Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Material

Non-noble-metal TiC nanoparticles promoted charge separation and photocatalytic degradation performance on Bi_2O_3 microrods: degradation pathway and mechanism investigation

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Photoelectrochemical detection

The electrochemical impedance spectroscopy (EIS) was performed on an electrochemical workstation (CHI660E) with a three-electrode cell system. In this electrode system, the platinum foil and standard calomel electrode were used as the counter electrode and reference electrode, respectively. The fabrication of working electrode was as follows: 15 mg sample, 0.75 mg carbon black and 0.75 mg polyvinylidene fluoride (PVDF) were dissolved in 1-methyl-2-pyrrolidione (NMP) to obtain slurry. Then, the slurry was evenly coated on a 1.0 × 1.0 cm^2 fluoride-doped tin oxide glass electrode, which was then heated at 60 °C for 5 h. Na_2SO_4 aqueous solution (0.1 $mol \cdot L^{-1}$) was employed as the electrolyte. The EIS test was performed by using the sinusoidal voltage pulse with amplitude of 5 mV with frequency range from 10^{-2} to 10^5 Hz.

Table S1 The Fukui index (nucleophilic index f^{+}, electrophilic index f^{-} and f^{0}) and the condensed dual descriptor (CDD) of AO7

No	Atom	q(N)	q(N+1)	q(N-1)	f^{-}	f^{+}	f^{0}	CDD
1	C	-0.039	-0.066	0.0047	0.0437	0.027	0.0353	-0.0166
2	C	-0.0366	-0.059	0.0127	0.0493	0.0224	0.0359	-0.0268
3	C	-0.0021	-0.0141	0.0099	0.012	0.012	0.012	0
4	C	-0.0024	-0.0088	0.0056	0.008	0.0064	0.0072	-0.0015
5	C	-0.0378	-0.0402	0.0044	0.0422	0.0024	0.0223	-0.0398
6	C	-0.0348	-0.0655	0.0105	0.0453	0.0307	0.038	-0.0145
7	H	0.051	0.0255	0.0809	0.0299	0.0255	0.0277	-0.0044
8	H	0.0479	0.0276	0.0752	0.0273	0.0203	0.0238	-0.007
9	H	0.0466	0.029	0.072	0.0255	0.0176	0.0215	-0.0079
10	C	-0.0287	-0.0772	0.0375	0.0662	0.0484	0.0573	-0.0177
11	C	0.0205	0.0155	0.0653	0.0448	0.005	0.0249	-0.0398
12	H	0.0432	0.0387	0.0616	0.0183	0.0046	0.0114	-0.0138
13	H	0.0496	0.0298	0.0762	0.0267	0.0197	0.0232	-0.007
14	C	0.0722	0.0466	0.1131	0.0408	0.0257	0.0333	-0.0152
15	C	-0.0499	-0.0686	-0.0144	0.0355	0.0187	0.0271	-0.0168
16	H	0.053	0.0323	0.0787	0.0256	0.0207	0.0232	-0.0049
17	O	-0.2143	-0.2235	-0.1859	0.0284	0.0092	0.0188	-0.0192
18	H	0.1794	0.1636	0.2001	0.0207	0.0157	0.0182	-0.005
19	N	-0.0571	-0.187	0.0026	0.0598	0.1298	0.0948	0.07
20	N	-0.0594	-0.2091	0.0258	0.0852	0.1498	0.1175	0.0646
21	C	0.046	0.0329	0.0496	0.0036	0.0131	0.0084	0.0095
22	C	-0.0181	-0.0519	0.0006	0.0187	0.0338	0.0263	0.015
23	C	-0.0317	-0.0593	-0.0159	0.0158	0.0276	0.0217	0.0118
24	C	-0.0103	-0.0409	0.0088	0.0191	0.0306	0.0249	0.0115
25	H	0.0642	0.0429	0.0765	0.0122	0.0213	0.0168	0.0091
26	C	-0.0242	-0.0535	-0.0056	0.0186	0.0293	0.024	0.0107
27	H	0.0518	0.0347	0.0612	0.0094	0.0171	0.0132	0.0077
28	C	-0.0078	-0.0492	0.0198	0.0275	0.0415	0.0345	0.0139
29	H	0.0652	0.0436	0.0798	0.0147	0.0216	0.0181	0.0069
30	H	0.0577	0.0356	0.0735	0.0158	0.0221	0.019	0.0063
31	S	0.5201	0.4996	0.5319	0.0119	0.0205	0.0162	0.0086
32	O	-0.361	-0.3975	-0.3264	0.0347	0.0365	0.0356	0.0018
33	O	-0.3641	-0.4043	-0.325	0.0391	0.0402	0.0397	0.0011
34	O	-0.1959	-0.2124	-0.1833	0.0126	0.0165	0.0145	0.004
35	H	0.2066	0.1901	0.2179	0.0114	0.0165	0.0139	0.0051

