Supporting Information

Enhanced adsorption of hydroxyl- and amino-substituted aromatic chemicals to nitrogen doped multiwall carbon nanotubes: A combined batch and theoretical calculation study

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Table S1. Adsorbate Water Solubility (S_W), *n*-Octanol-Water Partition Coefficient (K_{OW}), *n*-Hexadecane-Water Partition Coefficient (K_{HW}), and Acid Dissociation Constants (pK_a).

Compound	S_W (mmol/L)	K_{OW} (L/L)	K_{HW} (L/L)	pK_a
2-naphthol	6.93×10^{0}[a]	5.01×10^{2}[a]	1.80×10^{0}[c]	9.51[a]
1-naphthylamine	1.20×10^{1}[a]	1.78×10^{2}[a]	1.58×10^{1}[c]	3.92[a]
naphthalene	2.50×10^{-1}[a]	2.14×10^{3}[a]	2.57×10^{3}[d]	/
1,3-dinitrobenzene	2.88×10^{0}[a]	3.09×10^{1}[a]	4.30×10^{1}[e]	/
triethanolamine	6.7×10^{3}[b]	1×10^{-1}[b]	/	7.76[b]
n-octanol	4.15×10^{0}[b]	1×10^{3}[b]	4.17×10^{1}[f]	/

[a]From Schwarzenbach et al.[1]

[b]Adopted from the U.S. National Library of Medicine Hazardous Substance Data Bank (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB).

[c]From Chen et al.[2]

[d]From Zhu and Pignatello.[3]

[e]From Liu et al.[4]

[f] From Abraham et al.[5]

Table S2. Freundlich Model Parameters (K_F and n ± Standard Deviation) and Ranges of Solid-to-Solution Distribution Coefficient (K_d) for Adsorption of Different Compounds on N-doped multiwall carbon nanotubes (N-MCNT) and non-doped multiwall carbon nanotubes (MCNT).

Compound	**Adsorbent**	K_F **(mmol^{1-n} L/kg)**	n	R^2	K_d[a] **(L/kg)**
2-naphthol	N-MCNT	1500±59	0.460±0.014	0.9875	10^3-10^5
	MCNT	270±13	0.350±0.012	0.9806	10^3-10^4
1-naphthylamine	N-MCNT	2300±51	0.184±0.005	0.9925	10^4-10^6
	MCNT	1200±51	0.280±0.012	0.9813	10^3-10^5
naphthalene	N-MCNT	370±16	0.570±0.011	0.9947	10^3-10^4
	MCNT	170±5	0.380±0.011	0.9916	10^3
1,3-dinitrobenzene	N-MCNT	210±12	0.570±0.016	0.9899	10^2-10^3
	MCNT	250±18	0.470±0.018	0.9809	10^3-10^4
triethanolamine	N-MCNT	400±103	1.300±0.104	0.9285	10^3
	MCNT	170±15	0.860±0.040	0.9714	10^3
n-octanol	N-MCNT	400±143	0.900±0.102	0.8321	10^2-10^3
	MCNT	270±55	0.700±0.041	0.9660	10^3

