Electronic Supplementary Information For

Covalently functionalized carbon nanotubes supported Pd nanoparticles for catalytic reduction of 4-nitrophenol

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Table S1 The XPS data summary of different samples.

Sample	O (at. %)	O1 (C=O) (at. %)	O2 (O=C-O) (at. %)	O3 (C-OH) (at. %)	C2 (C-OH)/%[b]
NF-CNT	0.77	0.16	0.22	0.38 (49.8%)[a]	10.1
CNT-160	2.36	0.33	0.72	1.31 (55.6%)[a]	11.6
CNT-200	5.11	0.50	1.32	3.29 (64.5%)[a]	14.9
CNT-220	5.36	0.45	1.24	3.68 (68.6%)[a]	15.3

a. the percentage is relative intensity of C-OH groups from O1s core level spectra of different samples; b the percentage is relative intensity of C-OH groups from C1s core level spectra of different;

Table S2 Sample denotations and comparison of the fit parameters from the peaks fitted in the Raman spectra of CNT samples.

Sample	Description	Position [cm^{-1}]	Area (a.u.)	FWHM [cm^{-1}]	I_D/I_G
NF-CNT	D	1318.7	14.1	27.8	2.61
	G	1569.4	5.4	22.6	
	D’	1600.7	2.7	16.6	
	D3	1504.1	0.9	59.0	
CNT-160	D	1319.1	13.5	29	2.55
	G	1570	5.3	24.1	
	D’	1601.2	2.6	16.8	
	D3	1502.6	1.1	60.3	
CNT-200	D	1320.3	14.1	27.7	2.43
	G	1571.4	5.8	24.3	
	D’	1602.1	2.5	16	
	D3	1483.2	1.4	69.5	
CNT-220	D	1323.2	13.9	29.3	2.39
	G	1573.4	5.8	24.6	
	D’	1604.8	2.7	16.9	
	D3	1497.9	2.0	69.5	

Table S3 Summary of XPS Pd 3d core level of different composites.

Sample		$3d_{5/2}$ /eV	$3d_{3/2}$ /eV	Pd^0 /%	Pd^{2+} /%
Pd NPs/NF-CNT	Pd^0	335.7	341	86.9	13.1
	Pd^{2+}	337.8	343		
Pd NPs/O-CNT	Pd^0	336	341.3	83.4	16.6
	Pd^{2+}	337.7	342.9		
Pd NPs/CNT-220[a]	Pd^0	335.8	341.1	81.3	18.7
	Pd^{2+}	338.2	343.4		
Pd NPs/CNT-220[b]	Pd^0	335.9	341.2	84.2	15.8
	Pd^{2+}	338	343.2		

a. this sample used before catalytic reaction; b this sample used after catalytic reaction.

