# **Electronic Supplementary Information (ESI)**

# Hydrogenation of cinnamaldehyde to hydrocinnamaldehyde over Pd nanoparticles deposited on nitrogen-doped mesoporous carbon

Atul S. Nagpure, Lakshmiprasad Gurrala, Pranjal Gogoi and Satyanarayana V. Chilukuri\*

Catalysis & Inorganic Chemistry Division, CSIR-National Chemical Laboratory, Dr. Homi Bhabha Road, Pune-411008, India, Tel.: +91-20-25902019; Fax: +91-20-25902633. E-mail: sv.chilukuri@ncl.res.in

#### **1. Experimental section:**

### 1.1. Characterization techniques

XRD patterns of the samples were obtained using a PANalytical X'pert Pro dual goniometer. Nickel filtered Cu K $\alpha$  radiation ( $\lambda = 1.5406$  Å, 40 kV, 30 mA) was used and the data was collected using a flat holder in Bragg–Brentano geometry. The data were recorded in the 20 range of 5–90° (with 0.02° step size). The BET surface area of the samples was examined by using N<sub>2</sub> sorption isotherm at -196 °C (Quantachrome Autosorb IQ). The samples were evacuated at 250 °C for 3 h at a residual pressure of 2 x 10<sup>-3</sup> Torr prior to N<sub>2</sub> sorption analysis. Raman spectra of all the samples were collected using LabRAM HR800 (Jobin Yvon Horiba, France) with laser wavelength of 632.84 nm (He-Ne Laser, 20 mW of power) and 2 µm spot size. TEM images were obtained using a FEI Technai TF-30 instrument operating at 300 kV. The samples for TEM analysis were prepared by placing a droplet of the sample suspension prepared in 2-propanol using ultrasonication on a carbon coated copper grid and by leaving them for drying at room temperature. XPS analysis of the materials were performed using a VG Microtech Multilab ESCA 3000 with Mg Ka radiation (hv = 1253.6 eV). The base pressure in analyzing chamber was maintained at 3-6 x 10<sup>-10</sup> mbar. The peak related to carbon 1s (at 284.5 eV) was taken as reference in calculating the binding energy values of different elements in the catalyst. FT-IR analysis of the samples was performed using a Bruker Optic (TENSOR-27). All samples were mixed with KBr and determined in the 500-4000 cm<sup>-1</sup> range. The amount of Pd present in the samples was estimated by ICP-OES (Spectro Arcos, FHS-12).



Scheme S1 Schematic illustration of NMC synthesis.



Scheme S2 Synthesis of Pd-NMC catalyst by modified ultrasonic-assisted method.



Fig. S1 XRD patterns of the fresh and spent Pd-NMC catalyst.



**Fig. S2** TEM images and the Pd nanoparticles size distribution for fresh Pd-NMC (a and b) and reused Pd-NMC after 6 cycles (c and d), respectively.

Table S1 Elemental analysis results of MC and NMC						
Sample	Elemental analysis (wt%)					
	С	Ν	Н	O (cal.)		
МС	86.3	0	1.3	12.4		
NMC	73.0	11.6	0.7	14.7		

## 2. Calculation of Pd dispersion (%) using average Pd particle size:

The average particle size of Pd nanoparticles in Pd-NMC, Pd-AC and Pd-MC catalysts were used to calculate dispersion (%) of Pd assuming spherical shape of particles and using the formula described by Isaifan et al.<sup>[1]</sup>

Dispersion (%) = 
$$(600 \cdot M_{Pd}) / (\rho \cdot d_{nm} \cdot a_{pd} \cdot N_a)$$
 ----- (1)

Where  $M_{Pd}$  is the molecular weight of Pd (106.42 g/mol),  $a_{pd}$  is the atomic surface area of Pd (6.8×10<sup>-20</sup> m<sup>2</sup>/atom),  $\rho$  is the metal density (12.023 g/cm<sup>3</sup> of Pd),  $N_a$  is Avogadro's number and  $d_{nm}$  is the average metal particle diameter estimated from TEM in nanometers.

Table S2 Physico-chemical characteristics of catalysts					
Catalyst	Pd content <sup>[a]</sup> (wt%)	Average Pd particle size <sup>[b]</sup> (nm)	Pd metal dispersion <sup>[c]</sup> (%)		
Pd-NMC	2.05	2.4	54.0		
Pd-MC	1.97	7.7	16.8		
Pd-AC	1.94	4.6	28.2		
[a] Determined by ICP-OES. [b] Calculated based on TEM analysis. [c] Estimated on the basis of average Pd particle size using TEM analysis and using equation 1.					

#### **References:**

[1] R. J. Isaifan, H. A. E. Dole, E. Obeid, L. Lizarrag, P. Vernoux and E. A. Baranova, *Electrochem. Solid-State Lett.*, 2012, 15 (3) E14-E17.