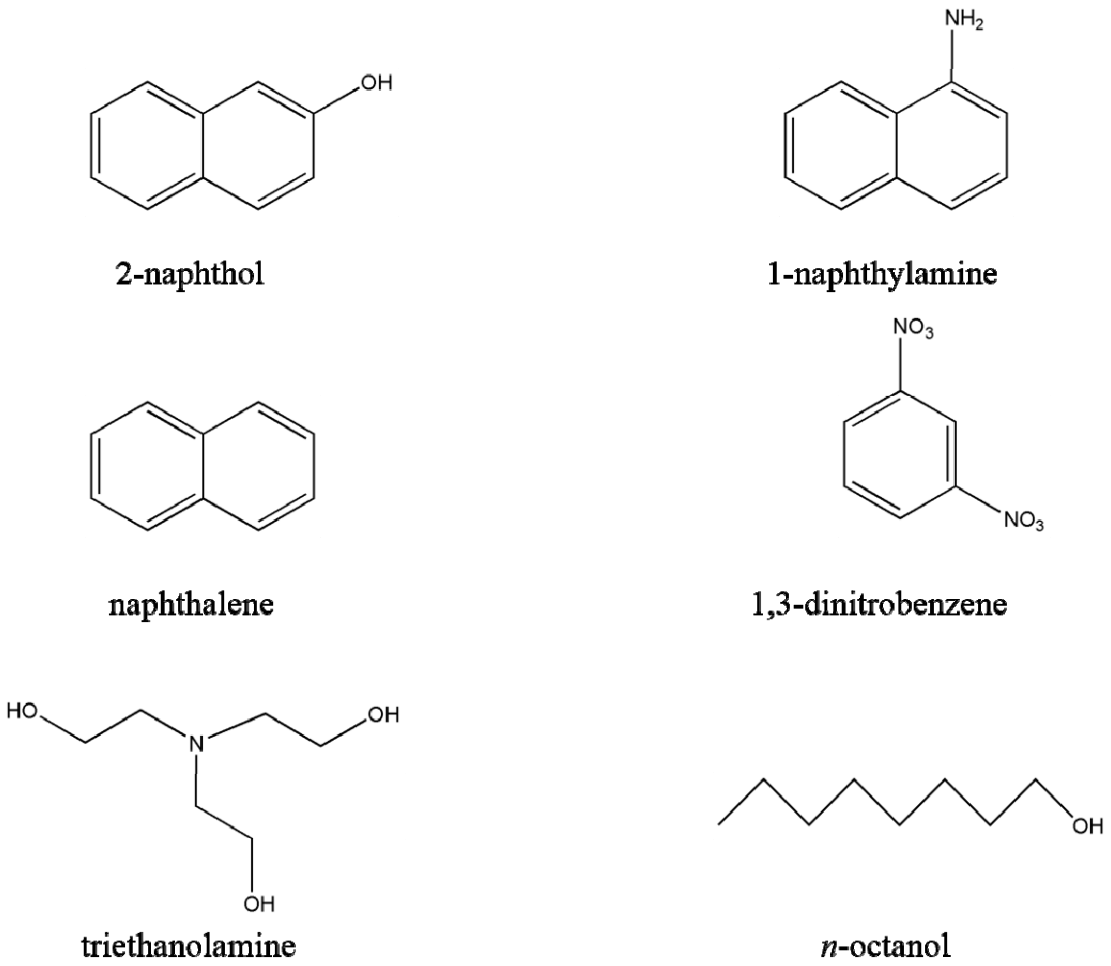

Figure S1. Chemical structures of adsorbate molecules.