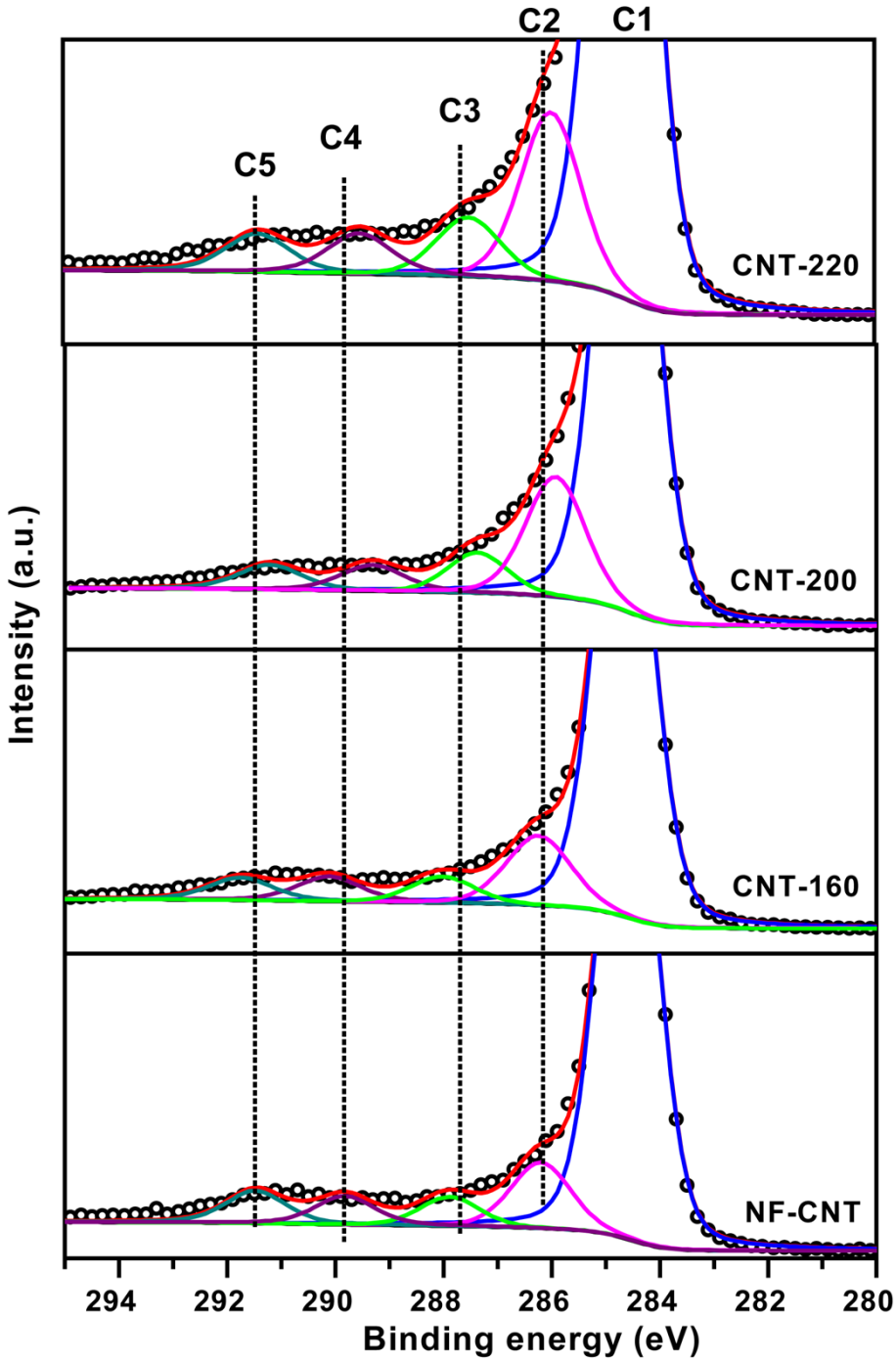

Figure S1 The curve fitted C1s XPS of NF-CNT, CNT-160, CNT-200 and CNT-220. To visualize the component and shakeup peaks, component peaks C1 are shown as cut-out.

