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:

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

Where $C_{\text{PBB-29, 0 min}}$ is the initial concentration of PBB-29, $C_{\text{biphenyl/monoPBB/diPBB}, t}$ 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.

<table>
<thead>
<tr>
<th>Name</th>
<th>HOMO (eV)</th>
<th>LUMO (eV)</th>
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<tbody>
<tr>
<td>PBB-29</td>
<td>-0.2546</td>
<td>-0.0540</td>
</tr>
<tr>
<td>PBB-7</td>
<td>-0.2521</td>
<td>-0.0468</td>
</tr>
<tr>
<td>PBB-3</td>
<td>-0.2430</td>
<td>-0.0466</td>
</tr>
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**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.