Electronic Supportive Information

Robust Charge Carrier Engineering Via Plasmonic effect and Conjugated II-Framework on Au loaded ZnCr-LDH/RGO Photocatalyst towards H₂ and H₂O₂ Production

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S1. Calculation of Number of H₂ evolved (theoretical) and apparent conversion efficiency (ACE).

(a) Number of H₂ molecules generated over Au@LDH/RGO composite was calculated by the reported literature of Deka et al.: [3]

Number of H₂ produced from Au@LDH/RGO composite:

Volume of H₂ generated during the reaction period = 20.6 ml = 0.0206 L

Form standard gas equation, we have \( PV = nRT \)

\( n \) (no. of H₂ gas evolved) = 0.0206 L x 1 atm / 0.082 L.atm mol⁻¹ K⁻¹ x 298 K

The corresponding amount of hydrogen in moles/2h = 0.000843 moles/2h

As we know, 1 mole of H₂ gas = 6.023 x 10²³ molecules of H₂

Therefore, 0.000843 moles = 6.023 x 10²³ x 0.000843 H₂ molecules

H₂ molecule (per cm² per s) = \( \frac{6.023 \times 10^{23} \times 0.000843}{14.13 \times 2 \times 60 \times 60} \)

= \( 4.9903 \times 10^{15} \) cm⁻² s⁻¹

Number of H₂ molecule (per s) = \( \frac{6.023 \times 10^{23} \times 0.000843}{2 \times 60 \times 60} \)

= \( 7.0513 \times 10^{16} \) s⁻¹

(b) Apparent conversion efficiency (ACE) of Au@LDH/RGO hybrid for H₂ production (918.76 µmol/2h in methanol solution) under 125W Hg lamp irradiation was calculated by following the below given formula. [2]

\[ \text{ACE} = \frac{\text{Stored chemical energy (SCE)}}{\text{Incident photon intensity (IPI)}} \]

\[ \text{SCE} = \text{Number of H₂ generated (moles/sec) \times} \text{Heat of combustion of H₂ (kJ/mole)} \]

= \( 0.127 \times 10^{-6} \text{ mole/sec} \times 285.8 \times 10^{3} \text{J/mole} \)

= 0.0362 W
\[ \text{IPI} = \text{Intensity of 125 W Hg lamp} \times \text{Distance between lamp and reaction suspension surface} \times \text{spherical surface area on which light is irradiated} (2\pi r) \]

\[ = 0.027 \times 9 \times 2 \times 3.14 \times (1.5)^2 \]

\[ = 0.3433 \text{W} \]

\[ \Rightarrow \text{ACE} = \frac{\text{SCE}}{\text{IPI}} \]

\[ 0.0362 \text{W} \]

\[ \Rightarrow \frac{0.0362 \text{W}}{0.3433 \text{W}} = 10.5\% \]

**Fig. S2**  Picture of photoreactor for \( \text{H}_2\text{O}_2 \) generation.

**S3. Calculation of solar to chemical conversion efficiency (SCC %).**

Solar to chemical conversion efficiency (SCC %) of Au@LDH/RGO composite towards \( \text{H}_2\text{O}_2 \) production under 250 W Hg lamp was calculated by following the below mention equation:
\[
\text{SCC} \% = \left( \frac{[\Delta G^\circ \text{ for } H_2O_2 \text{ production (J/mol)}] \times [H_2O_2 \text{ formed (mol)]}}{([\text{Input energy (W)]} \times [\text{reaction time(s)]})} \right) \times 100
\]

Input energy = Intensity of used Hg lamp \times Distance of lamp from catalyst mixed solution (9 cm) \times Surface area of the spherical region on which light is focused (2\pi r, r = 1.5 cm)

\[= 1.33 \times 9 \times 2 \times 3.14 \times (1.5)^2 \]

\[= 169.13 \text{ W} \]

\[
\frac{117 \times 10^3 \times 24.3 \times 10^{-6}}{169.13 \times 2 \times 3600} \times 100
\]

\[= 0.23\%
\]

Fig. S4  XRD pattern of (a) GO and (b) LDH.
**Fig. S5** (a) FESEM image and (b) colour elemental mapping image of Au@LDH/RGO.

