Supporting Information for

Porphyrin-based porous polyimide polymers/Pd nanoparticles composites as efficient catalysts for Suzuki-Miyaura coupling reactions

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Fig. S1 ¹H NMR of 5, 10, 15, 20-Tetrakis(4-aminobiphenyl)porphyrin (TBPP).



Fig. S2 ¹³C NMR of 5, 10, 15, 20-Tetrakis(4-aminobiphenyl)porphyrin (TBPP).



Fig. S3 Pore size distribution for **PPPP-1**, **Pd@PPPP-1**, **PPPP-2** and **Pd@PPPP-2** calculated based on collected N₂ isotherms.



Fig. S4 TGA data of Pd@PPPP-1 and Pd@PPPP-2 under N₂ atmosphere.



Fig. S5 FT-IR spectra of **Pd@PPPP-1** after treatment for 3 days in HCl (6 M) solutions, NaOH (6 M) solutions, and boiling water.



Fig. S6 FT-IR spectra of **Pd@PPPP-2** after treatment for 3 days in HCl (6 M) solutions, NaOH (6 M) solutions, and boiling water.



Fig. S7 TEM images of Pd@PPPP-1 after treatment for 3 days in NaOH (6 M).



Fig. S8 TEM images of Pd@PPPP-2 after treatment for 3 days in NaOH (6 M).



Figure S9 Filtration test of Pd@PPPP-1 for the coupling phenylboronic and p-iodonitrobenzene.



Figure S10 Yield of catalytic recyclability studies for the coupling phenylboronic and p-iodonitrobenzene by Pd@PPPP-2.



Figure S11 TEM image of Pd@PPPP-2 after 5rd cycle.

| Table S1. PPPP-1 eclipsed stacking | | | | | |
|------------------------------------|---------|------------|---------|--|--|
| Space group P_4/mmm | | | | | |
| a = 34.1122 Å | | | | | |
| c = 3.4871 Å | | | | | |
| Atom | x/a | <i>y/b</i> | z/c | | |
| C1 | 0.10195 | 0 | 0.00000 | | |
| C2 | 0.14739 | 0 | 0.00000 | | |
| C3 | 0.08126 | -0.03638 | 0.00000 | | |
| C4 | 0.42439 | 0.96782 | 0.00000 | | |
| C5 | 0.46534 | 0.97970 | 0.00000 | | |
| C6 | 0.29577 | 0.96462 | 0.00000 | | |
| C7 | 0.33670 | 0.96466 | 0.00000 | | |
| 08 | 0.41302 | 0.93395 | 0.00000 | | |
| N9 | 0.04165 | 0.95835 | 1.00000 | | |
| C10 | 0.07205 | 0.90000 | 1.00000 | | |
| C11 | 0.16953 | 1.03490 | 1.00000 | | |
| C12 | 0.21045 | 1.03519 | 1.00000 | | |
| C13 | 0.23142 | 1.00000 | 1.00000 | | |
| N14 | 0.59983 | 1.00000 | 1.00000 | | |
| C15 | 0.35775 | 1.00000 | 1.00000 | | |
| C16 | 0.27483 | 1.00000 | 1.00000 | | |
| C17 | 0.50000 | 0.04235 | 0.00000 | | |

