Tailoring the structure, pH sensitivity and catalytic performance in Suzuki-Miyaura cross-couplings of Ln/Pd MOFs based on the 1,1'-di(p-carboxybenzyl)-2,2'-diimidazole linker

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Fig. S1 TGA plots for different samples

Fig. S2 X-ray powder diffraction patterns of 1-4
Fig. S3 (a) Complex 1 (0.4% mmol), \( \text{K}_2\text{CO}_3 \) (2.0 mmol) in H\(_2\)O (6.0 mL); (b) acidified with diluted HCl (2.0 mol L\(^{-1}\)) to pH = 4; (c) the mixture (b) after centrifugation.

Fig. S4 X-ray powder diffraction patterns of 1. Simulated (black); recovered after reaction in ethanol (red); precipitate [Fig. S3(c)] recovered from water after phase switch with acid (blue).

Fig. S5 TEM images of catalyst 1 after the reaction in water-ethanol (left) and water (right).

Fig. S6 XPS spectra of catalyst 1 after the reaction in water
Fig. S7 XPS spectra of catalyst 1 after the reaction in water-ethanol

Fig. S8 IR spectra of 1, before and after the cross-coupling reaction in ethanol

**GC-yield Standard Curve**

The response peak area ratios of the product and internal standard, n-hexadecane (Ap/Ad) were obtained from Agilent 7890A GC spectrometer. All the GC-yields were calculated by the formula of curve fitting.

**GC-Yield Standard Curve of biphenyl**

<table>
<thead>
<tr>
<th>Ap/Ad</th>
<th>0.0806</th>
<th>0.2106</th>
<th>0.4497</th>
<th>0.6333</th>
<th>0.6953</th>
<th>0.7448</th>
</tr>
</thead>
<tbody>
<tr>
<td>Yields</td>
<td>0.1</td>
<td>0.30</td>
<td>0.60</td>
<td>0.81</td>
<td>0.90</td>
<td>1.00</td>
</tr>
</tbody>
</table>
GC-Yield Standard Curve of 4-Phenyltoluene

<table>
<thead>
<tr>
<th>$A_p/A_d$</th>
<th>0.0833</th>
<th>0.2243</th>
<th>0.4362</th>
<th>0.6207</th>
<th>0.7095</th>
<th>0.7776</th>
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</thead>
<tbody>
<tr>
<td>Yields</td>
<td>0.1</td>
<td>0.30</td>
<td>0.60</td>
<td>0.80</td>
<td>0.90</td>
<td>1.00</td>
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$y = 1.2986x + 0.00921$

GC-Yield Standard Curve of 4-Phenylacetophenone

<table>
<thead>
<tr>
<th>$A_p/A_d$</th>
<th>0.0730</th>
<th>0.2305</th>
<th>0.4982</th>
<th>0.6735</th>
<th>0.7293</th>
<th>0.8697</th>
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</table>

$y = 1.2728x + 0.01179$
Yields

<table>
<thead>
<tr>
<th></th>
<th>0.1</th>
<th>0.30</th>
<th>0.60</th>
<th>0.80</th>
<th>0.90</th>
<th>1.00</th>
</tr>
</thead>
</table>
| **y** = 1.149x + 0.02783

^1HNMR Spectra of products

**Biphenyl**: ^1^H NMR (500 MHz, DMSO-d6): δ = 7.35 (t, 2H), 7.45(t, 4H), 7.64 (d, 4H).
4-Methyl-1,1'-biphenyl: $^1$H NMR (500 MHz, DMSO-$d_6$): $\delta = 2.33 \, (s, \, 3H)$, 7.26 \,(d, \, 2H), 7.32 \,(t, \, 1H), 7.43 \,(t, \, 2H), 7.53 \,(d, \, 2H), 7.61 \,(d, \, 2H)$.

4-Acetyl-1,1'-biphenyl: $^1$H NMR (500 MHz, DMSO-$d_6$): $\delta = 2.60 \,(s, \, 3H)$, 7.42 \,(t, \, 2H), 7.50 \,(t, \, 2H), 7.73 \,(d, \, 2H), 7.82 \,(d, \, 2H), 8.03\,(d, \, 2H)$.