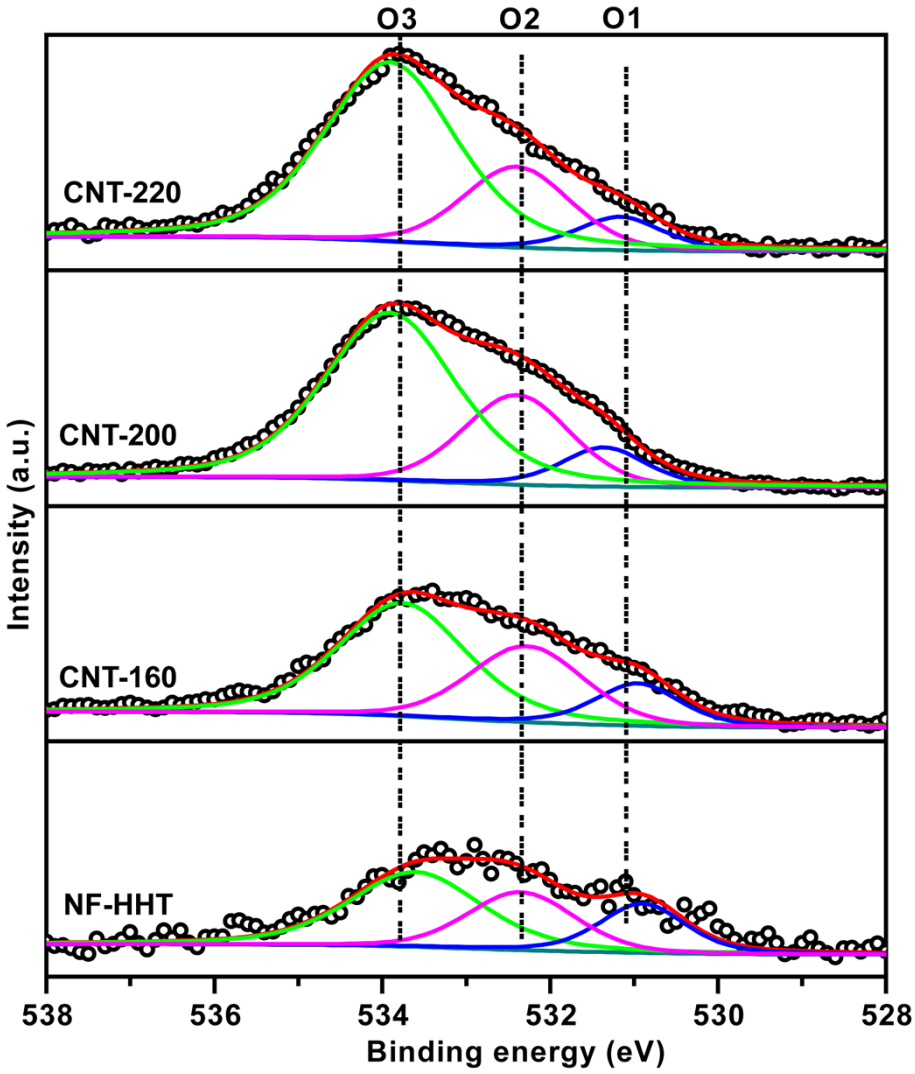

Figure S2 T The curve fitted O1s XPS of NF-CNT, CNT-160, CNT-200 and CNT-220.

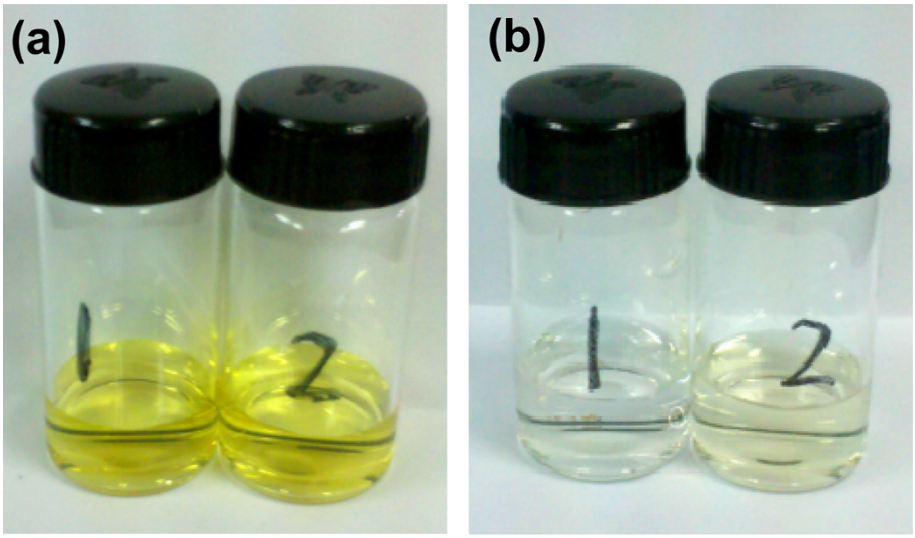

Figure S3 Photograph of solution color Pd NPs supported CNTs before (a) and after (b); CNT-220 was added in the **bottle 1** and NF-CNT was added in the **bottle 2**.

