Zr-doped BaTaO$_2$N photocatalyst modified with Na-Pt cocatalyst for efficient hydrogen evolution and Z-scheme water splitting

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Table S1. Chemical compositions of three BaTaO$_2$N samples.

<table>
<thead>
<tr>
<th>Sample</th>
<th>Atomic ratio (at%)</th>
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<tbody>
<tr>
<td></td>
<td>Ba$^a$</td>
</tr>
<tr>
<td>BaTaO$_2$N</td>
<td>20.24</td>
</tr>
<tr>
<td>BaTaO$_2$N:Zr0.01</td>
<td>19.19</td>
</tr>
<tr>
<td>BaTaO$_2$N:Zr0.1</td>
<td>18.29</td>
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</tbody>
</table>

$^a$Measured by ICP-OES

$^b$Measured by the N-O combustion analyzer
Figure S1. Ta 4f XPS spectra of BaTaO$_2$N and BaTaO$_2$N:Zr0.01.
Figure S2. The action spectrum of Cr₂O₃ (0.9 wt% Cr)/0.23 wt% Na-0.3 wt% Pt/BaTaO₃N:Zr0.01 (100 mg) for photocatalytic water reduction in an aqueous 50 mM sodium phosphate buffer solution at pH 6 (150 mL) containing 6 mM K₄[Fe(CN)₆] under 300 W xenon lamp (420 nm < λ < 800 nm) equipped with various band-pass filters.
Figure S3. Time courses of H$_2$ evolution over Cr$_2$O$_3$ (0.9 wt% Cr)/0.23 wt% Na-0.3 wt% Pt/BaTaO$_2$N:Zr0.01 (100 mg) in an aqueous 50 mM sodium phosphate buffer solution at pH 6 (150 mL) containing 6 mM K$_4$[Fe(CN)$_6$] and O$_2$ evolution over CoO$_x$ (0.5 wt% Co)/0.2 wt% Au/BiVO$_4$ (100 mg) in the same sodium phosphate buffer solution but containing 6 mM K$_3$[Fe(CN)$_6$]. Light source: 300 W xenon lamp (420 nm < $\lambda$ < 800 nm).
Figure S4. Dependence curve of AQY as a function of irradiation wavelength and diffuse reflectance spectra of the HEP and OEP. The gas evolution over ZOWS consisted of 0.9 wt% Cr$_2$O$_3$/0.23 wt% Na-0.3 wt% Pt/BaTaO$_2$N:Zr0.01 (70 mg), 0.5 wt% CoO$_x$/0.2 wt% Au/BiVO$_4$ (100 mg), and 150 mL 25 mM sodium phosphate buffer solution (pH 6.0) containing K$_4$[Fe(CN)$_6$]$_3$ (6 mM) was performed under 300 W xenon lamp (420 nm < $\lambda$ < 800 nm) equipped with various band-pass filters.
Figure S5. (A) XRD pattern and (B) Ta 4f, (C) O 1s, and (D) Pt 4f XPS spectra of BaTaO$_2$N:Zr0.01 (a) before and (b) after a HER reaction in an aqueous 50 mM sodium phosphate buffer solution at pH 6 (150 mL) containing 6 mM K$_4$[Fe(CN)$_6$] under visible light irradiation.
Figure S6. XRD pattern of as-prepared BiVO$_4$. 