Electronic Supplementary Material (ESI) for RSC Advances
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Supplementary Material (ESI) for

Electroless reductions on carbon nanotubes: how critical is the diameter of a nanotube

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1. Experimental and theoretical sections

1. 1. Synthesis of K_2PdCl_4 by mixing $PdCl_2$ and KCl

5mg $PdCl_2$ and 10 mg KCl were added into a vial with 5 ml deionized water, followed by the stirring. 10 hours later, a clearly yellow solution was acquired and no precipitate was found on the bottom of vial. Ultra Violet-Visible Spectrophotometer was used to identify if K_2PdCl_4 was formed since it had a specific UV absorption at 207 nm.

1. 2. Synthesis of Pd/CFCNT5 and Pd/CFCNT15 composites

The commercial CFCNT5 and CFCNT15 samples were characterized with Fourier-transform infrared (FTIR) spectra, transmission electron microscopy (TEM), Raman spectrometer (Horiba Jobin Yvon/Labram Aramis), cyclic voltammetry (CV) method and inductively-coupled plasmaspectrometer (ICP).

10 mg commercial CFCNT5 was added into the as-synthesized K_2PdCl_4 solution (5 ml), followed by stirring at room temperature for 1 hour. For exploring the time effect on the size of Pd on CFCNT5, another reaction was performed with the same strategy except for that the reaction time was 24 hours. The synthesized Pd/CFCNT5 composites were characterized by TEM, Raman and ICP. The Pd/CFCNT15 composites were synthesized with the same way.

1.3. Computational method

B3LYP/STO-3G method in Gaussian 09 program was used to investigate the charge distribution on the surfaces of carbon nanotube and the acid-treated carbon nanotube. Since the reaction proceeded in water, solvent effect had been considered in all optimizations by using PCM model with water as solvent. For simplicity, single-walled carbon nanotube models with different diameters were constructed to simulate the structures of CNT5, CNT15, CFCNT5 and CFCNT15. The unsaturated carbon atoms at the edge of carbon nanotube were saturated with H atoms.

These complex structures were drawn with Gview program based on the optimized results.

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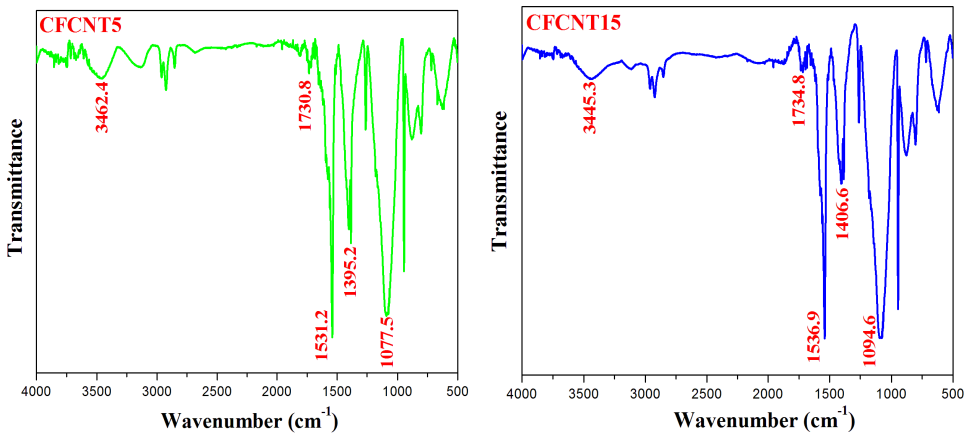

Fig. S1 FTIR spectras of CFCNT5 and CFCNT15 samples.