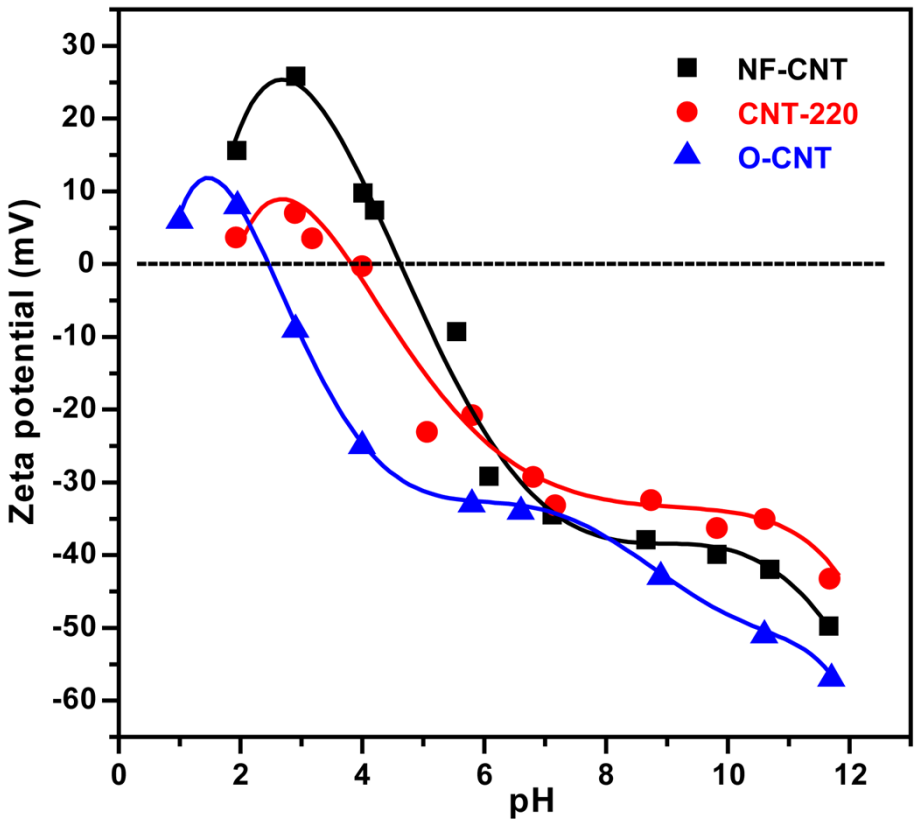

Figure S4 The Zeta potential for NF-CNT, CNT-220 and O-CNT as function of pH.

