Electronic Supplementary Material (ESI) for Environmental Science: Nano.

SUPPLEMENTARY DATA

Photocatalytic degradation of polybrominated biphenyls (PBBs) on metal doped TiO_2 nanocomposites in aqueous environment: Mechanisms and solution effects

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4 pages, 5 Figures, 1 Table

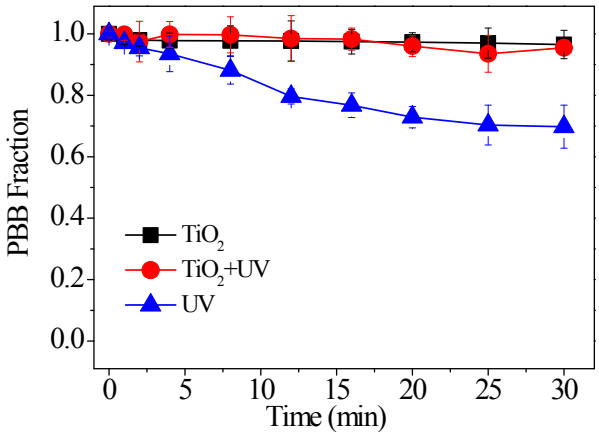

Fig. S1. The degradation of PBB-29 by direct UV light, TiO_2 only, and TiO_2 with UV light.

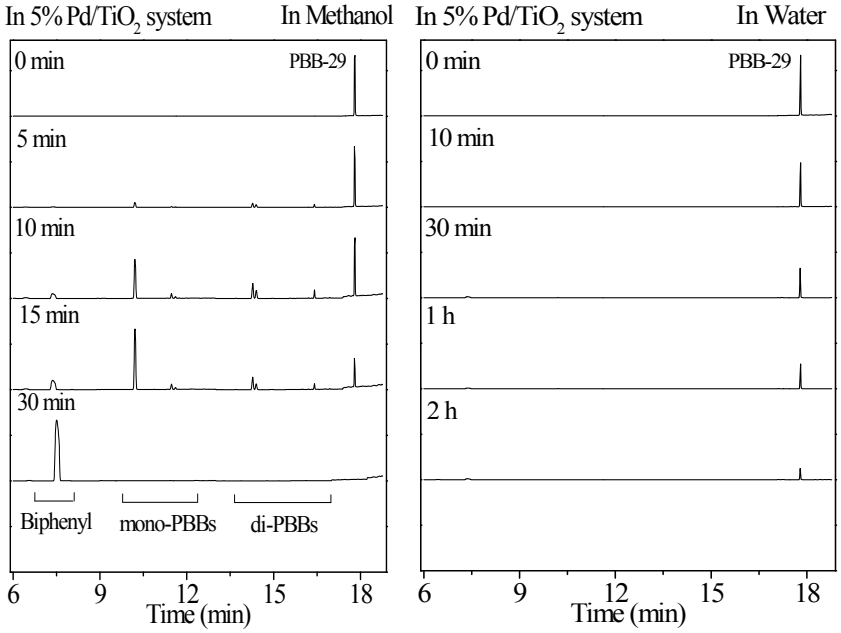

Fig.S2 The chromatograms of the degradation of PBB-29 in 5% Pd/TiO_2 systems with methanol and water solutions.

