Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Adsorption of Aromatic Carboxylic Acids on Carbon Nanotubes: Impact of Surface Functionalization, Molecular Size and Structure

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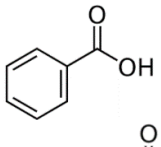
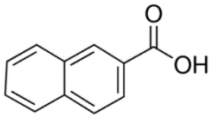
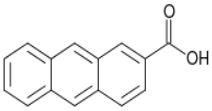
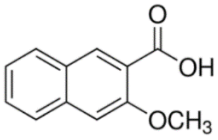
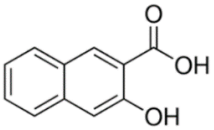
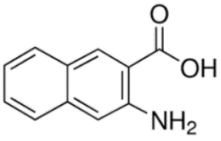
Table S1*. Physiochemical Properties of three Multi-carbon Nanotube Tubes

Compounds	G-MWNTs	COOH-MWNTs	OH-MWNTs
Purity	>99.9 wt%	> 99.9 wt%	> 99.9 wt%
Outside diameter	10-20 nm	10-20 nm	10-20 nm
Inside diameter	5-10 nm	5-10 nm	5-10 nm
Length	10-30 um	10-30 um	10-30 um
SSA	> 100 m^2/g	> 100 m^2/g	> 100 m^2/g
Ash content	< 0.1 wt%	< 0.1 wt%	< 0.1 wt%
True density	~2.1 g/cm^3	~2.1 g/cm^3	~2.1 g/cm^3
Functional group density	N/A	1.00wt%	2.48wt%
Manufacturing method	CVD	CVD	CVD

*Selected properties of MWNTs are reported by the vendor: the US Research Nanomaterials Inc. (https://www.us-nano.com)

Table S2. Molecular structures and key chemical parameters of the organic acids investigated in this study

Compounds	Structure	Log K_{ow}	D_{ow}[#]	Henry constant (atm-m^3/mole)	pK_a
BA		1.87	-0.041	1.08E-007	4.19
2-NA		3.28	0.201	1.06E-008	4.16
2-AA		4.23	0.123	1.03E-009	N/A
3-M-2-NA		2.79	-0.356	6.26E-010	2.73
3-H-2-NA		3.05	-0.206	1.06E-008	2.79
3-A-2-NA		2.54	0.188	3.74E-012	5.02

[*]: All values listed in the table are from Chemspider unless otherwise noticed. Henry constants in this table were measured by bond method with the unit atm-m^3/mole. BA: benzoic acid; 2-NA: 2-Napththoic acid; 2-AA: 2-Anthroic acid; 3-M-2-NA: 3-Methoxyl-2-Napthoic acid; 3-H-2-NA: 2 Hydroxy-2-Naphthoic acid; 3-A-2-NA: 3-Amino-2-Naphthoic acid.

[#]: Estimated pH dependent octanol-water partitioning coefficient at the pH values used in this study. Detailed approach for D_{ow} estimation is elaborated in the manuscript.

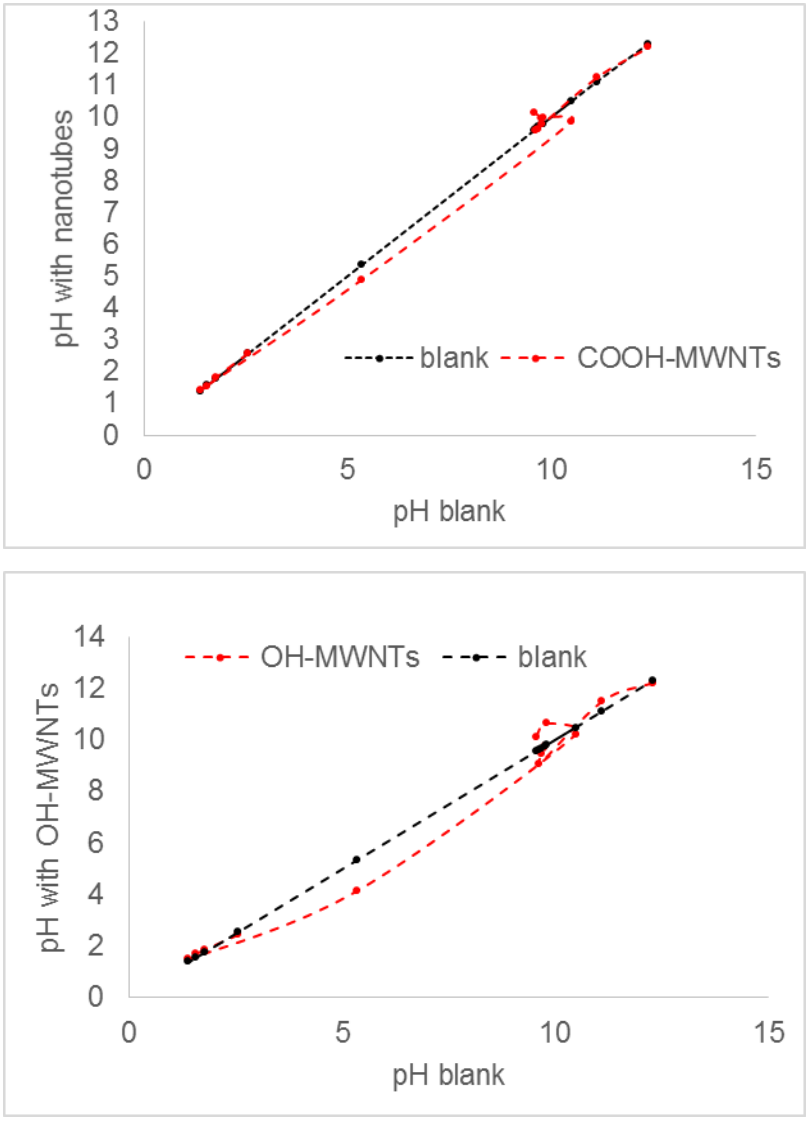


Figure S1: Titration curves for the determination of hydroxide ion consumption by two functionalized multi-walled carbon nanotubes (MWNTs). (A): COOH-MWNTs, (B): OH-MWNTs.

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