**Supplementary Materials**

# Sorption and desorption analysis of nitrobenzene on differently functionalized multiwalled carbon nanotubes and implications on the stability

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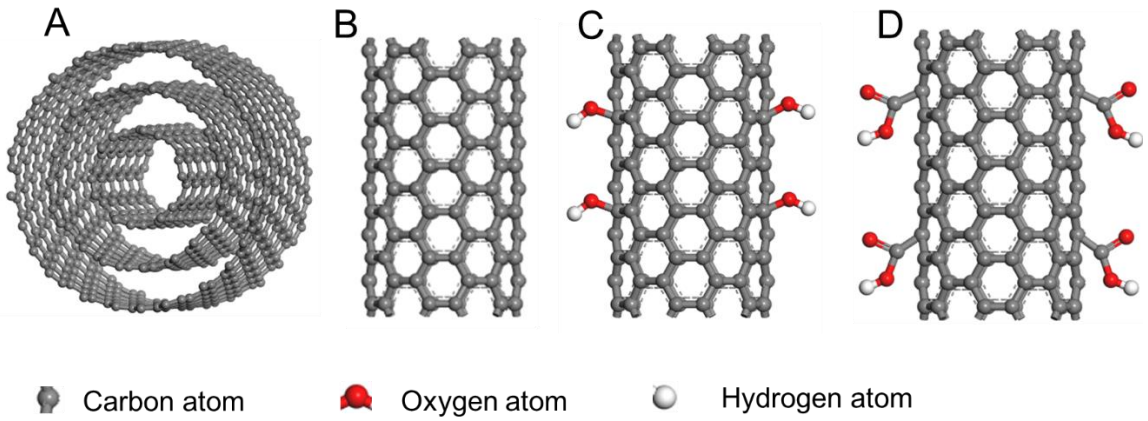
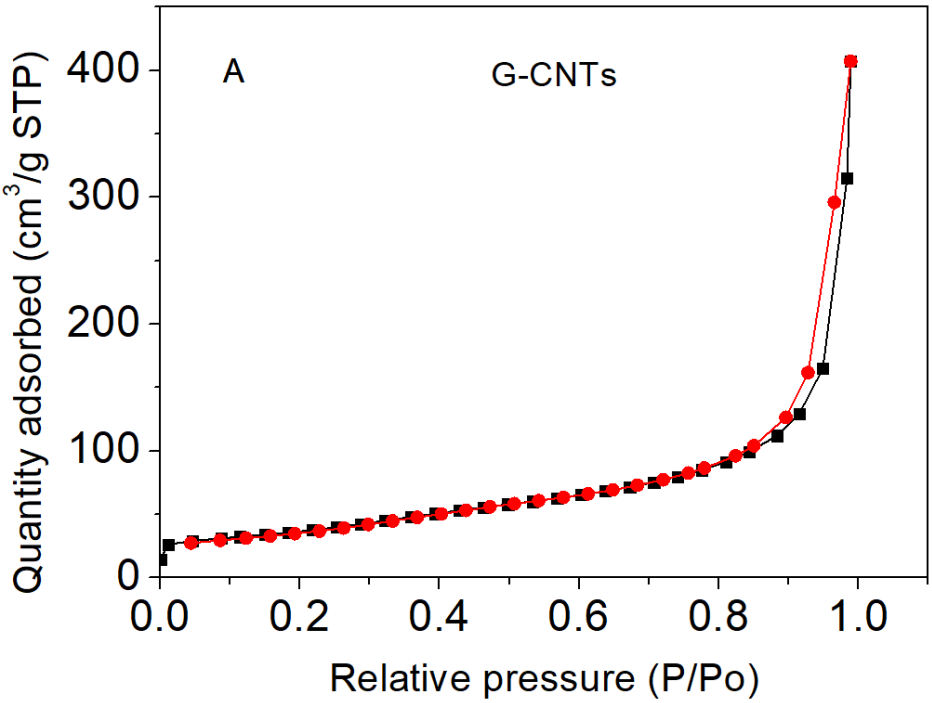


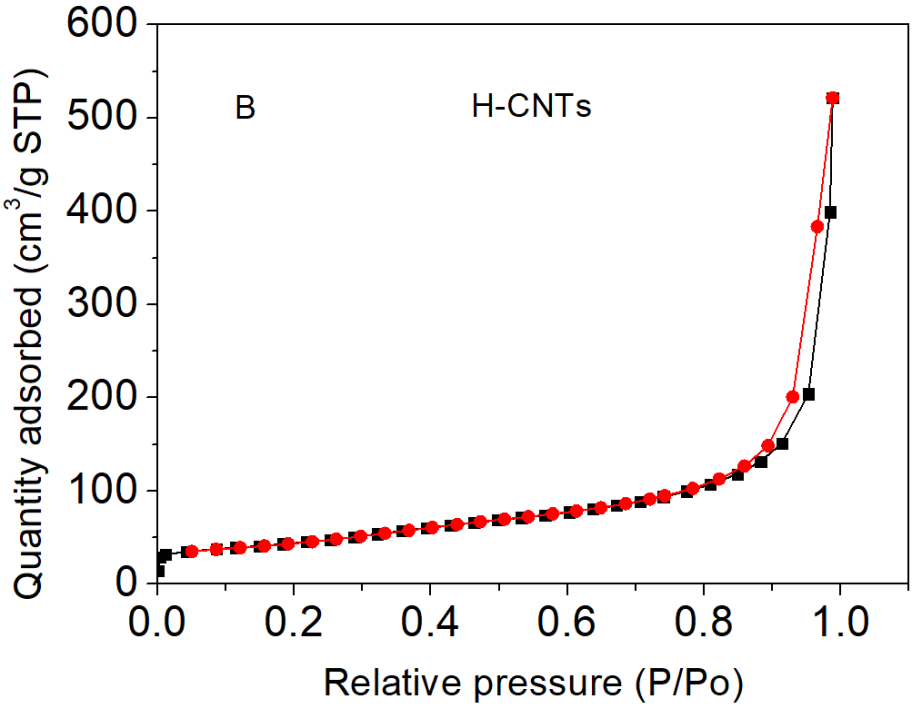

**Figure S1.** The chemical structure sketches of three functionalized carbon nanotubes: (**A**) multiwalled structure of three carbon nanotubes; (**B**) the surface of G−CNTs; (**C**) the surface of H−CNTs; (**D**) the surface of C−CNTs.

**Table S1.** Selected physicochemical properties of CNTs.

| CNTs | Surface O [a] (wt%) | Functionalized surface C [b] (wt%) | Total O [c] (wt%) | L [d] (μm) | OD [e] (nm) | ID [f] (nm) | SSA [g] ($m^2/g$) |
|---|---|---|---|---|---|---|---|
| G−CNTs | 0.7 | <0.7 | <0.1 | 5−30 | 10−20 | 5−10 | 133.6 |
| H−CNTs | 4.1 | 4.28 | 2.9 | 5−30 | 10−20 | 5−10 | 159.4 |
| C−CNTs | 4.2 | 2.19 | 0.5 | 5−30 | 10−20 | 5−10 | 145.5 |
| **CNTs** | **$S_{mic}$ [h] ($m^2/g$)** | **$S_{mes}$ [i] ($m^2/g$)** | **$V_{total}$ [j] ($cm^3/g$)** | **$V_{mic}$ [k] ($cm^3/g$)** | **$V_{mes}$ [l] ($cm^3/g$)** | **$D_{average}$ [m] (nm)** | **$D_{mes}$ [n] (nm)** |
| G−CNTs | 6.4 | 133.9 | 0.257 | 0.002 | 0.627 | 3.8 | 9.4 |
| H−CNTs | 12.7 | 155.2 | 0.310 | 0.005 | 0.800 | 3.9 | 10.3 |
| C−CNTs | 10.2 | 140.6 | 0.280 | 0.004 | 0.636 | 3.9 | 9.0 |

[a] Surface O, Surface oxygen content, was measured by X-ray photoelectron spectroscopy (XPS);[b] Functionalized surface carbon (wt%) was calculated according to XPS result, functionalized surface carbon (wt%) = the ratio of oxidized carbon atoms to total carbon atoms; [c] Total O, Total oxygen content was measured by Elemental Analyzer; [d] L, length of the CNTs; [e] OD, outer diameter of the CNTs; [f] ID, inner diameter of the CNTs; [g] SSA, Special surface area, was measured by $N_2$ adsorption using the Brunauer-Emmett-Teller (BET) method; [h] $S_{mic}$, micropore surface area, was obtained using the t-plot theory; [i] $S_{mes}$, mesopore surface area, was calculated using the Barrett-Johner- Halendar (BJH) theory; [j] $V_{total}$, total pore volume was measured by $N_2$ adsorption using the BET method; [k] $V_{mic}$, micropore volume, was obtained using the t-plot theory; [l] $V_{mes}$, mesopore volume, was calculated using the Barrett-Johner- Halendar (BJH) theory; [m] $D_{average}$, average pore diameter of the CNTs, was measured by N2 adsorption using the BET method; [n] $D_{mes}$, the mesopore diameter, was calculated using the Barrett-Johner- Halendar (BJH) theory.


A
G-CNTs
Quantity adsorbed (cm3/g STP)
0
100
200
300
400
0.0
0.2
0.4
0.6
0.8
1.0
Relative pressure (P/Po)


B
H-CNTs
Quantity adsorbed (cm3/g STP)
0
100
200
300
400
500
600
0.0
0.2
0.4
0.6
0.8
1.0
Relative pressure (P/Po)

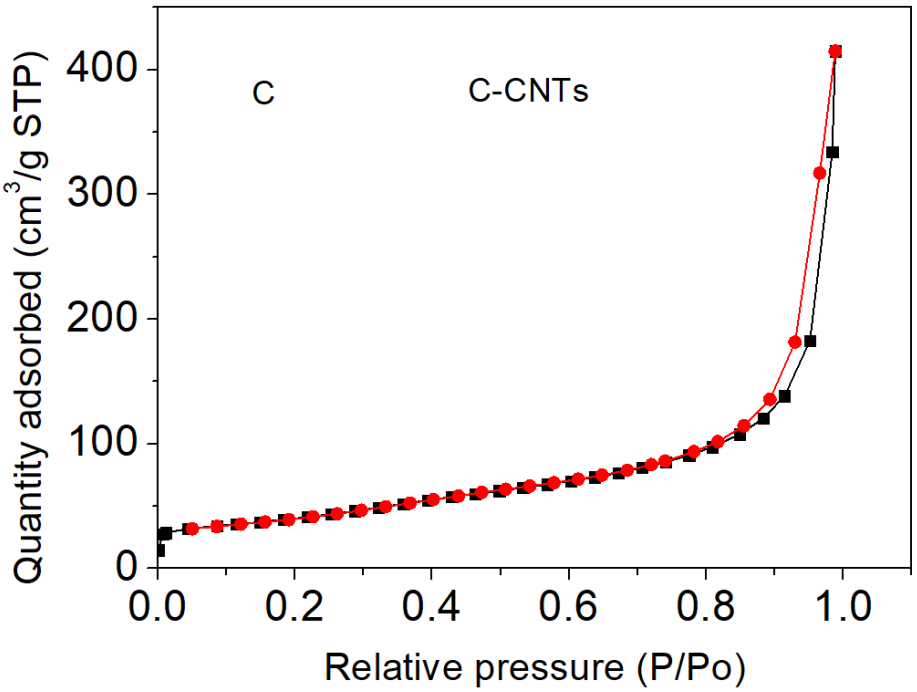
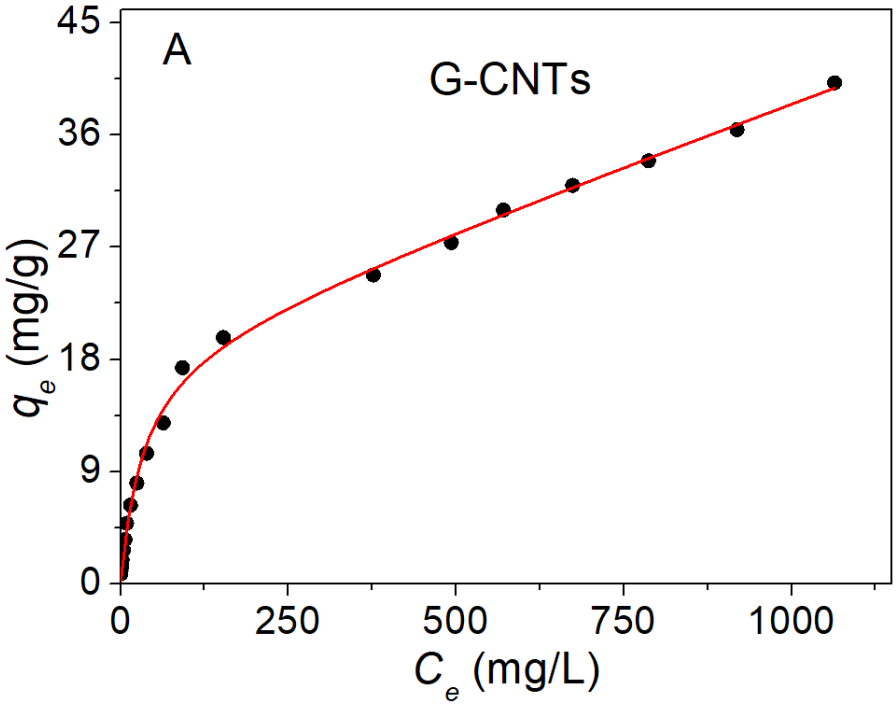



**Figure S2.** The nitrogen adsorption–desorption isotherms that were obtained using a surface area and porosimetry analyzer (ASAP 2460, Micromeritics, USA): (**A**) G–CNTs; (**B**) H–CNTs; (**C**) C–CNTs.



