Supporting Information

One-step Synthesis of the Nanostructured AgI/BiOI Composites with Highly Enhanced Visible-Light Photocatalytic Performances

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**Figure S1.** The UV–vis absorption spectrum of methyl orange with the initial concentration of 20 mg L\(^{-1}\).

**Figure S2.** The UV–vis absorption spectrum of phenol with the initial concentration of 20 mg L\(^{-1}\).
Figure S3. XPS spectra of Ag 3d for (a) the fresh 20%AgI/BiOI and (b) after photodegradation of MO under visible light irradiation.

Figure S4. Irradiation time dependence of 20%AgI/BiOI composite upon repeated runs.
2. Band position calculations

For a compound, at the point of zero charge, the valence band (VB) position can be calculated by the following empirical formula [1-3]:

\[ E_{VB} = X - E^e + 0.5E_g \]  

(2)

where \( X \) is the absolute electronegativity of the semiconductor, which is defined as the geometric mean of the absolute electronegativity of the constituent atoms, \( E^e \) is the energy of free electrons on the hydrogen scale (ca. 4.5 eV), \( E_{VB} \) is the VB edge potential and \( E_g \) is the band gap of the semiconductor. The conduction band (CB) position can be deduced by \( E_{CB} = E_{VB} - E_g \). Given the equations above, the top of the VB and the bottom of the CB of AgI are calculated to be –6.75 and –3.95 eV with respect to the absolute vacuum scale (AVS), respectively. Accordingly, in the case of BiOI, the VB and CB are estimated to be –6.81 and –5.08 eV, respectively. The calculated band positions of AgI and BiOI are summarized in Table S1 and compared in Figure S5.

<table>
<thead>
<tr>
<th>oxide semiconductors</th>
<th>electronegativity (X)</th>
<th>estimated ( E_g ) (eV)</th>
<th>calculated VB position (eV)</th>
<th>calculated CB position (eV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>AgI</td>
<td>5.354</td>
<td>2.8</td>
<td>2.25 (NHE) -6.75 (AVS)</td>
<td>–0.55(NHE) –3.95(AVS)</td>
</tr>
<tr>
<td>BiOI</td>
<td>5.941</td>
<td>1.73</td>
<td>2.31(NHE) -6.81(AVS)</td>
<td>0.58(NHE) –5.08(AVS)</td>
</tr>
</tbody>
</table>
Figure S5. The CB and VB position comparisons of BiOI and AgI.

References:

