# Pd doped Ni nanoparticles modified N-doped carbon nanocatalyst with high Pd atom utilization for transfer hydrogenation of nitroarenes

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#### **Preparation of mCN**

Firstly, 2.12 g PAN was added to 50 mL DMF at 100°C and vigorously stirred for 30min. Secondly, 30 g melamine was added to the above solution, and continues to stir for another 1h to obtain a thick slurry. Then, the obtained thick slurry was dried in the oven overnight at 120°C and ground into powder. Finally, the powder was pyrolyzed at 900°C for 1h by programmed heating in a nitrogen atmosphere at 5°C/min in a tubular furnace. Thus the mCN was prepared.

## **Preparation of Pd/mCN**

50 mg of mCN was dispersed in 100 mL of deionized water by ultrasonic dispersion. Then, 0.4 mL Pd(AcO)<sub>2</sub> solution (contains 2 mg Pd<sup>2+</sup>) was added to the mCN dispersion mixture. Then, the solution was evaporated and dried in the oven overnight. The obtained Pd<sup>2+</sup>/mCN was reduced at 350°C for 2h in a nitrogen/hydrogen ( $V_{N2}$ : $V_{H2}$ =9:1) atmosphere in a tubular furnace.

### **Preparation of Ni/AC**

450 mg of AC was dispersed in 100 mL of deionized water by ultrasonic dispersion. Then, 280mg  $(Ni(NO_3)_2 \cdot 6H_2O)$  was added to the AC dispersion mixture. Then, the solution was evaporated and dried in the oven overnight. The obtained Ni<sup>2+</sup>/AC was reduced at 350°C for 2h in a nitrogen/hydrogen  $(V_{N2}:V_{H2}=9:1)$  atmosphere in a tubular furnace.

#### Preparation of NiPd/AC

The PdNi/AC nanocatalyst was prepared according to the same spontaneous reduction preparation process of PdNi/mCN.



**Fig. S1.** The TEM images of Ni/mCN with different pyrolysis temperatures (a) 600°C, (b) 700°C, (c) 800°C and (d) 900°C.



Fig. S2. The (a) Fe 2p spectrum (Fe/mCN), (b) Co 2p spectrum (Co/mCN).



Fig. S3. The EDS spectrum of PdNi/mCN nanocatalysts.



Fig. S4. High resolution XPS spectroscopy of C 1s in different nanocatalysts.



Fig. S5. The curve of the conversion over different times.



**Fig. S6.** The TEM images of (a) Pd/AC, (c) PdNi/AC, (e) Pd/mCN nanocayalysts, and the corresponding NPs size distribution of Pd/AC (b), PdNi/AC (d), Pd/mCN nanocayalysts (f).



**Fig. S7.** The TEM image (a), VSM curve (b), BET isotherm (c) and XRD pattern (d) of the used PdNi/mCN nanocatalyst.