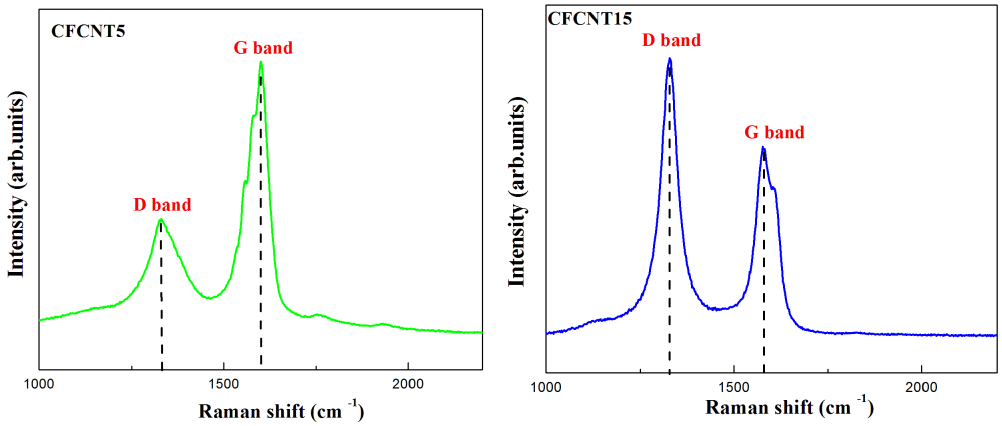

Fig. S2 Raman spectras of CFCNT5 and CFCNT15 samples.

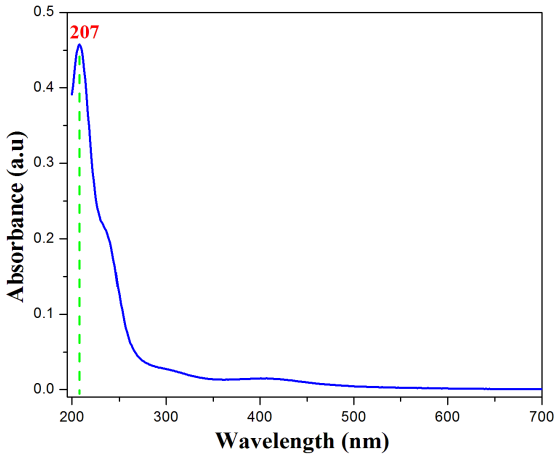

Fig. S3 UV spectra of the as-synthesized K_2PdCl_4.

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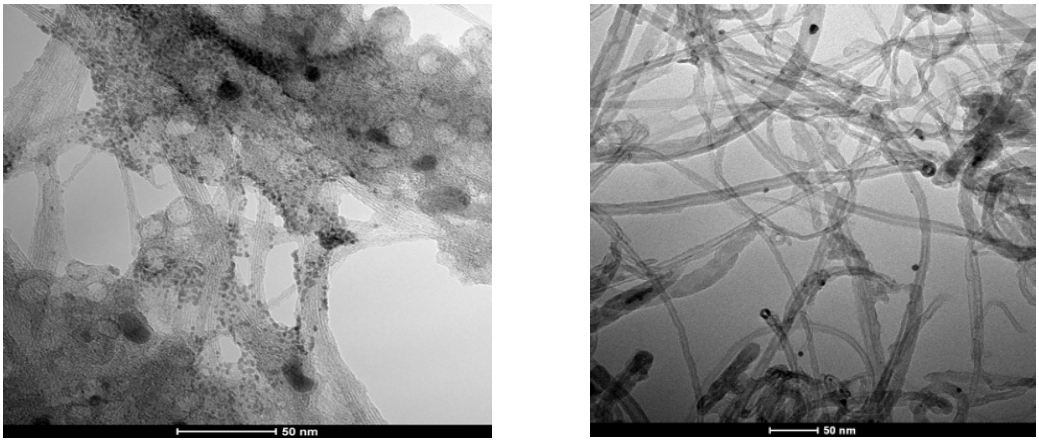

Fig. S4 TEM images of Pd/CFCNT5 (left) and Pd/CFCNT15 (right) produced with the reaction time of 1 hour. The Pd particle in Pd/CFCNT5 is more than that in Pd/CFCNT15.