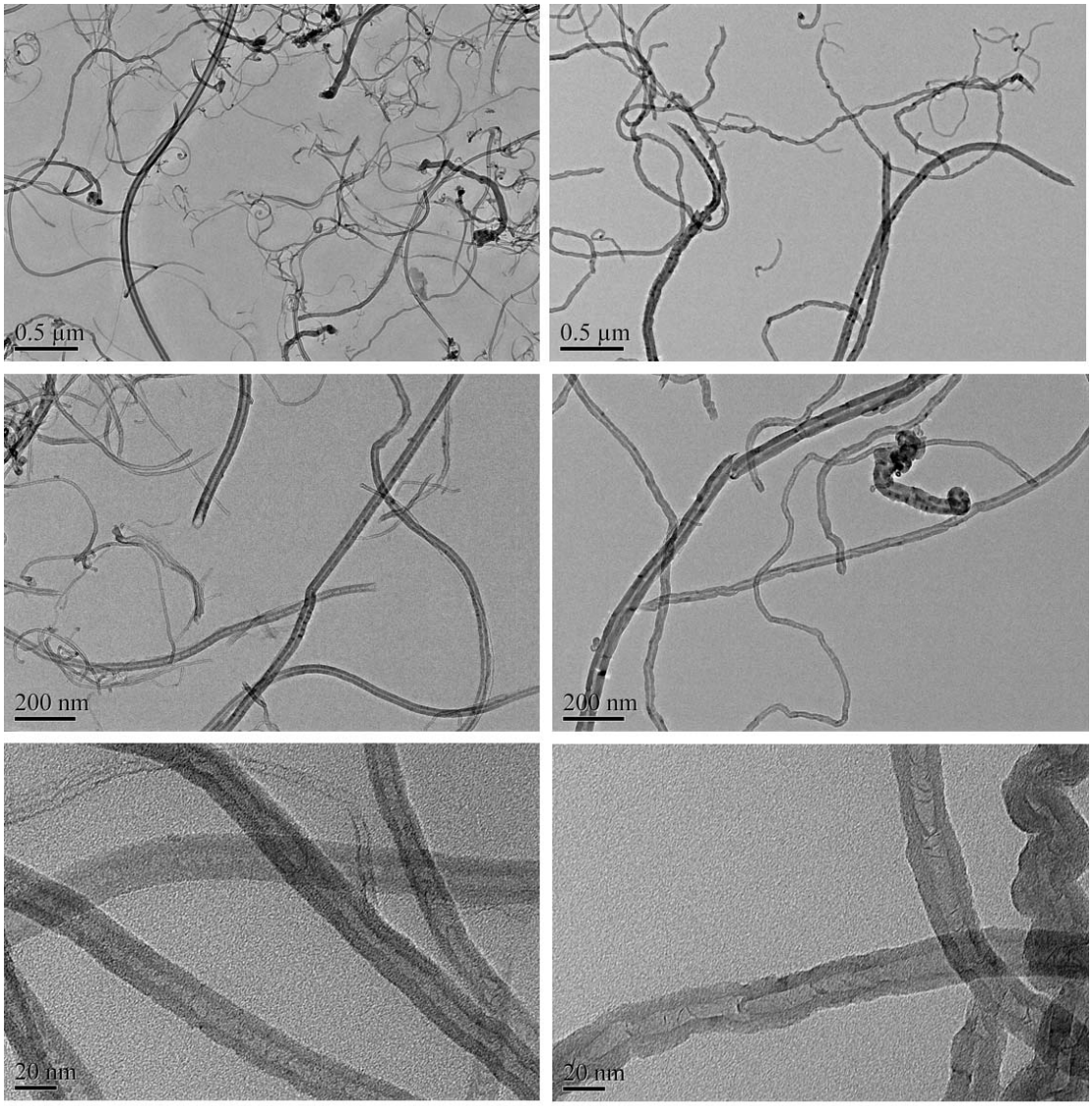

Figure S2. Transmission electron microscopy (TEM) images of N-doped multiwall carbon nanotubes (N-MCNT, left column) and non-doped multiwall carbon nanotubes (MCNT, right column).

