

Supplementary Materials: The effect of carbon nanofibers surface properties in hydrogenation and dehydrogenation reactions

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1. Supplementary Information

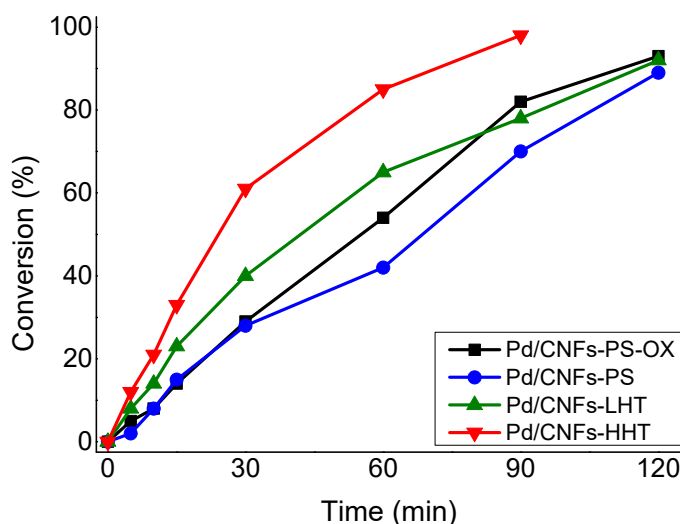


Figure S1. Time on line conversion of the four catalysts in the cinnamaldehyde hydrogenation reaction.

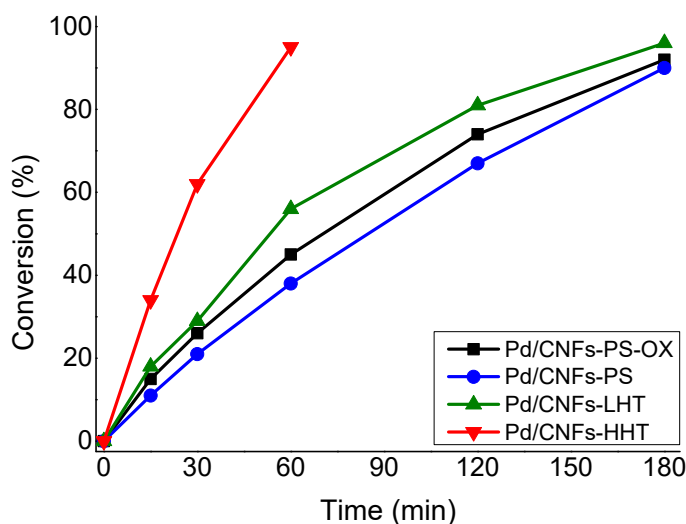


Figure S2. Time on line conversion of the four catalysts in the cinnamyl alcohol dehydrogenation reaction.

2. Calculation of the number of surface exposed atoms

Pd surface atoms abundance was calculated assuming that all nanoparticles had cubo-octahedral morphology with cubic close-packed structure in this size range; the model of full-shell nanoparticles was adopted [1]. The total number of Pd atoms in the cluster for a given cluster size was calculated following Equation (1),

$$d_{NPS} = 1.105 d_{Pd} N_T^{1/3} \quad (1)$$

where d_{NPS} is the mean diameter of the Pd particles obtained from TEM analysis and d_{Pd} is the atom diameter of Pd, 0.262 nm. The number of surface atoms (N_S) and n can be calculated from equations (2) and (3), based on the values of N_T :

$$N_T = \frac{10n^3 - 15n^2 + 11n - 3}{3} \quad (2)$$

$$N_S = 10n^2 - 20n + 12 \quad (3)$$

Finally, the Pd surface atoms abundance (Pd_{SURF}) that represent the fraction of atoms lying on the surface was calculated following the Equation (4):

$$Pd_{SURF} = \frac{N_S}{N_T} 100 \quad (4)$$

3. Calculation of the Turnover Frequency

Turnover frequency (TOF) values were calculated based on the total Pd content (TOF_{TOT}) and on the surface atoms only (TOF_{SURF}). In particular, TOF_{TOT} was calculated following the Equation (5):

$$TOF_{TOT} = \frac{mol_{Sub}}{mol_{Pd} t} \quad (5)$$

Where mol_{Sub} is the moles of substrate converted after a set time “ t ”, and mol_{Pd} are the moles of Pd in the catalyst. The TOF_{SURF} , on the other hand, was calculated based on the fraction of atoms lying at the surface (Pd_{SURF}):

$$TOF_{SURF} = \frac{TOF_{TOT}}{Pd_{SURF}} 100 \quad (6)$$

References

1. K. Mori, T. Hara, T. Mizugaki, K. Ebitani, K. Kaneda, Hydroxyapatite-Supported Palladium Nanoclusters: A Highly Active Heterogeneous Catalyst for Selective Oxidation of Alcohols by Use of Molecular Oxygen, *J. Am. Chem. Soc.* **2004**, *126*, 10657–10666.