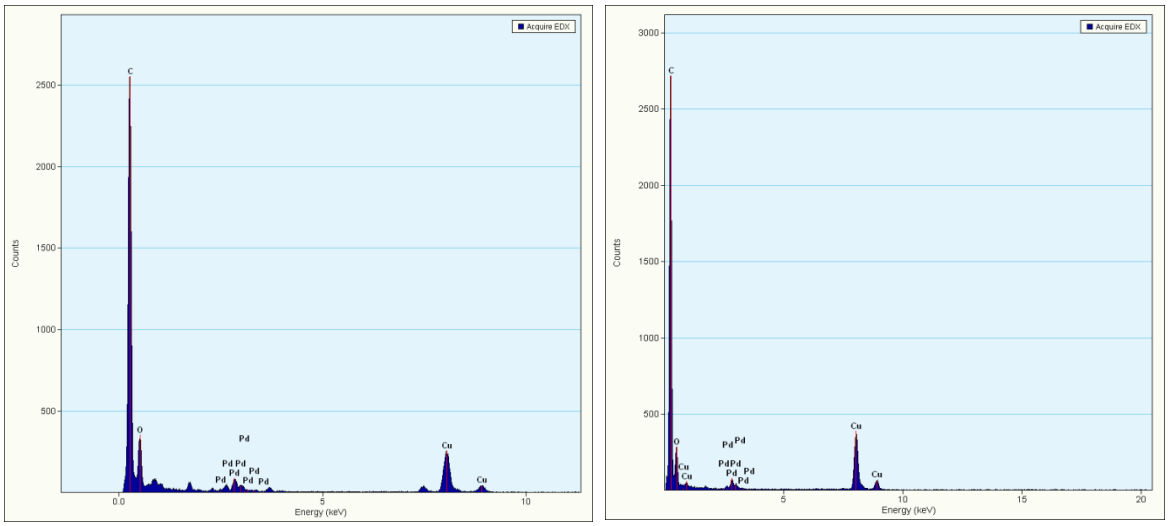

Fig. S5 EDX of Pd/CFCNT5 (left) and Pd/CFCNT15 (right) produced with the reaction time of 24 hours.

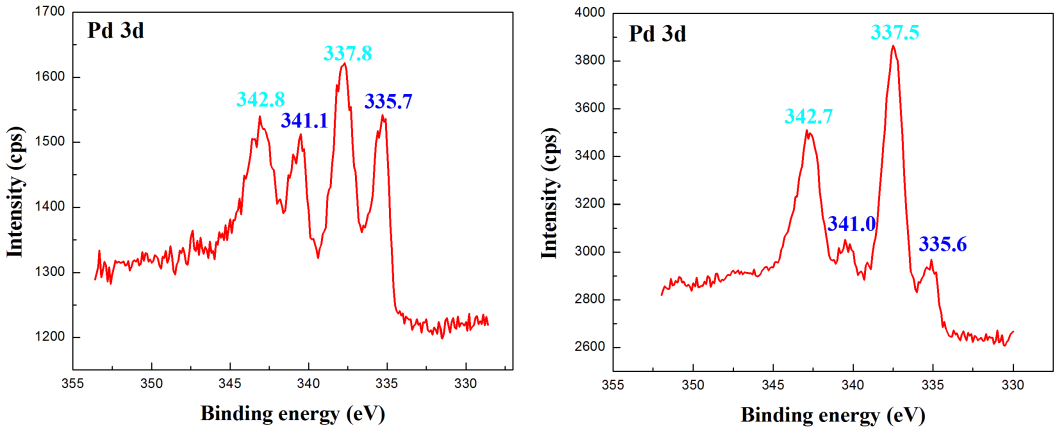

Fig.S6 XPS spectras of Pd/CFCNT5 (left) and Pd/CFCNT15 (right).

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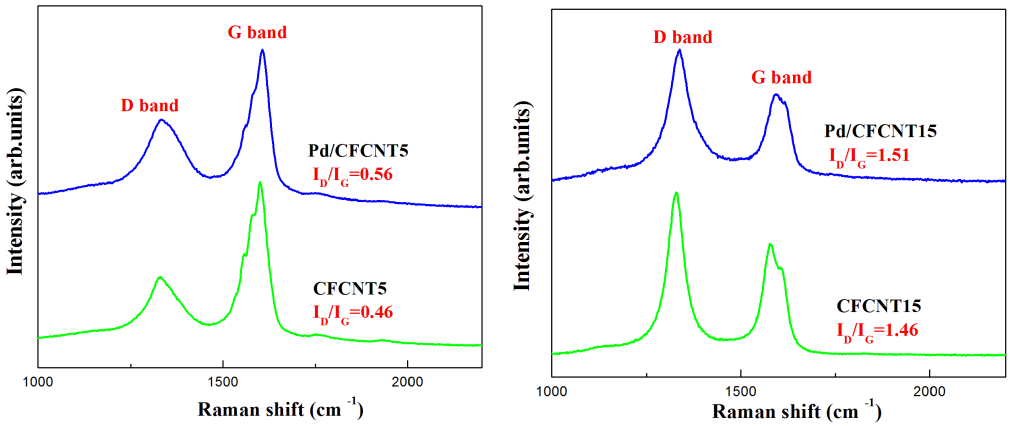

Fig. S7 Raman spectras of CFCNT5, Pd/CFCNT5, CNFCNT15 and Pd/CFCNT15.

