Electronic Supplementary Information for:

Separation of CO_2/CH_4 mixture on defective single walled carbon nanohorn – tip does matter

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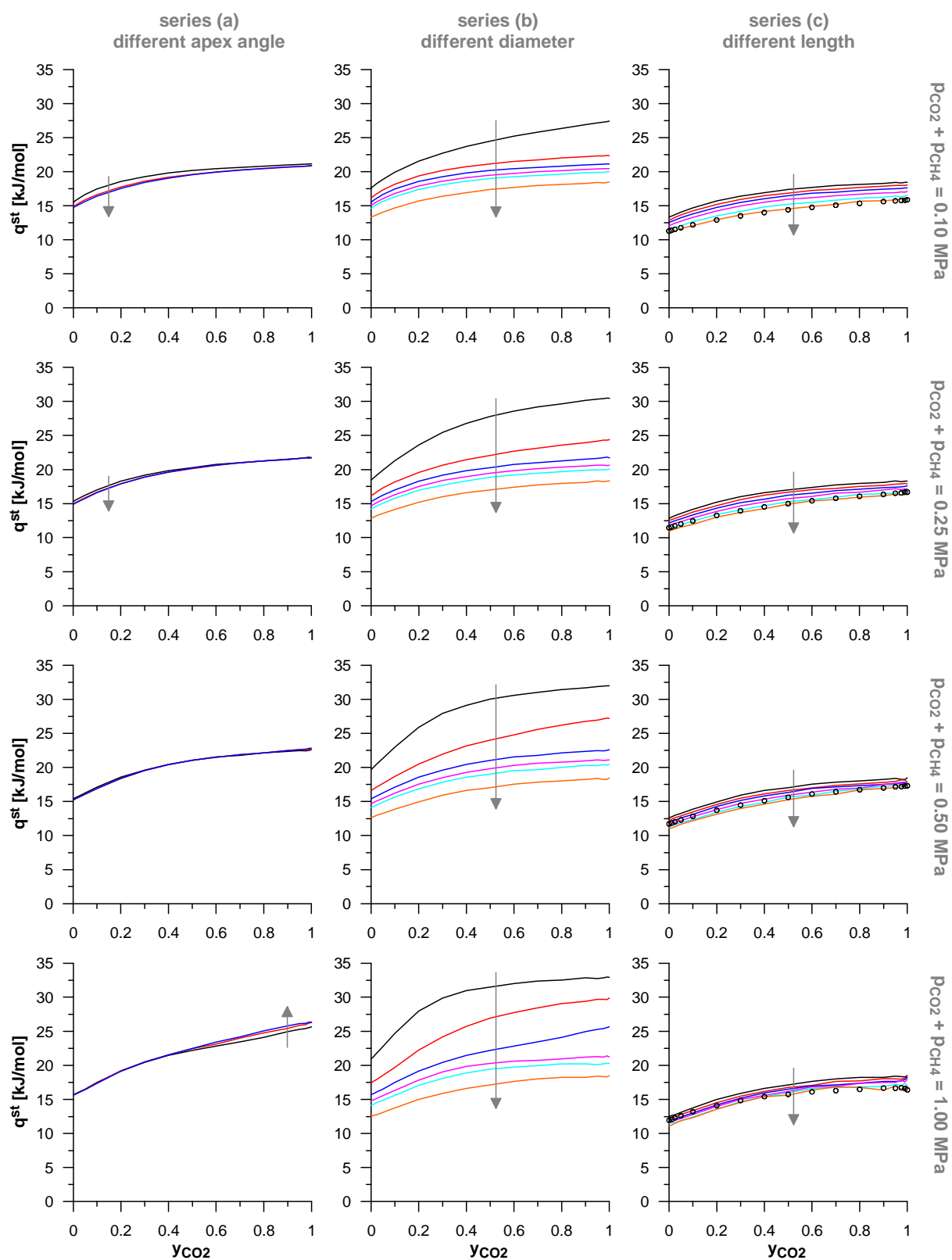
Number of pages: 5

**Number of Tables: 1**

Number of Figures: 3

Table 1S.

The values of LJ potential parameters and point charges applied in simulations

| Molecule	Centre	σ [nm]	ε/k_B [K]	q/e	Reference
CO_2	C	0.2824	28.680	+ 0.664	1
	O	0.3026	82.000	− 0.332	
CH_4	C	0.3400	55.055	− 0.660	2
	H	0.2650	7.901	+ 0.165	
	C-H[*]	0.3025	30.600	−	
nanohorn	C	0.3400	28.000	−	3 and references therein