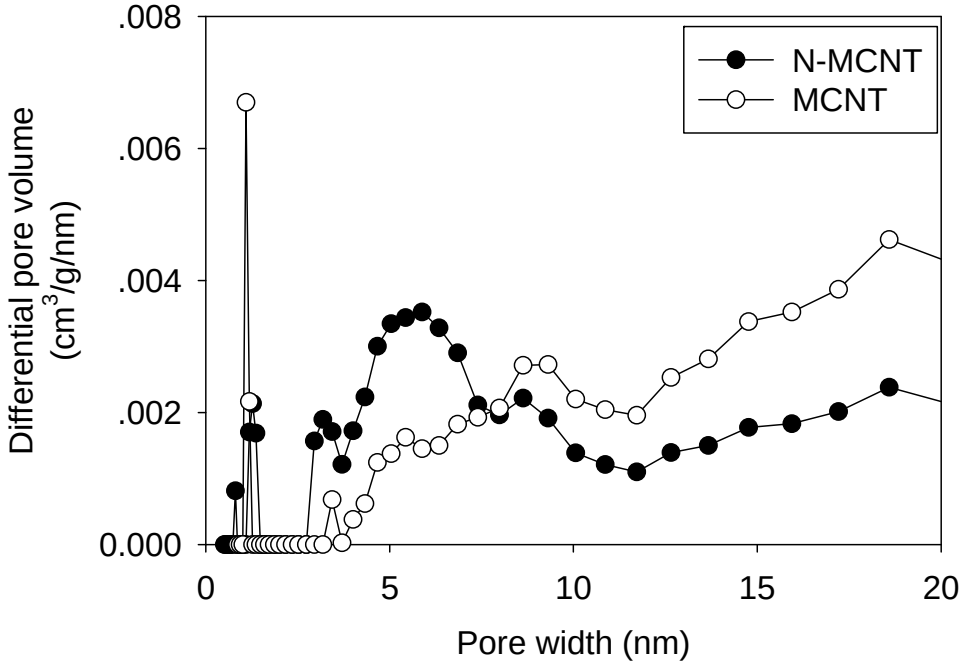

Figure S3. Pore size distribution of N-doped multiwall carbon nanotubes (N-MCNT) and non-doped multiwall carbon nanotubes (MCNT), plotted as differential pore volume vs. pore width. Lines are visual clarity only.

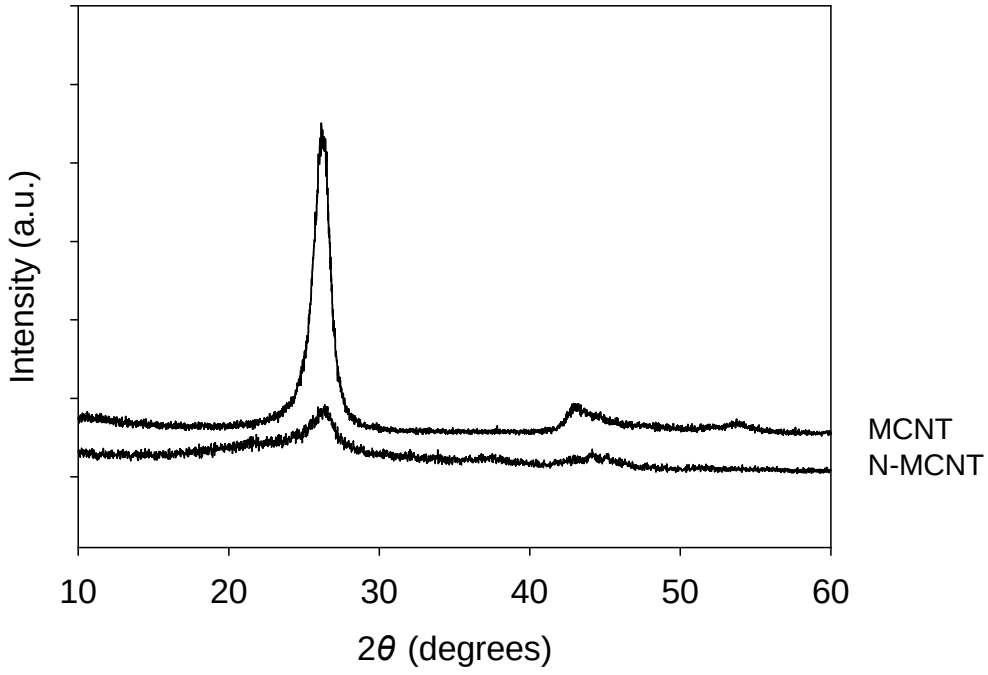

Figure S4. X-ray diffraction (XRD) patterns of N-doped multiwall carbon nanotubes (N-MCNT) and non-doped multiwall carbon nanotubes (MCNT). XRD patterns were performed on a Philips X'Pert Pro diffractometer (Eindhoven, Netherlands) using Cu Kα radiation across a range of 10-70°. The diffraction peak at 26.3° (002) is characteristic of the graphitization structure. N-MCNT shows much weaker (002) diffraction peak compared with MCNT. This illustrates the nitrogen atoms in N-MCNT partially disorders the graphitization structure.[6]

