Electronic Supplementary information (ESI)

Highly water-dispersible Pd nanoparticles and single atoms magnetite-supported as excellent catalysts for Suzuki and hydrogenation reactions

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Figures:

**Fig. S1** Pd3d core level XPS of the catalysts. The black lines represent the experimental data, whereas the red, blue and green show the fitted Pd(0), Pd(II) and Pd(IV) components, respectively.
Tables:

**Table S1.** Temperature effect on Suzuki-Miyaura coupling with Fe$_3$O$_4$ dpa@Pd$_{0.5}$ as catalyst.

<table>
<thead>
<tr>
<th>Temperature (ºC)</th>
<th>TOF (h$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>204</td>
</tr>
<tr>
<td>65</td>
<td>110000</td>
</tr>
<tr>
<td>80</td>
<td>182000</td>
</tr>
</tbody>
</table>

Bromobencene (3 mmol), phenylboronic acid (3.6 mmol), K$_3$PO$_4$ (9 mmol), catalyst (9.4×10$^{-5}$ mmol Pd), 65 ºC and EtOH:water.

**Table S2.** Base effect on Suzuki-Miyaura coupling with Fe$_3$O$_4$ dpa@Pd$_{0.5}$ as catalyst.

<table>
<thead>
<tr>
<th>Base</th>
<th>TOF (h$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>KOH</td>
<td>122</td>
</tr>
<tr>
<td>K$_3$PO$_4$</td>
<td>110000</td>
</tr>
<tr>
<td>K$_2$CO$_3$</td>
<td>100000</td>
</tr>
<tr>
<td>AcONa</td>
<td>28900</td>
</tr>
<tr>
<td>NaHCO$_3$</td>
<td>63500</td>
</tr>
</tbody>
</table>

Bromobencene (3 mmol), phenylboronic acid (3.6 mmol), base (9 mmol), catalyst (9.4×10$^{-5}$ mmol Pd), 65 ºC, and EtOH:water.

**Table S3.** Solvent effect on Suzuki-Miyaura coupling with Fe$_3$O$_4$ dpa@Pd$_{0.5}$ as catalyst.

<table>
<thead>
<tr>
<th>Solvent</th>
<th>TOF (h$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EtOH</td>
<td>384</td>
</tr>
<tr>
<td>Water</td>
<td>1470</td>
</tr>
<tr>
<td>EtOH:Water</td>
<td>110000</td>
</tr>
</tbody>
</table>

Bromobencene (3 mmol), phenylboronic acid (3.6 mmol), K$_3$PO$_4$ (9 mmol), catalyst (9.4×10$^{-5}$ mmol Pd), 65 ºC, and solvent (60 mL).

**Table S4.** Temperature effect on Suzuki-Miyaura coupling with Fe$_3$O$_4$ dpa@Pd$_{0.5}$ as catalyst in water.

<table>
<thead>
<tr>
<th>Temperature (ºC)</th>
<th>TOF (h$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>65</td>
<td>3150</td>
</tr>
<tr>
<td>100</td>
<td>14950</td>
</tr>
</tbody>
</table>

Bromoaryl (0.5 mmol), phenylboronic acid (0.6 mmol), K$_3$PO$_4$ (1.5 mmol), 2.0×10$^{-4}$ mmol Pd, water, air atmosphere.