Supporting Information

Two-Dimensional Confined Electron Donor–Acceptor Co-intercalated Inorganic/Organic Nanocomposites: An Effective Photocatalyst for Dye Degradation

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1. Structural characterization and optical absorption spectra of CuPcTS-PTCB(x %)/LDHs

Table S1. The elemental composition of CuPcTS-PTCB(x %)/LDHs

<table>
<thead>
<tr>
<th>Nominal (x %)</th>
<th>Chemical Composition</th>
<th>Zn/Al Ratio</th>
<th>Determined (x %)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>Zn_{0.585}Al_{0.415}(OH)<em>{2} (C</em>{32}H_{12}N_{6}CuO_{12}S_{4})<em>{0.073} (OH)</em>{0.123} · 3.316H_{2}O</td>
<td>1.41</td>
<td>0.00</td>
</tr>
<tr>
<td>10</td>
<td>Zn_{0.595}Al_{0.405}(OH)<em>{2}(C</em>{24}H_{18}O_{8})<em>{0.037} (C</em>{32}H_{12}N_{6}CuO_{12}S_{4})<em>{0.064} · 2.197H</em>{2}O</td>
<td>1.47</td>
<td>36.63</td>
</tr>
<tr>
<td>30</td>
<td>Zn_{0.603}Al_{0.397}(OH)<em>{2}(C</em>{24}H_{18}O_{8})<em>{0.049} (C</em>{32}H_{12}N_{6}CuO_{12}S_{4})<em>{0.050} · 1.741H</em>{2}O</td>
<td>1.52</td>
<td>49.75</td>
</tr>
<tr>
<td>50</td>
<td>Zn_{0.605}Al_{0.395}(OH)<em>{2}(C</em>{24}H_{18}O_{8})<em>{0.063} (C</em>{32}H_{12}N_{6}CuO_{12}S_{4})<em>{0.036} · 1.873H</em>{2}O</td>
<td>1.53</td>
<td>63.64</td>
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<tr>
<td>70</td>
<td>Zn_{0.611}Al_{0.389}(OH)<em>{2}(C</em>{24}H_{18}O_{8})<em>{0.075} (C</em>{32}H_{12}N_{6}CuO_{12}S_{4})<em>{0.022} · 1.718H</em>{2}O</td>
<td>1.57</td>
<td>77.32</td>
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<tr>
<td>90</td>
<td>Zn_{0.606}Al_{0.394}(OH)<em>{2}(C</em>{24}H_{18}O_{8})<em>{0.090} (C</em>{32}H_{12}N_{6}CuO_{12}S_{4})<em>{0.009} · 2.313H</em>{2}O</td>
<td>1.54</td>
<td>90.91</td>
</tr>
<tr>
<td>100</td>
<td>Zn_{0.595}Al_{0.405}(OH)<em>{2}(C</em>{24}H_{18}O_{8})<em>{0.101} · 0.507H</em>{2}O</td>
<td>1.47</td>
<td>100.00</td>
</tr>
</tbody>
</table>

Figure S1 The FT-IR spectra, (a) PTCD and PTCB, (b) a-CuPcTS/LDHs; b-CuPcTS-PTCB(36.63 %)/LDHs; c-CuPcTS-PTCB(49.75 %)/LDHs; d-CuPcTS-PTCB(63.64 %)/LDHs; e-CuPcTS-PTCB(77.73 %)/LDHs; f-CuPcTS-PTCB(90.91 %)/LDHs; g-PTCB/LDHs.

For the FT-IR spectrum of pristine PTCD (Figure S1a), the strong band at 1773 cm\(^{-1}\) was the characteristic CO–O–CO stretching vibration of the anhydride, and the bands at 1596 cm\(^{-1}\) and 1508 cm\(^{-1}\) were due to the skeleton vibration of phenyl ring. When the PTCD was hydrolyzed into PTCB, two bands corresponding to the vibrations of C=O in the –COOH group could be observed at 1687 cm\(^{-1}\) and 1590 cm\(^{-1}\) (Figure S1a), and the in plane deformation vibration of O–H appeared at 1433 cm\(^{-1}\). For the CuPcTS-PTCB(x %)/LDHs that included PTCB, the bands at 1550 cm\(^{-1}\) and 1424 cm\(^{-1}\)
were due to the antisymmetric and symmetric stretching vibration of C–O– in the –COO– group. The skeleton vibration of the phenyl ring also appeared at 1592 cm\(^{-1}\). All those indicated that the PTCB was intercalated into Zn\(_{1.5}\)Al-LDHs. The appearance of the characteristic absorption peak of –SO\(_3\)\(^{-1}\) at 1193 cm\(^{-1}\) (Figure S1b) suggested the successful intercalation of CuPcTS into the Zn\(_{1.5}\)Al-LDHs.\(^2\)

