Electronic Supplementary Information

Ni nanoparticles confined covalent organic polymer directed diaryl-selenides synthesis

Deepika Yadav^a, A.K. Dixit^b, S. Raghothama^c, Satish Kumar Awasthi^{*a}

^a*Chemical Biology Laboratory, Department of Chemistry, University of Delhi,

Delhi- 110007, India, E-mail: satishpna@gmail.com

^bVSSD College, Kanpur University, Kanpur, India.

^cNMR Research Centre, Indian Institute of Science, Bangalore-560012, India.

Table of Contents						
Materials and Instrumentation						
Figure S1. (a) EDX pattern and (b) TGA of Ni@CGP. (c) PXRD patterns of						
CGP after successive treatments in MeCN, DMSO, THF, NaOH, HCl, and H ₂ O for 2 days (d) XPS Complete survey spectrum of Ni@CGP						
Figure S2 (a) FTIR (b) PXRD (c) SEM and (d) TEM of reused Ni@CGP	S 3					
Figure S3. Recyclability graph of Ni@CGP	S3					
Table S1. Reusability of Ni@CGP.	S4					
¹ H and ¹³ C NMR chemical shifts for compounds 1-14.	S4-S5					
¹ H and ¹³ C NMR spectra of compounds 1-14.	S6-S19					

Materials All the reagents, starting materials and organic substrates for hydrogenation were purchased from Sigma-Aldrich USA /Spectrochem Pvt. Ltd. India and used as picked up. Double distilled water was used from USIC, University of Delhi by a Milli-Q pore water purification system.

Instrumentation IR experiments were carried out in the range of 400-4000 cm⁻¹ (Thermo Scientific; Model: INCOLET iS50) spectrometer. PXRD experiments were performed using D8 DISCOVER X-ray diffractometer. N₂ adsorption-desorption isotherm and Pore size distribution was measured by Quantachrome Instruments; Model: ASI-CT-11. Thermo Gravimetric Analysis dataset was obtained through Perkin Elmer, Model: TG/DTA. UV/VIS and UV-DRS experiments were performed using Schimadzu instrument, Model: UV-2600. X-Ray photoelectron spectroscopy (XPS) results were obtained using OMICRON Multi probe Surface Analysis System in UHV. TEM images were obtained using FEI, Germany equipped with digital imaging and Field Emission Scanning Electron Microscope (FESEM) Model: ZEISS Gemini SEM-500 were used to study the sur-face morphological pattern of Pd@CCTP. ¹³C CP-MAS, ¹H and ¹³C NMR data was obtained through JEOLECX400 spectrophotometer.



Figure S1. (a) EDX pattern and (b) TGA of Ni@CGP, (c) PXRD patterns of CCTP after successive treatments in MeCN, DMSO, THF, NaOH, HCl, and H₂O for 2 days, (d) XPS Complete survey spectrum of Ni@CGP.



Figure S2. (a) FTIR spectrum, (b) PXRD pattern, (c) SEM and (d) TEM micrographs of reused Ni@CGP.



Figure S3. Recyclability graph of Ni@CGP.

Table S1. Reusability of Ni@CGP.

Runs	1	2	3	4	5	6	7	8	9	
Yield %	90	90	89	88	88	87	86	85	85	
^a Reaction conditions: Iodobenzene (2 mmol), K ₂ CO ₃ (1.5 eq), Se Powder (1 mmol)										
Ni@CGP (10 mg, 1.23 mol% Ni), DMSO: H ₂ O [1:1, (2.5 mL)].										

¹H and ¹³C NMR chemical shifts for 1-14.

¹H-NMR (400 MHz, CDCl₃-d) δ 7.73 (d, J = 8.2 Hz, 4H), 7.33-7.37 (m, 2H), 7.12 (t, J = 7.8 Hz, 4H)

¹³C-NMR (101 MHz, CDCl₃-*d*) δ 137.60, 130.39, 127.60

HRMS-ESI: calculated: 233.9902, Observed [M+H]: 234.8992.

2) ¹H-NMR (400 MHz, CDCl₃-d) δ 7.38 (d, J = 8.4 Hz, 4H), 7.05 (d, J = 8.0 Hz, 4H), 2.31 (s, 6H)

¹³C-NMR (101 MHz, CDCl₃-*d*) δ 136.87, 131.33, 130.92, 119.15, 21.03

HRMS-ESI: calculated: 262.0262, Observed [M+H]: 263.0992.

3) ¹H-NMR (400 MHz, CDCl₃-d) δ 7.23 (d, J = 8.8 Hz, 4H), 6.55 (d, J = 8.7 Hz, 4H), 3.61 (s, 4H)

¹³C-NMR (101 MHz, CDCl₃-*d*) δ 145.58, 131.83, 116.86, 110.23

HRMS-ESI: calculated: 264.0166, Observed [M+H]: 265.1227.