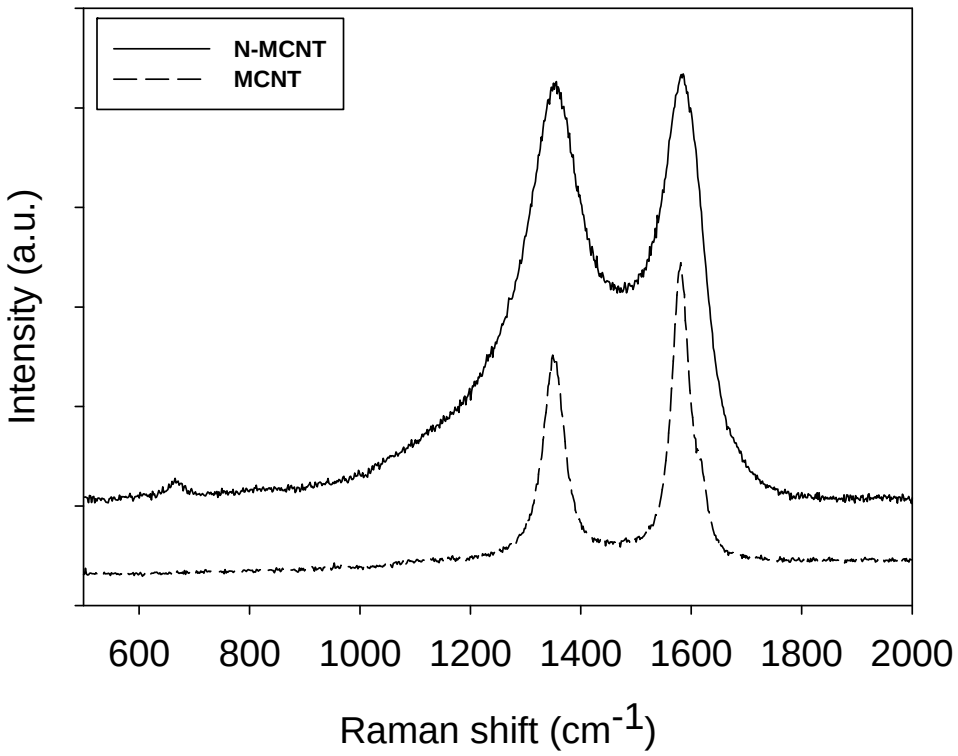

Figure S5. Raman spectra of N-doped multiwall carbon nanotubes (N-MCNT) and non-doped multiwall carbon nanotubes (MCNT). Raman spectra were recorded on a LabRAM-HR Raman spectrometer (Horiba Jobin Yvon, France) with a laser excitation wavelength of 514 nm. The two carbon nanotubes show Raman peaks around 1336 cm^{-1} and 1590 cm^{-1}, which correspond to the D band and G band of carbonaceous materials. The ratio of I_G/I_D reflects the graphitization degree of the carbon nanotubes. MCNT has significant higher graphitization degree (I_G/I_D = 1.42) than N-MCNT (I_G/I_D = 1.04). The Raman results indicate that N-doping decreases the order of the graphitic structures.[7]