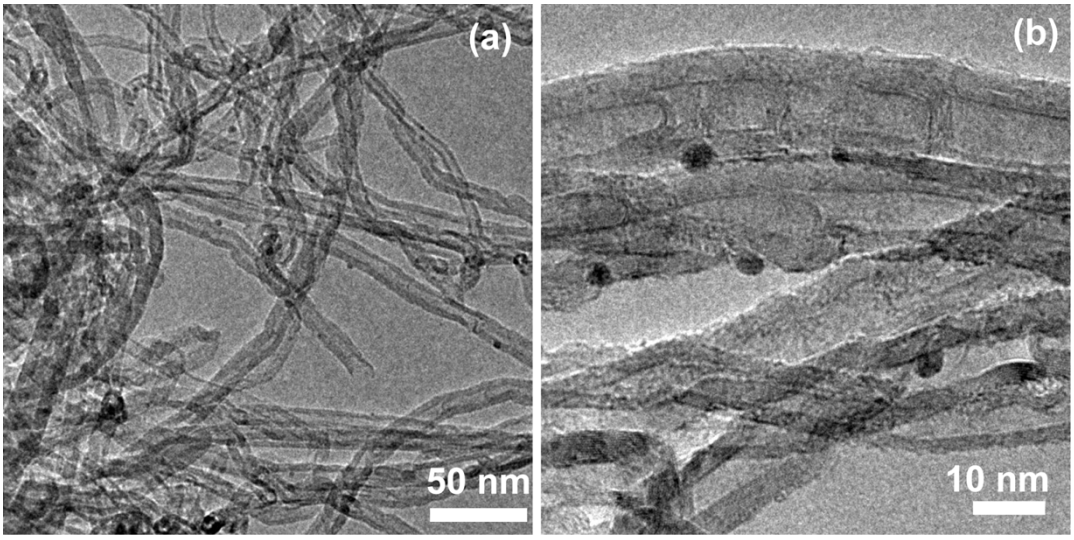

Figure S5 The TEM images of Pd NPs/O-CNT composites.