**Fig. S6** EDAX of (a) LDH/RGO and (b) Au@LDH/RGO.
Fig. S7 XPS plot of LDH (a) C 1s, (b) O 1s, (c) Zn 2p and (d) Cr 2p.
**Fig. S8** Mott-Schottky graph of LDH at different frequency.

**Table S9.** Table represents the comparison study for photocatalytic H\textsubscript{2} evolution over present ternary heterostructure with the reported LDH, RGO and Au based system.

<table>
<thead>
<tr>
<th>Photocatalyst</th>
<th>Light irradiation and sacrificial agents</th>
<th>H\textsubscript{2} evolution (\mu mol g\textsuperscript{-1} h\textsuperscript{-1})</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>rGO/La\textsubscript{2}Ti\textsubscript{2}O\textsubscript{7}/NiFe-LDH</td>
<td>simulated solar irradiation, AM 1.5, TEOA</td>
<td>532.2</td>
<td>1</td>
</tr>
<tr>
<td>NiAl-LDH/g-C\textsubscript{3}N\textsubscript{4}/Ag\textsubscript{3}PO\textsubscript{4}</td>
<td>250 W quartz tungsten halogen lamp ($\lambda \geq 420$), CH\textsubscript{3}OH</td>
<td>268</td>
<td>2</td>
</tr>
<tr>
<td>CdIn\textsubscript{2}S\textsubscript{4}/In(OH)\textsubscript{3}/Ni Cr-LDH</td>
<td>300 W Xe lamp ($\lambda \geq 400$), Na\textsubscript{2}S and Na\textsubscript{2}SO\textsubscript{3}</td>
<td>1093</td>
<td>3</td>
</tr>
</tbody>
</table>
Table S10. Table represents the comparison study for photocatalytic \( H_2O_2 \) evolution over present ternary heterostructure with the reported RGO and Au based system.

<table>
<thead>
<tr>
<th>Photocatalyst</th>
<th>Light irradiation and sacrificial agents</th>
<th>( H_2O_2 ) production</th>
<th>Ref</th>
</tr>
</thead>
<tbody>
<tr>
<td>CN/rGO@black phosphorus quantum dot</td>
<td>300 W arc Xe lamp (420&lt;( \lambda &lt;780 ) nm)</td>
<td>181.69 ( \mu )mol/L, 3h</td>
<td>9</td>
</tr>
<tr>
<td>CoPi/rGO/TiO2</td>
<td>300 W Xe arc lamp (( \lambda \geq 320 ) nm), 2-propanol</td>
<td>850 ( \mu )mol, 3h</td>
<td>10</td>
</tr>
<tr>
<td>TiO2/rGO/Carbon dots</td>
<td>simulated solar irradiation AM 1.5, 2-propanol</td>
<td>350 ( \mu )mol, 1h</td>
<td>11</td>
</tr>
<tr>
<td>System</td>
<td>Reaction Conditions</td>
<td>Product</td>
<td>Time</td>
</tr>
<tr>
<td>-------------------------</td>
<td>--------------------------------------------</td>
<td>---------</td>
<td>------</td>
</tr>
<tr>
<td>TiO$_2$/WO$_3$/rGO</td>
<td>simulated solar irradiation AM 1.5, 2-propanol</td>
<td></td>
<td>270 µmol, 1h</td>
</tr>
<tr>
<td>Au/SnO$_2$-TiO$_2$</td>
<td>UV light, alcohol</td>
<td></td>
<td>15000 µmol, 3h</td>
</tr>
<tr>
<td>Au@LDH/RGO</td>
<td>125 W Xe lamp, (λ≥420), CH$_3$OH</td>
<td>24.3 µmol, 2h</td>
<td>Present Work</td>
</tr>
</tbody>
</table>

*Fig. S11* XRD plot of Au@LDH/RGO sample after and before use.
References