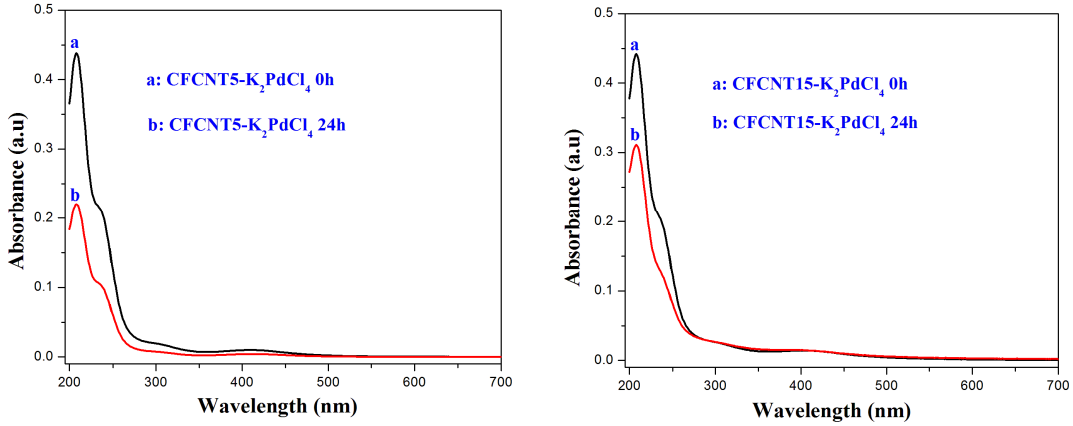

Fig.S8 UV spectras of the K_2PdCl_4 before and after the addition of CFCNT5 and CFCNT15.

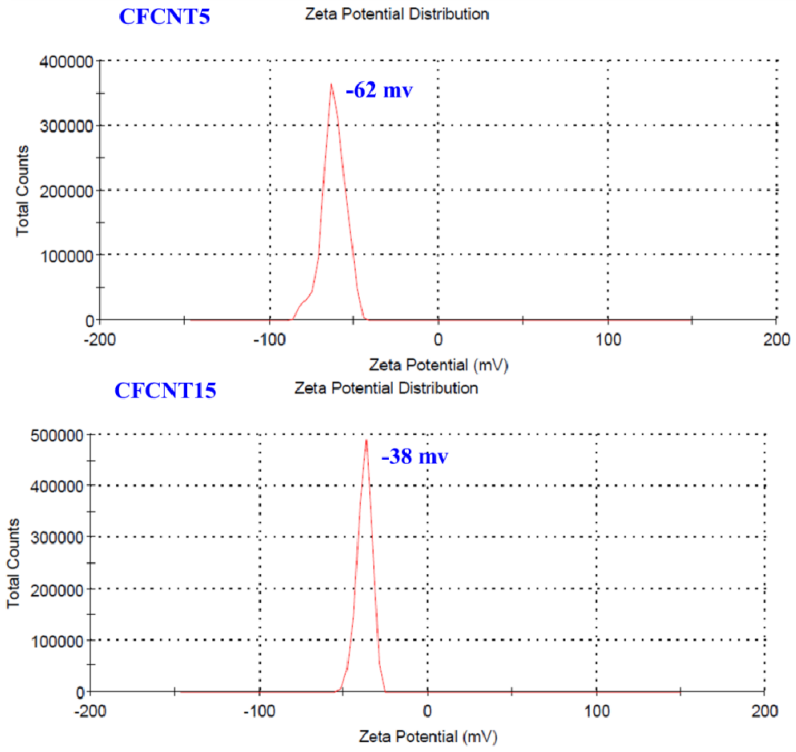

Fig.S9 Zeta potential results of CFCNT5 (up) and CFCNT15 (down) materials.

