ELECTRONIC SUPPORTING INFORMATION (ESI)

Palladium Nanoparticle Embedded in Metal Organic Framework Derived Porous Carbon: Synthesis and Application for Efficient Suzuki-Miyaura Coupling Reaction

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Fig. S1 The nitrogen adsorption-desorption isotherms of Zn-free MOF-5-NPC-900.



Fig. S2 Element mappings images of Zn-free MOF-5-NPC-900-Pd.



Fig. S3 TEM (A) and HRTEM (B) images of the catalyst after 5 cycles.



Fig. S4 XPS image of the catalyst after 5 cycles.

NMR data of the obtained products:

Biphenyl: ¹H NMR (400 MHz, CDCl₃): δ = 7.64 (d, 4H, *J* = 7.32 Hz, ArH), δ = 7.49(t, 4H, *J* = 7.23 Hz, ArH), δ = 7.39 (d, 2H, *J* = 6.72 Hz, ArH).

4-Methoxybiphenyl: ¹HNMR (400 MHz, CDCl₃): δ = 7.57-7.51 (m, 4H, ArH), δ = 7.48 (t, 2H, *J* = 7.37 Hz, ArH), δ = 7.31 (t, 1H, *J* = 7.31 Hz, ArH), δ = 6.92 (d, 2H, *J* = 8.73 Hz, ArH), δ = 3.88 (s, 3H, -OCH₃).

4-Hydroxybiphenyl: ¹H NMR (400 MHz, CDCl₃): δ= 7.61 (d, 2H, *J* = 7.27 Hz, ArH), δ = 7.51 (d, 2H, *J* = 8.45 Hz, ArH), δ = 7.41 (t, 2H, *J* = 7.46 Hz, ArH), δ = 7.32 (t, 1H, *J* = 7.33 Hz, ArH), δ = 6.9 (d, 2H, *J* = 8.5 Hz, ArH), δ = 4.82 (s, 1H, -OH).

4-Hydroxy-2'-methylbiphenyl: ¹H NMR (400 MHz, CDCl₃): δ= 7.54 (d, 2H, *J* = 7.29 Hz, ArH), δ = 7.45 (d, 2H, *J* = 8.35 Hz, ArH), δ =7.35-7.29 (m, 4H, ArH), δ = 4.85 (s, 1H, -OH), δ = 2.58 (s, 3H, -CH₃).

2-Methylbiphenyl. ¹H NMR (400 MHz, CDCl₃): δ = 7.63 (d, 2H, *J* = 7.64 Hz, ArH), δ = 7.45-7.39 (m, 4H, ArH), δ = 7.35-7.29 (m, 2H, ArH), δ = 7.28 (d, 1H, *J* = 7.02 Hz, ArH), δ = 2.56 (s, 3H, - CH₃).

4'-Methyl-4-nitro-biphenyl: ¹H NMR (400 MHz, CDCl₃): $\delta = 8.28$ (d, J = 8.6 Hz, 2H, ArH), $\delta = 7.72$ (d, J = 8.6 Hz, 2H, ArH), $\delta = 7.53$ (d, J = 7.9 Hz, 2H, ArH), $\delta = 7.31$ (d, J = 7.8 Hz, 2H, ArH), $\delta = 2.43$ (s, 3H, -CH₃).

4-methoxy-4'-nitrobiphenyl: ¹H NMR (400 MHz, CDCl₃): δ = 7.04 (2H, d, *J* = 8.7 Hz, ArH), δ = 7.61 (2H, d, *J* = 8.8 Hz, ArH), δ = 7.72 (2H, d, *J* = 8.8 Hz, ArH), δ = 8.30 (2H, d, *J* = 8.7 Hz, ArH), δ = 3.90 (s, 3H, OCH₃).

1-(Biphenyl-4-yl)ethanone: ¹H NMR (400 MHz, CDCl₃): $\delta = 8.12$ (d, 2H, J = 8.19 Hz), $\delta = 7.62$ (d, 2H, J = 8.41 Hz, ArH), $\delta = 7.58$ (d,2H, J = 7.25 Hz, ArH), $\delta = 7.50-7.43$ (m, 2H, ArH), $\delta = 7.42-7.39$ (m, 1H), $\delta = 2.57$ (s, 3H, -CH₃).

4-Hydroxy-3'-methylbiphenyl: ¹H NMR (400 MHz, CDCl₃): δ= 7.56 (d, 2H, *J* = 7.26 Hz, ArH), δ = 7.48 (d, 2H, *J* = 8.31 Hz, ArH), δ =7.40 (s, 1H, ArH), δ =7.31-7.22 (m, 3H, ArH), δ = 4.83 (s, 1H, -OH), δ = 2.57 (s, 3H, -CH₃).

4-carbaldehydebiphenyl: ¹H NMR (400 MHz, CDCl₃): δ = 10.09 (s, 1H, -CHO), δ = 7.99 (d, *J*=8.0Hz, 2H, ArH), δ = 7.79 (d, *J*=8Hz, 2H, ArH), δ = 7.67 (d, *J*=7.2Hz, 2H, ArH), δ = 7.52 (t, *J*=6.8Hz, 2H, ArH), δ = 7.45 (t, *J*=7.2Hz, 1H, ArH).

4-carbaldehyde-4'-nitrobiphenyl: ¹H NMR (400 MHz, CDCl₃): δ = 10.15 (s, 1H, -CHO), δ = 8.45(d, *J* = 8.7Hz, 2H, ArH), δ = 8.24 (d, *J* = 8.7Hz, 2H, ArH), δ = 8.04 (d, *J* = 8.5Hz, 2H, ArH), δ = 7.78 (t, *J*=8.4Hz, 2H, ArH).

1-(4'-nitroBiphenyl-4-yl)ethanone: ¹H NMR (400 MHz, CDCl₃): $\delta = 8.15$ (d, 2H, J = 8.21 Hz), $\delta = 7.64$ (d, 2H, J = 8.43 Hz, ArH), $\delta = 7.75$ (t, J = 8.4Hz, 2H, ArH), $\delta = 7.55$ (d, 2H, J = 8.20 Hz, ArH), $\delta = 2.55$ (s, 3H, -CH₃).