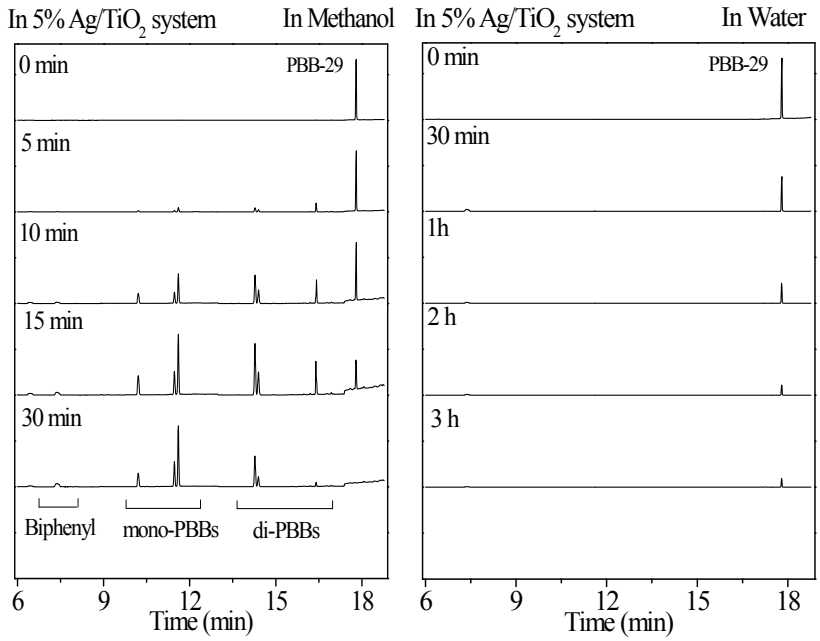

Fig. S3. The chromatograms of the degradation of PBB-29 in 5% Ag/TiO_2 systems with methanol and water solutions.

Note for Fig. S3: Since the degradation of PBBs in methanol systems only underwent debromination process, we have calculated the debromination efficiency of PBBs based on the equation below:

$$Debromination\ efficiency\ (t) = \frac{C_{biphenyl,\ t} \times 3 + C_{monoPBB,\ t} \times 2 + C_{diPBB,t} \times 1}{C_{PBB-29,\ 0\ min} \times 3}$$

Where $C_{PBB\text{-}29,\ 0\ min}$ is the initial concentration of PBB-29, $C_{biphenyl/monoPBB/diPBB,t}$ refers to the concentration of certain PBBs at t min. All the concentration should be converted into molar fraction. In 30 min, PBB-29 in 5% Pd/TiO_2 systems can reach to 100% debromination efficiency (Fig. S2), while that in 5% Ag/TiO_2 systems can only reach to 53 % (Fig. S3). This is because the lower PBBs by e-transfer process is more difficult to be debrominated than the higher PBBs (See our discussion about LUMO in main text).

Table S1. The energies of highest occupied molecular orbitals (HOMO) and lowest

unoccupied molecular orbitals (LUMO) of PBB-29, PBB-7 and PBB-3.

Name	HOMO (eV)	LUMO (eV)
PBB-29	-0.2546	-0.0540
PBB-7	-0.2521	-0.0468
PBB-3	-0.2430	-0.0466

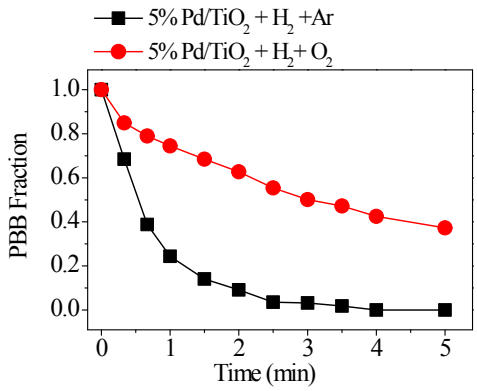

Fig. S4. The degradation of PBB-29 in Pd/TiO_2-H_2 system with Ar or O_2 purging.

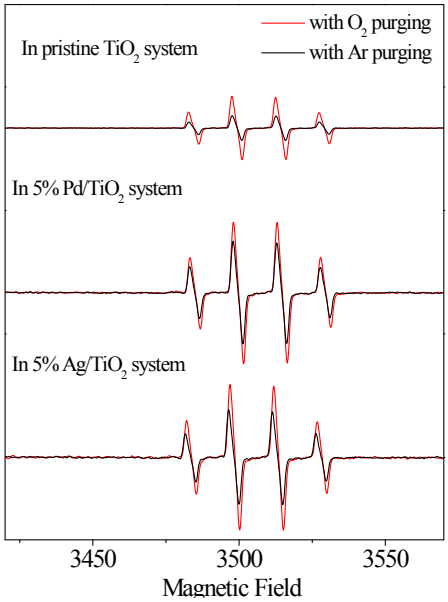

Fig. S5. Electron paramagnetic resonance spectra of pristine TiO_2, Pd/TiO_2 and Ag/TiO_2 in water with O_2 or Ar purging.