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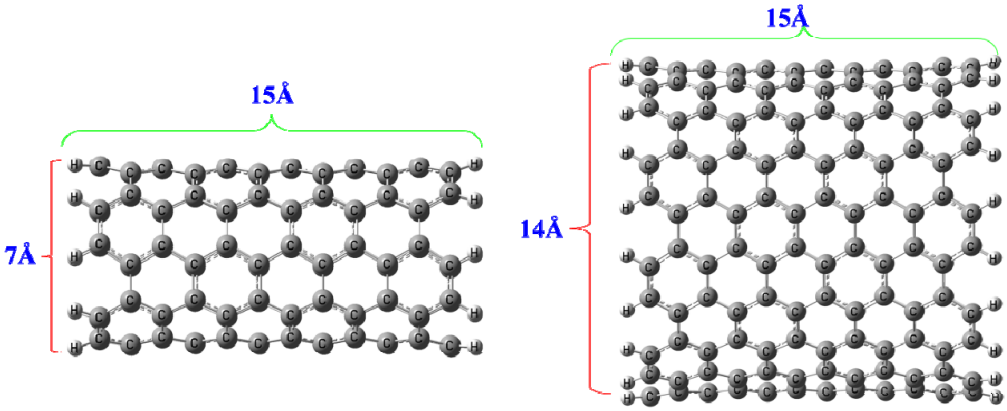

Fig.S10 The optimized CNT5 and CNT15 models.

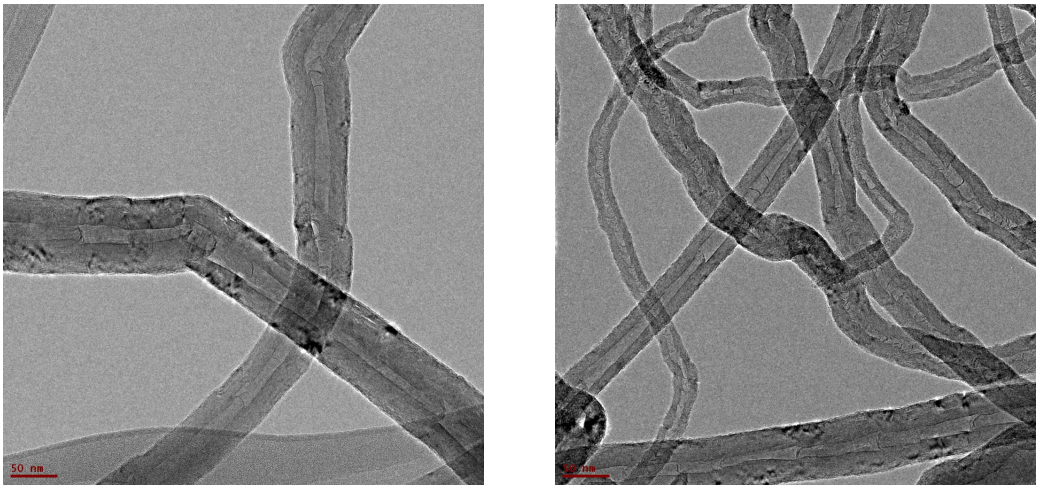

Fig. S11 TEM images of Pd/CFCNT50 (left) and Pd/CFCNT50 (right) produced with the reaction time of 24 hour.

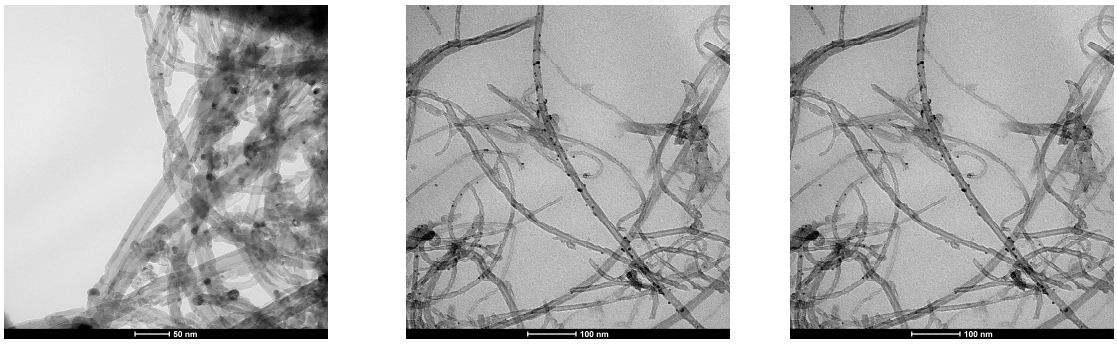

Fig. S12 TEM images of Pd/CFCNT15 at different locations of the same sample. Picture 1 also confirms the formation of CNT bundles in CFCNT15.