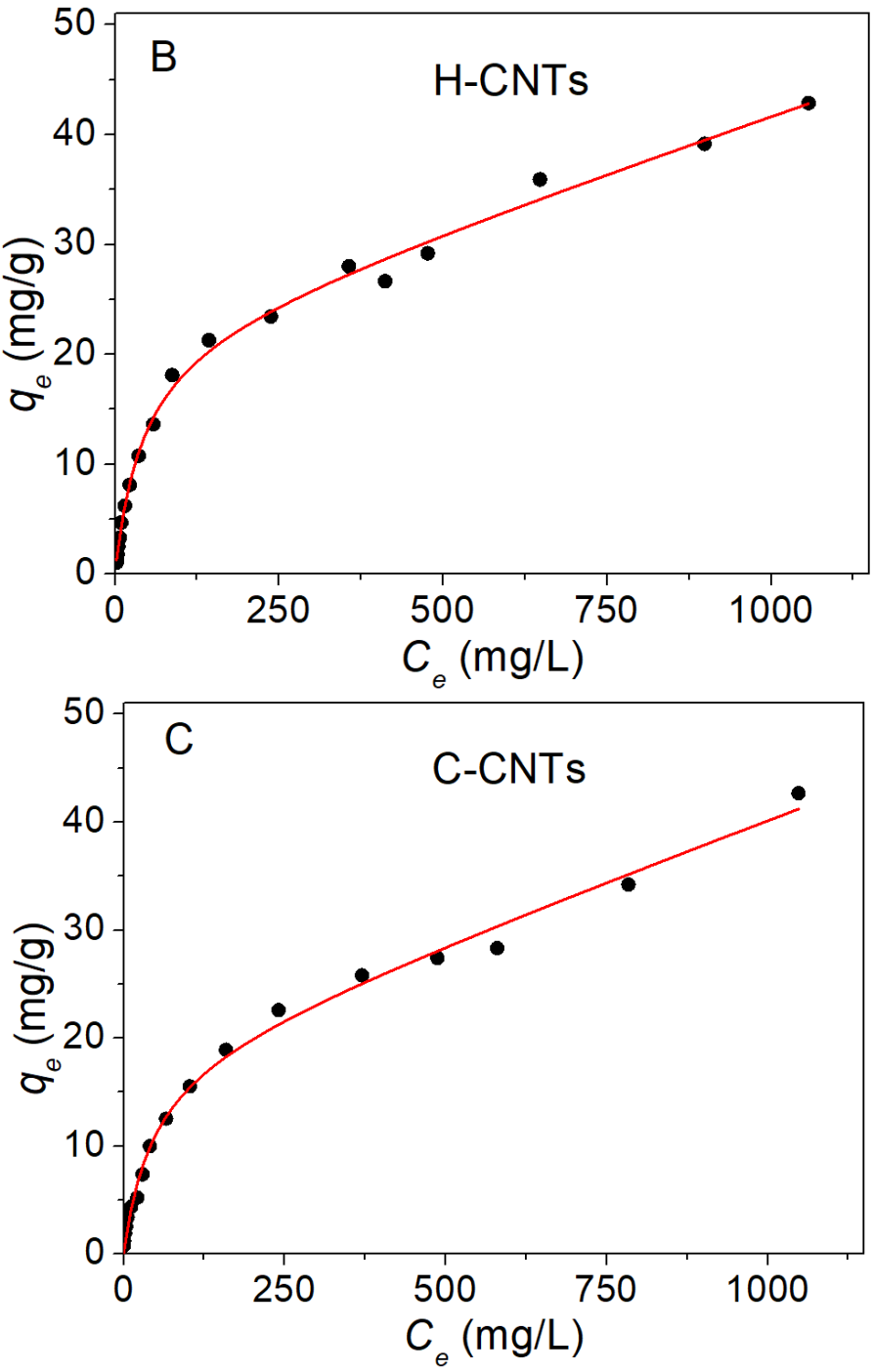



**Figure S3.** Sorption isotherms of nitrobenzene by three functionalized carbon nanotubes: (**A**) G–CNTs; (**B**) H–CNTs; (**C**) C–CNTs. Solid lines are the isotherms fitted by DMM model.