![Figure S2. The layer spacing of CuPcTS-PTCB(x%)/LDHs.](image)

![Figure S3. The molecular models of CuPcTS and PTCB calculated by Gaussian 09 software.](image)
Figure S4. The UV-vis absorption spectra of CuPcTS (15 µmol/L), PTCB (15 µmol/L) and CuPcTS@PTCB (15 µmol/L) aqueous solutions.

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2. The photocatalytic degradation of organic dyes for CuPcTS-PTCB(x%)/LDHs

Figure S8. The comparison of photodegradation of MO under the simulated solar irradiation.
**Figure S9.** Photocatalytic degradation of MO (a), AO (c), AY (e), MB (b), MV (d) and RhB (f) for 
CuPcTS-PTCB(x%)/LDHs (no catalysts-black, CuPcTS/LDHs-red, 
CuPcTS-PTCB(36.63%)/LDHs-green, CuPcTS-PTCB(49.75%)/LDHs-blue, 
CuPcTS-PTCB(63.64%)/LDHs-cyan, CuPcTS-PTCB(77.32%)/LDHs-magenta, 
CuPcTS-PTCB(90.91%)/LDHs-navy, PTCB/LDHs-dark yellow).

**Figure S10.** Photocatalytic activity of (a) CuPcTS/LDHs, (b) PTCB/LDHs, and (c) P25 particles for 
MO.
**Figure S11.** Photocatalytic degradation of phenol for CuPcTS-PTCB(49.75%)/LDHs.

![Photocatalytic degradation graph](image)

**Figure S12.** Adsorption amounts of MO on CuPcTS-PTCB(x%)/LDHs (x = 0, 36.63, 49.75, 63.64, 77.32, 90.91, 100).

**Table S2.** The BET surface of CuPcTS-PTCB(x%)/LDHs (x = 0, 36.63, 49.75, 63.64, 77.32, 90.91, 100)

<table>
<thead>
<tr>
<th>Photocatalyst</th>
<th>BET specific surface area (m² g⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CuPcTS/LDHs</td>
<td>60.83</td>
</tr>
<tr>
<td>CuPcTS-PTCB(36.63%)/LDHs</td>
<td>61.24</td>
</tr>
<tr>
<td>CuPcTS-PTCB(49.75%)/LDHs</td>
<td>52.82</td>
</tr>
<tr>
<td>CuPcTS-PTCB(63.64%)/LDHs</td>
<td>62.92</td>
</tr>
<tr>
<td>CuPcTS-PTCB(77.32%)/LDHs</td>
<td>53.14</td>
</tr>
<tr>
<td>CuPcTS-PTCB(90.91%)/LDHs</td>
<td>64.46</td>
</tr>
<tr>
<td>PTCB/LDHs</td>
<td>66.61</td>
</tr>
</tbody>
</table>
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**Figure S14.** Cyclic voltammograms curves of CuPcTS, PTCB, CuPcTS/LDHs, and PTCB/LDHs. The CV curves of CuPcTS/LDHs and PTCB/LDHs single-intercalated samples were also measured, provided that no remarkable difference in energy levels between the co-intercalated and single-intercalated composites.
Figure S15. Cyclic voltammograms curves of MO, AO, AY, MB, MV, and RhB.

Figure S16. The Current–Voltage curves of CuPcTS-PTCB(49.75%)/LDHs in dark and light at a scanning rate of 50 mV·s⁻¹. Inset: the EIS curve of CuPcTS-PTCB(49.75%)/LDHs.
References