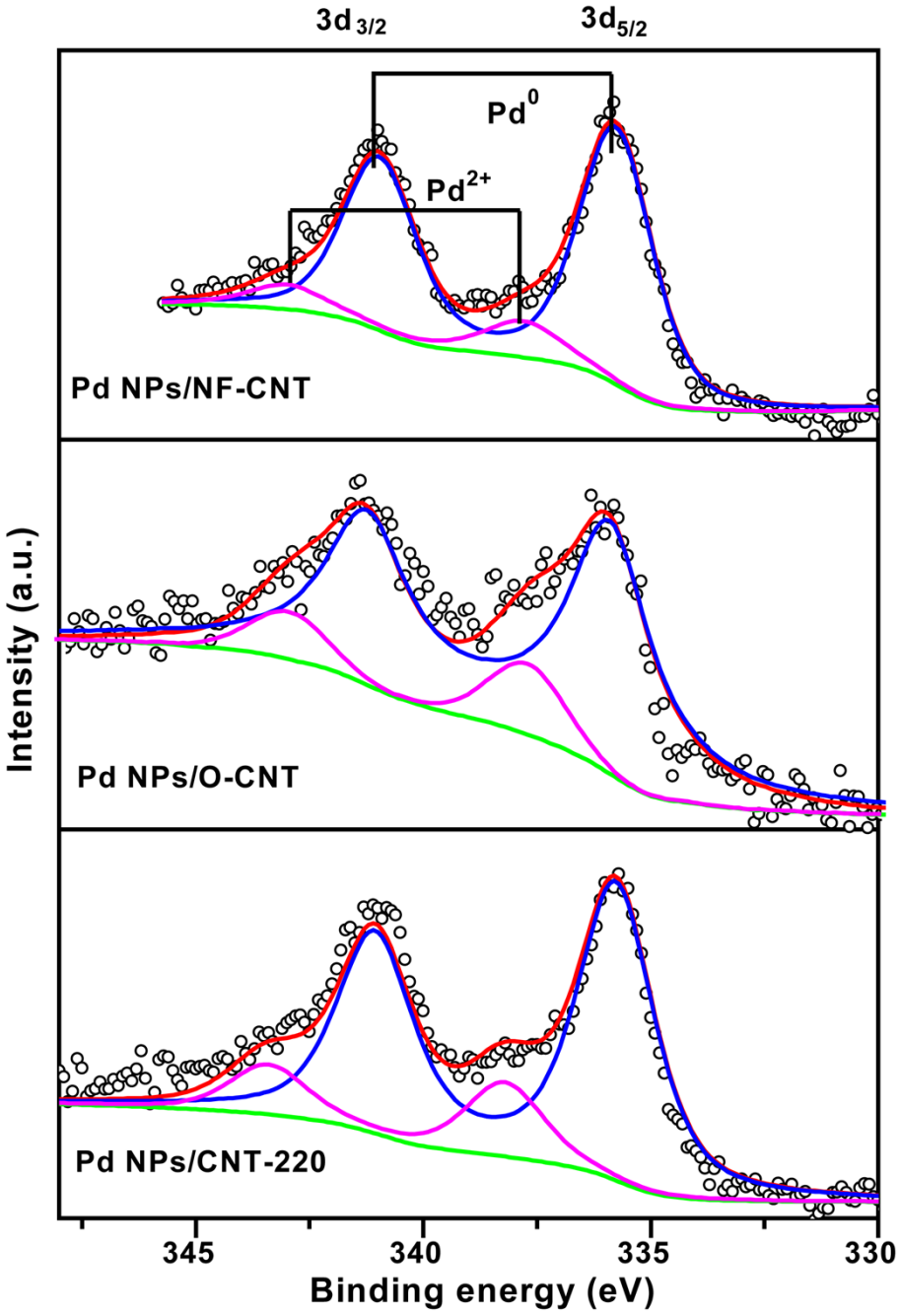

Figure S6 The curve fitted Pd3d XPS of different nanocomposites.

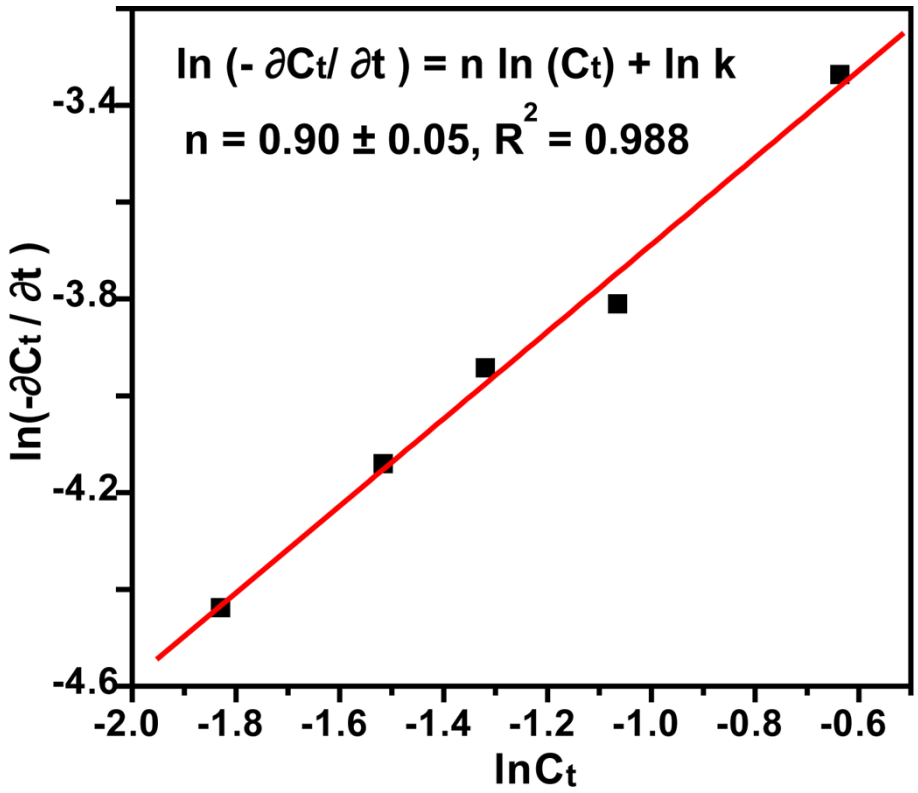

Figure S7 Reaction kinetics study of the reduction of 4-NP over Pd NPs/NF-CNT by UV-vis spectroscopy: the ln(-$\partial C_t/\partial_t$) versus ln(C_t) plot in which the slope of the linearly fitted line (0.90 ± 0.05) corresponds to the reaction order with respect to 4-NP (n), indicating pseudo-first-order reaction kinetics.