Crystallographic information of modeled PPPPs

| Table S2. PPPP-1 staggered stacking | | | | | |
|--|------------|------------|---------|--|--|
| Space group <i>I</i> ₄ / <i>mmm</i> | | | | | |
| <i>a</i> = 34.1269 Å | | | | | |
| c = 6.5904 Å | | | | | |
| Atom | <i>x/a</i> | <i>y/b</i> | z/c | | |
| C1 | 0.10199 | 0 | 0.00000 | | |
| C2 | 0.14745 | 0 | 0.00000 | | |
| C3 | 0.08130 | -0.03641 | 0.00000 | | |
| C4 | 0.33680 | 0.96467 | 0.00000 | | |
| C5 | 0.42447 | 0.96782 | 0.00000 | | |
| N6 | 0.04170 | 0.95830 | 1.00000 | | |
| C7 | 0.07208 | 0.89997 | 1.00000 | | |
| C8 | 0.16960 | 1.03489 | 1.00000 | | |
| С9 | 0.21051 | 1.03518 | 1.00000 | | |
| O10 | 0.41313 | 1.06604 | 1.00000 | | |
| C11 | 0.53462 | 1.02030 | 1.00000 | | |
| C12 | 0.29588 | 1.03537 | 1.00000 | | |
| C13 | 0.23150 | 1.00000 | 1.00000 | | |
| C14 | 0.27439 | 1.00000 | 1.00000 | | |
| C15 | 0.35785 | 1.00000 | 1.00000 | | |
| N16 | 0.40026 | 1.00000 | 1.00000 | | |
| C17 | 0.50000 | 0.04236 | 0.00000 | | |

| Table S3. PPPP-2 eclipsed stacking | | | | | |
|------------------------------------|---------|----------|---------|--|--|
| Space group P_4/mmm | | | | | |
| a = 34.6223 Å | | | | | |
| c = 3.4820 Å | | | | | |
| Atom | x/a | y/b | z/c | | |
| C1 | 0.10044 | 0.00000 | 0.00000 | | |
| C2 | 0.14522 | 0.00000 | 0.00000 | | |
| C3 | 0.08006 | -0.03585 | 0.00000 | | |
| C4 | 0.47984 | 0.93023 | 0.00000 | | |
| C5 | 0.54070 | 0.03487 | 0.00000 | | |
| C6 | 0.58347 | 0.03461 | 0.00000 | | |
| 07 | 0.59990 | 0.06578 | 0.00000 | | |
| C8 | 0.66827 | 0.03461 | 0.00000 | | |
| N9 | 0.04104 | 0.95896 | 1.00000 | | |
| C10 | 0.07099 | 0.90147 | 1.00000 | | |
| C11 | 1/6 | 1.03439 | 1.00000 | | |
| C12 | 0.20734 | 1.03467 | 1.00000 | | |
| C13 | 0.29142 | 1.03476 | 1.00000 | | |
| C14 | 0.22801 | 1.00000 | 1.00000 | | |
| C15 | 0.27078 | 1.00000 | 1.00000 | | |
| C16 | 0.35314 | 1.00000 | 1.00000 | | |
| C17 | 0.47957 | 1.00000 | 1.00000 | | |
| N18 | 0.39574 | 1.00000 | 1.00000 | | |

| Table S4. PPPP-2 staggered stacking | | |
|--|--|--|
| Space group <i>I</i> ₄ / <i>mmm</i> | | |
| <i>a</i> = 34.6786 Å | | |
| c = 6.7106 Å | | |

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|------|---------|----------|---------|
| Atom | x/a | y/b | z/c |
| C1 | 0.10037 | 0.00000 | 0.00000 |
| C2 | 0.14510 | 0.00000 | 0.00000 |
| C3 | 0.08000 | -0.03583 | 0.00000 |
| C4 | 0.29118 | 0.96526 | 0.00000 |
| N5 | 0.04104 | 0.95896 | 1.00000 |
| C6 | 0.07093 | 0.90156 | 1.00000 |
| C7 | 1/6 | 1.03434 | 1.00000 |
| C8 | 0.20717 | 1.03462 | 1.00000 |
| 09 | 0.40053 | 1.06697 | 1.00000 |
| C10 | 0.66855 | 1.03462 | 1.00000 |
| C11 | 0.45937 | 1.03515 | 1.00000 |
| C12 | 0.41677 | 1.03577 | 1.00000 |
| C13 | 0.52006 | 1.06988 | 1.00000 |
| C14 | 0.22782 | 1.00000 | 1.00000 |
| C15 | 0.27056 | 1.00000 | 1.00000 |
| C16 | 0.35260 | 1.00000 | 1.00000 |
| C17 | 0.47952 | 1.00000 | 1.00000 |
| N18 | 0.39484 | 1.00000 | 1.00000 |