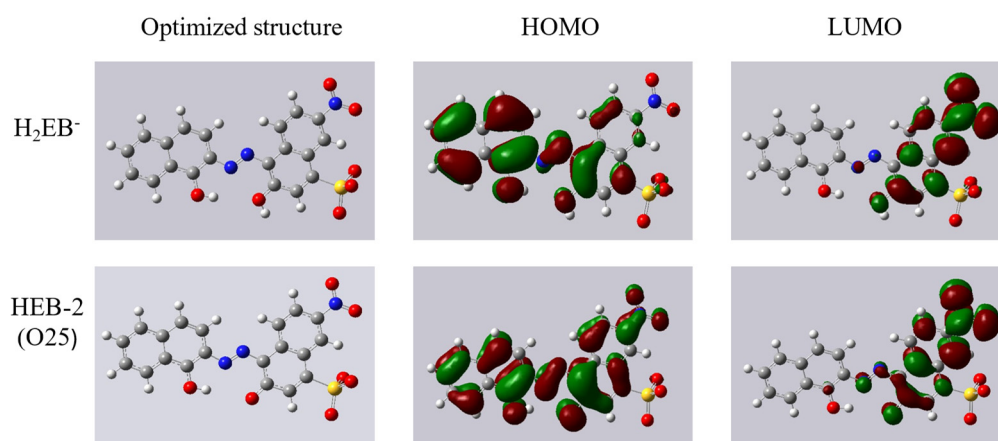


Figure S2. The optimized structures, FMO amplitudes (The LUMO and HOMO electron densities) for neutral EBT and protonated forms calculated by DFT/B3LYP/6-311++G(d,p) level.

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 ₂ EB ⁻	HEB ⁻² (O24)	HEB ⁻² (O25)	EB ⁻³
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

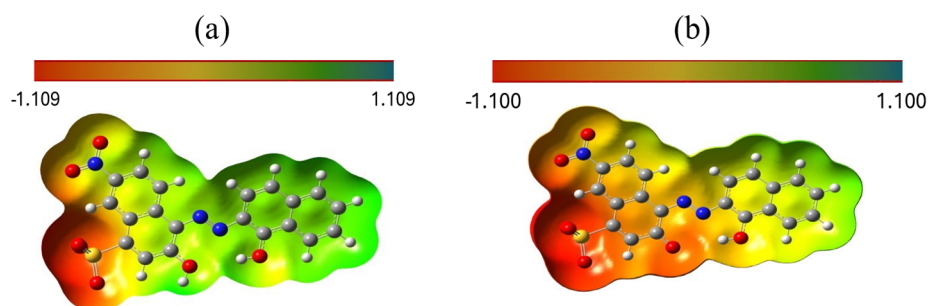


Figure S3. The contour representation of electrostatic potential regions of negative (positive) potential is red (green) for molecules; (a) H_2EB^- and (b) HEB^{2-} (O25) in the aqueous phase using the DFT/B3LYP/6-311++G(d,p) method.

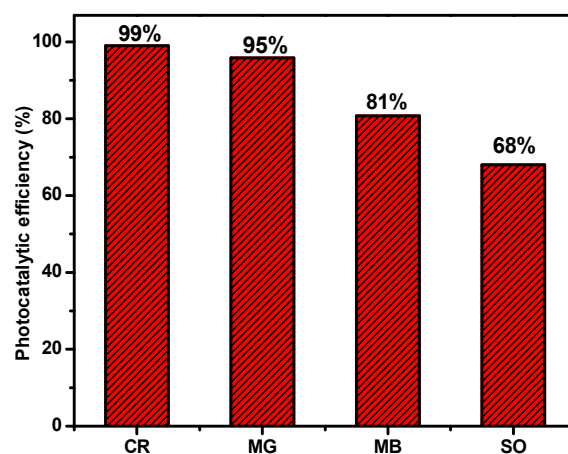


Figure S4. The photocatalytic activity of 10% Bi₂O₃@TiO₂ towards different dyes at the studied optimum conditions.

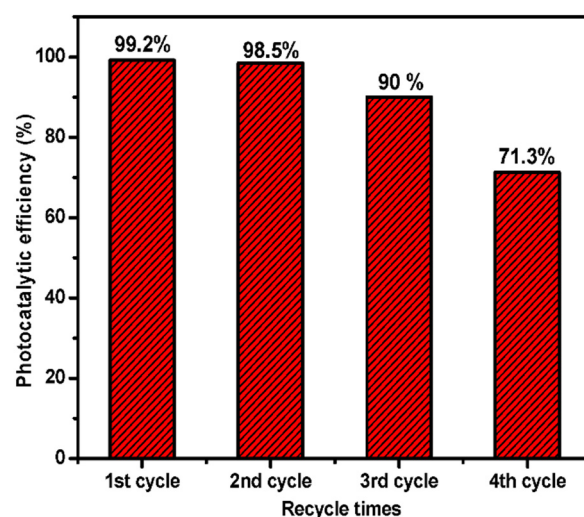


Figure S5. The cycling runs of the degradation of EBT dye over 10% Bi₂O₃@TiO₂ after regeneration.

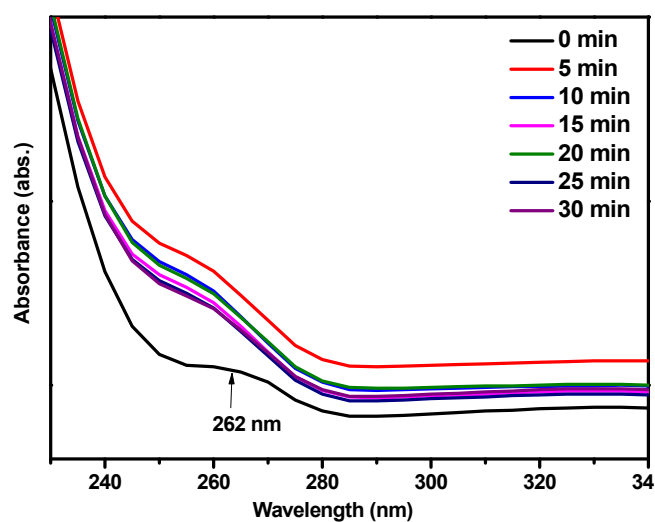


Figure S6. Decomposition of Lidocaine hydrochloride (0.05 g catalyst, 50 ppm 50 ml lidocaine hydrochloride solution, pH= 6, the irradiation time: 30 min) over 10% Bi₂O₃@TiO₂.