- 4) ¹H-NMR (400 MHz, CDCl₃-d) δ 7.57 (d, J = 8.7 Hz, 4H), 7.42 (d, J = 8.7 Hz, 4H)
 ¹³C-NMR (101 MHz, CDCl₃-d) δ 138.40, 132.80, 118.12, 111.57, 100.10
 HRMS-ESI: calculated: 283.9853, Observed [M+H]: 284.9902.
- **5)** ¹**H**-NMR (400 MHz, CDCl₃-*d*) δ 7.35 (d, J = 8.5 Hz, 4H), 7.13 (d, J = 8.5 Hz, 4H), 3.45 (s, 2H)

¹³C-NMR (101 MHz, CDCl₃-*d*) δ 132.19, 131.06, 130.04, 119.54

HRMS-ESI: calculated: 297.9489, Observed [M+H]: 298.9120.

6) ¹H-NMR (400 MHz, CDCl₃-d) δ 9.86 (s, 2H), 7.63 (dd, J = 6.9, 1.8 Hz, 4H), 7.56 (dd, J = 6.9, 1.8 Hz, 4H)
¹³C-NMR (101 MHz, CDCl₃-d) δ 191.22, 135.36, 132.51, 131.07, 129.87

HRMS-ESI: calculated: 289.9846, Observed [M+H]: 290.9753.

¹H-NMR (400 MHz, CDCl₃-*d*) δ 7.76 (d, J = 8.5 Hz, 4H), 6.60 (d, J = 8.5 Hz, 4H), 2.46 (s, 6H)
¹³C-NMR (101 MHz, CDCl₃-*d*) δ 196.84, 151.30, 130.91, 127.67, 113.43, 26.19

HRMS-ESI: calculated: 318.0159, Observed [M+H]: 318.9702.

- 8) ¹H-NMR (400 MHz, CDCl₃-d) δ 7.92 (ddd, J = 7.3, 1.8, 1.2 Hz, 2n), 7.59-7.67 (m, 4n), 2.64 (d, J = 1.8 Hz, 6n)
 ¹³C-NMR (101 MHz, CDCl₃-d) δ 198.60, 154.29, 141.05, 138.63, 131.86, 120.54, 25.82 HRMS-ESI: calculated: 320.0064, Observed [M+H]: 321.0023.
- 9) ¹H-NMR (400 MHz, CDCl₃-d) δ 8.32 (d, J = 8.5 Hz, 2H), 7.81-7.87 (m, 6H), 7.64 (t, J = 7.1 Hz, 2H), 7.55-7.58 (m, 2H), 7.33 (t, J = 7.8 Hz, 2H)
 ¹³C-NMR (101 MHz, CDCl₃-d) δ 134.80, 132.16, 130.09, 128.51, 128.14, 127.53, 127.26, 126.89, 126.36, 123.04
 HRMS-ESI: calculated: 334.0261, Observed [M+H]: 335.0115.
- 10) ¹H-NMR (400 MHz, CDCl₃-*d*) δ 10.03 (s, 2H), 8.54 (d, J = 8.2 Hz, 2H), 7.93 (d, J = 7.1 Hz, 4H), 7.49-7.59 (m, 8H), 7.36 (t, J = 8.5 Hz, 2H), 6.98-7.02 (t, 2H)
 ¹³C-NMR (101 MHz, CDCl₃-*d*) δ 164.99, 135.89, 134.63, 132.32, 129.06, 128.63, 127.22, 125.42, 121.94

HRMS-ESI: calculated: 472.0690, Observed [M+H]: 473.0226.

11) ¹H-NMR (400 MHz, CDCl₃-d) δ 7.46 (d, J = 10.6 Hz, 2H), 7.14 (d, J = 6.9 Hz, 2H), 6.71 (d, J = 33.5 Hz, 4H), 4.11 (s, 4H)

¹³C-NMR (101 MHz, CDCl₃-*d*) δ 146.54, 134.83, 130.71, 121.64, 118.00

HRMS-ESI: calculated: 264.0166, Observed [M+H]: 265.0021.

- 12) ¹H-NMR (400 MHz, CDCl₃-*d*) δ 7.95-7.89 (m, 8H)
 ¹³C-NMR (101 MHz, CDCl₃-*d*) δ 148.63, 135.91, 131.85, 120.53
 HRMS-ESI: calculated: 323.9649, Observed [M+H]: 324.9018.
- 13) ¹H-NMR (400 MHz, CDCl₃-d) δ 9.84 (s, 2H), 7.78 (s, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.18 (d, J = 8.1 Hz, 2H), 7.12 (t, J = 8.0 Hz, 2H), 2.14 (s, 6H)
 ¹³C-NMR (101 MHz, CDCl₃-d) δ 169.13, 130.29, 126.95, 122.53, 118.07, 40.73 HRMS-ESI: calculated: 348.0377, Observed [M+H]: 348.9902.
- 14) ¹H-NMR (400 MHz, DMSO-*d*₆) δ 12.37 (s, 1H), 7.69-7.73 (m, 2H), 7.55 (d, J = 16.1 Hz, 1H), 7.19 (t, J = 8.9 Hz, 2H), 6.45 (d, J = 15.9 Hz, 1H)

¹³C-NMR (101 MHz, DMSO-*d*₆) δ 168.07, 162.59, 143.22, 131.42, 131.05, 116.48,

116.27

HRMS-ESI: calculated: 374.0057, Observed [M+H]: 374.9983.

¹H and ¹³C NMR spectra.













