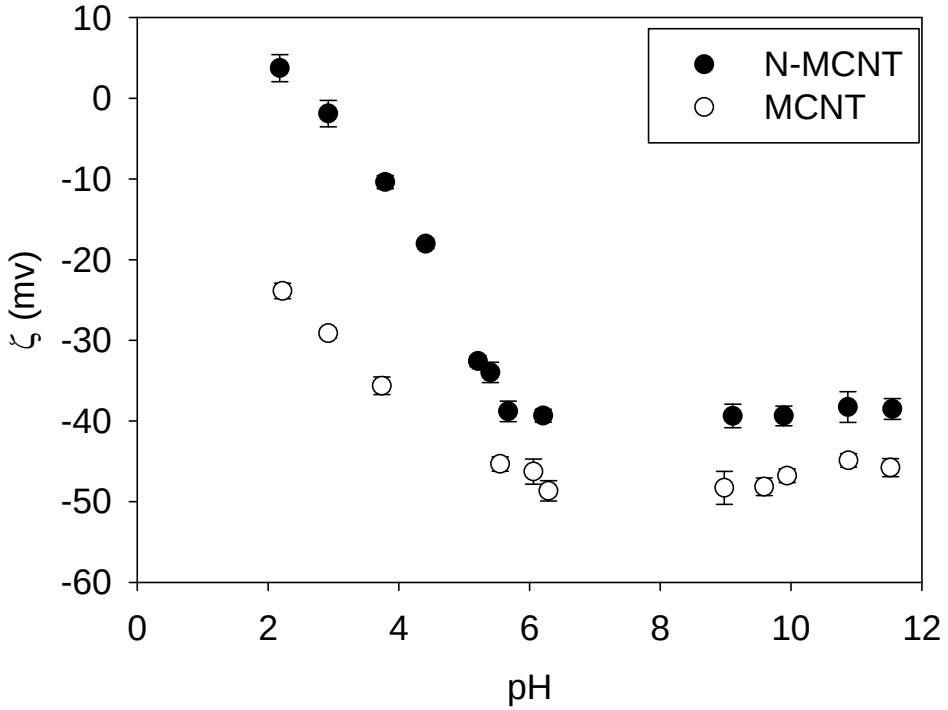

Figure S6. Single point measurements of Zeta potential (ζ) as a function of pH for N-doped multiwall carbon nanotubes (N-MCNT) and non-doped multiwall carbon nanotubes (MCNT).

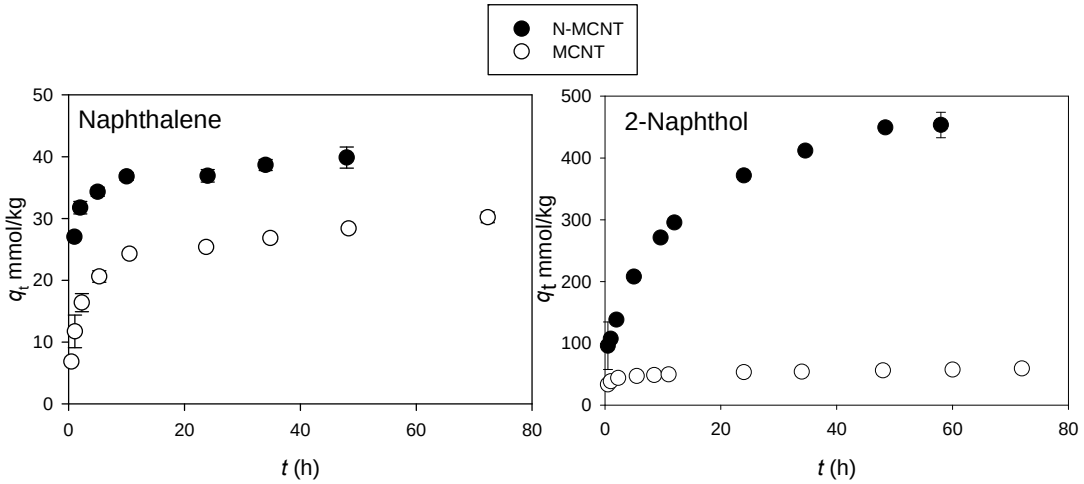

Figure S7. Adsorption kinetics plotted as adsorbed concentration (q_t, mmol/kg) at given time (t, h) to N-doped multiwall carbon nanotubes (N-MCNT) and non-doped multiwall carbon nanotubes (MCNT) for selected adsorbates.

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