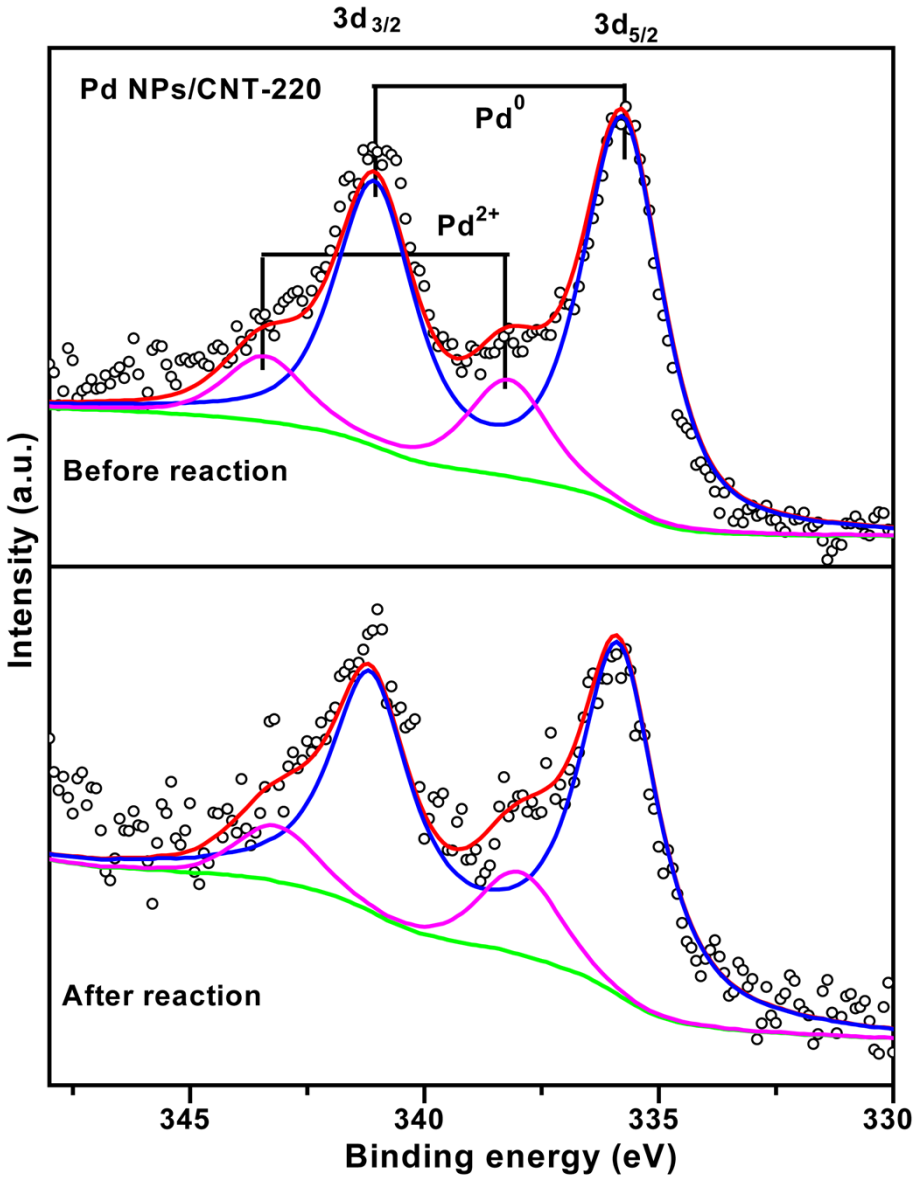

Figure S8 The curve fitted Pd3d XPS of Pd NPs/CNT-220 before and after the catalytic reaction.