[*] cross-interaction parameters

Figure 1S. Variations of the isosteric enthalpy of CO_2/CH_4 adsorption with total pressures of $CO2/CH4$ bulk mixtures and molar fractions of CO_2 in bulk mixtures computed for all studied series of SWCNHs (see Figure 1 in the main article).
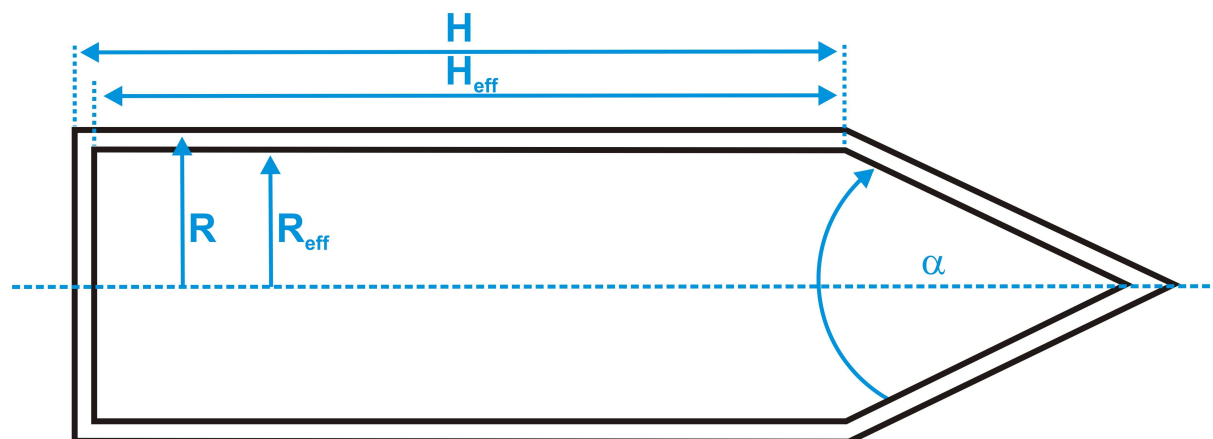
Figure 2S. The axial section of SWCNHs. H is the length of tubular part, R is the radius of tubular part ($H - H_{eff} = 0.17$ nm $= R - R_{eff}$), and α is the apex angle of horn-shaped tip.
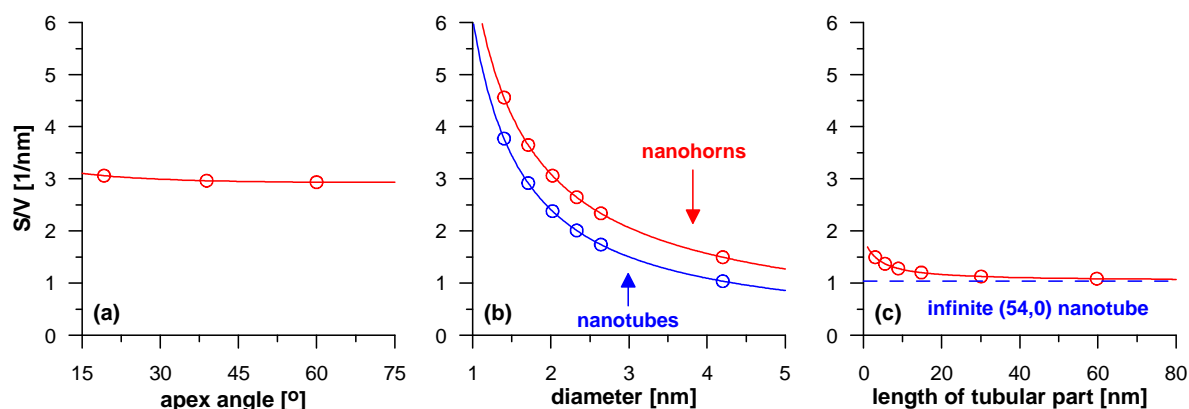
Figure 3S. The changes of surface to volume ratio calculated for model simplified geometry of SWCNHs (see Figure 2S, axial section) with the rise in apex angle, α (a), diameter, D (b), and length of tubular part (c). The points correspond with sizes of the studied systems – see Fig. 1. Panel (b) presents also the data calculated for infinite SWCNTs. The values of surface area or volume are calculated on the basis of the following equations: $S_{\mathrm{SWCNT}} = 2\pi R_{eff} H$,

$$V_{\mathrm{SWCNT}} = \pi R_{eff}^2 H \ , \ \ S_{\mathrm{SWCNH}} = \pi R_{eff}^2 + 2\pi R_{eff} H_{eff} + \frac{\pi R_{eff}^2}{\sin\frac{\alpha}{2}} \ , \text{ and } V_{\mathrm{SWCNH}} = \pi R_{eff}^2 H_{eff} + \frac{\pi R_{eff}^3}{3 tg\frac{\alpha}{2}} \ .$$

References

[1]   T. X. Nguyen, Ph.D. Thesis, University of Queensland, 2006.

[2]   A. P. Terzyk, S. Furmaniak, P. A. Gauden and P. Kowalczyk, *Adsorpt. Sci. Technol.*, 2009, **27**, 281.

[3]   S. Furmaniak, A. P. Terzyk, K. Kaneko, P. A. Gauden, P. Kowalczyk and T. Itoh, *Phys. Chem. Chem. Phys.*, 2013, **15**, 1232.