Table S2 Toxicity analysis result of AO7 and its intermediates

Substance	Acute toxicity	Bioaccumulation factor	Developmental toxicity	
	Daphnia magna LC_{50} (48h) (mg/L)	**Predicted value**	**Predicted value**	**Predicted result**
AO7	3.3	7.34	0.89	Developmental toxicant
P1	3.21	3.73	0.59	Developmental toxicant
P2	314.67	2.7	0.55	Developmental toxicant
P3	92.03	1.83	0.62	Developmental toxicant
P4	990.46	1.59	0.84	Developmental toxicant
P5	3180.55	0.01	0.61	Developmental toxicant
P6	239.77	2.81	0.88	Developmental toxicant
P7	1638.12	0.02	0.46	Developmental non-toxicant
P8	177.21	0.52	0.48	Developmental non-toxicant

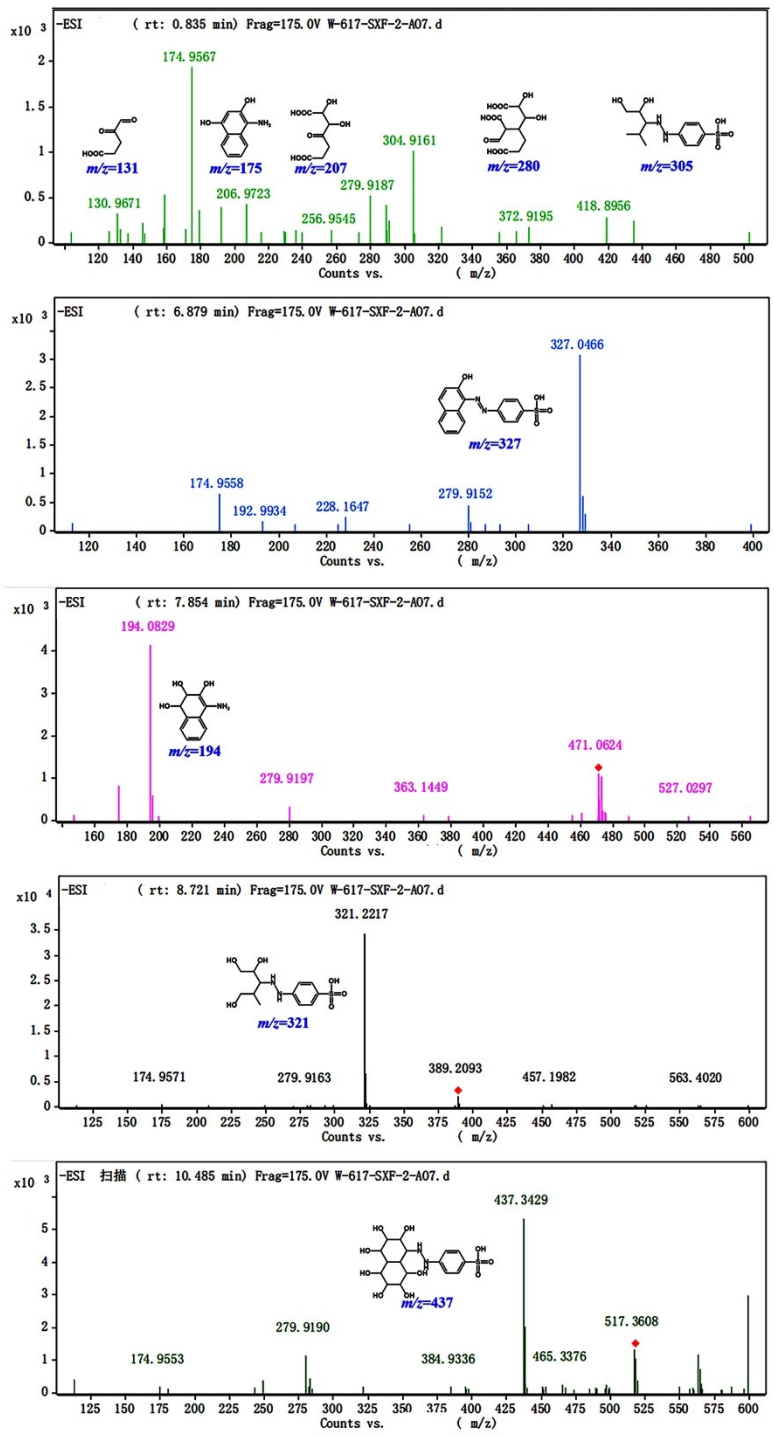

Fig. S1. The mass-to-charge ratio (m/z) of intermediates and the corresponding possible molecular structure

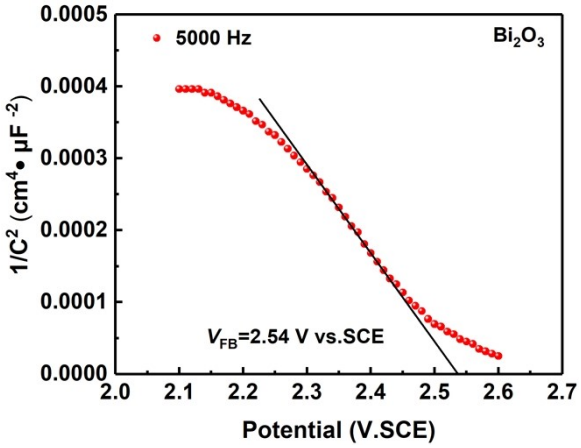

Fig. S2. Mott-Schottky (M-S) plot of bare Bi_2O_3