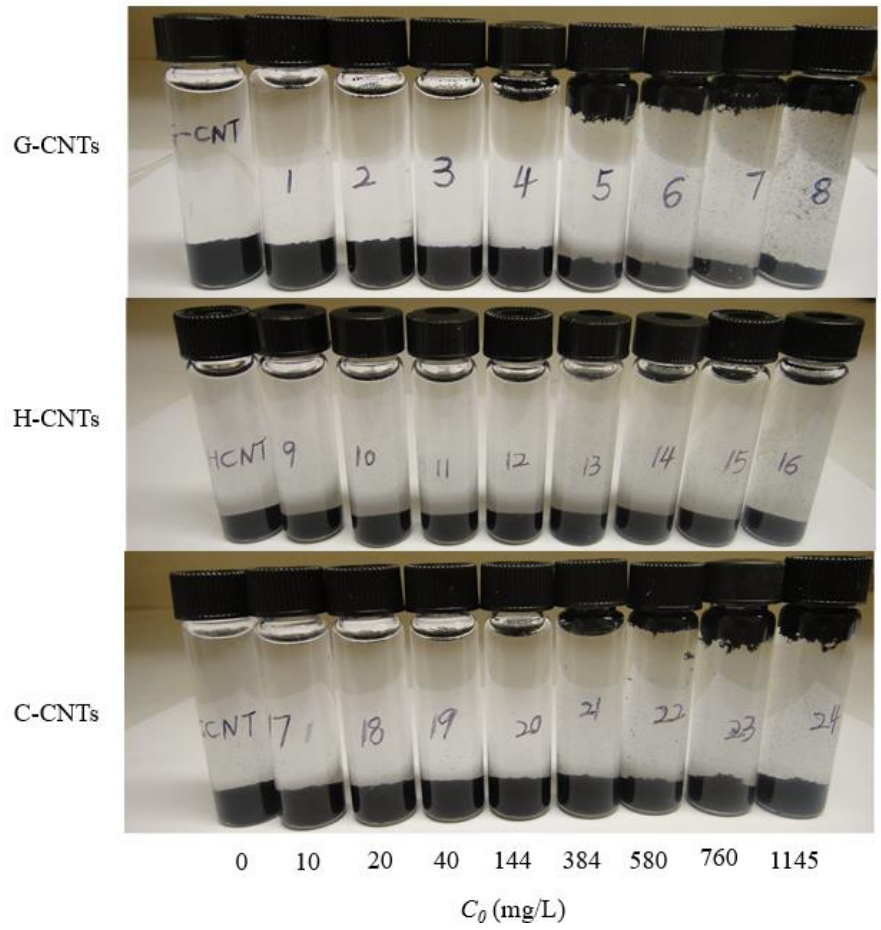



**Figure S4.** Photo of three functionalized MWCNTs suspension with different initial concentration of nitrobenzene after 72 h shaking and 1 hour′ settlement.

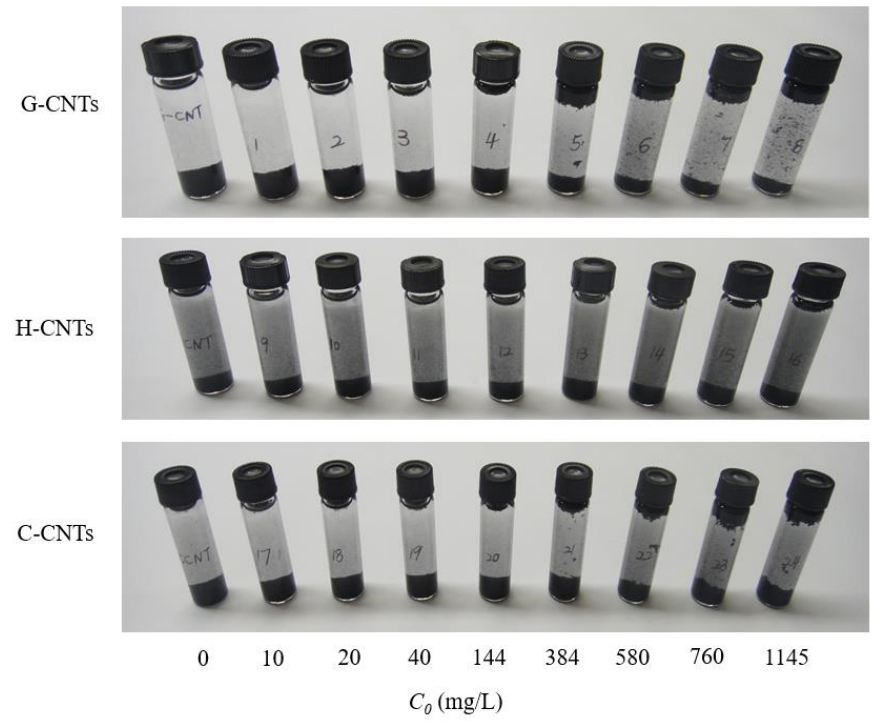



**Figure S5.** Photo of three functionalized MWCNTs suspension with different initial concentration of nitrobenzene after 72 h shaking and 5 minutes′ settlement [48].