Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics
This journal is © The Owner Societies 2014

On the thermodynamics of carbon nanotube single-file water loading: Free energy, Energy and Entropy calculations. Supplementary material.

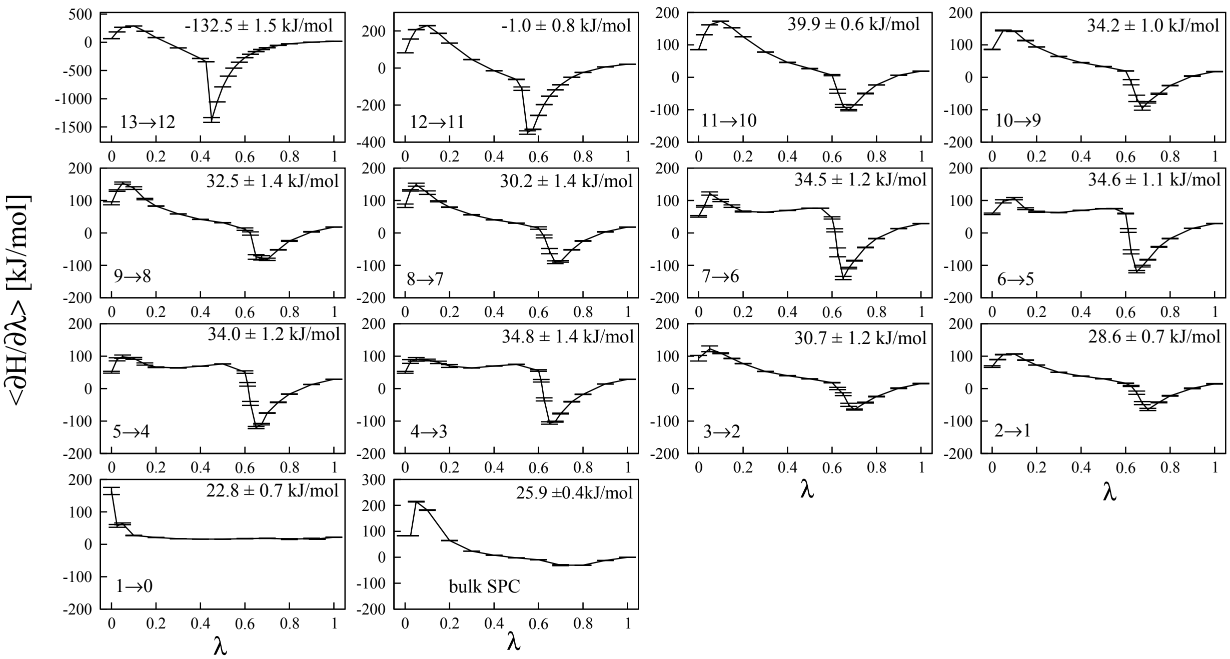
Jose Antonio Garate
Institute of Molecular Modelling and Simulation.
University of Natural Resources and Life Sciences
Vienna, Austria.
Computational Biology Lab.
Fundacíon Ciencia & Vida
Santiago, Chile.

Tomas Perez-Acle
Computational Biology Lab.
Fundacíon Ciencia & Vida
Santiago, Chile.

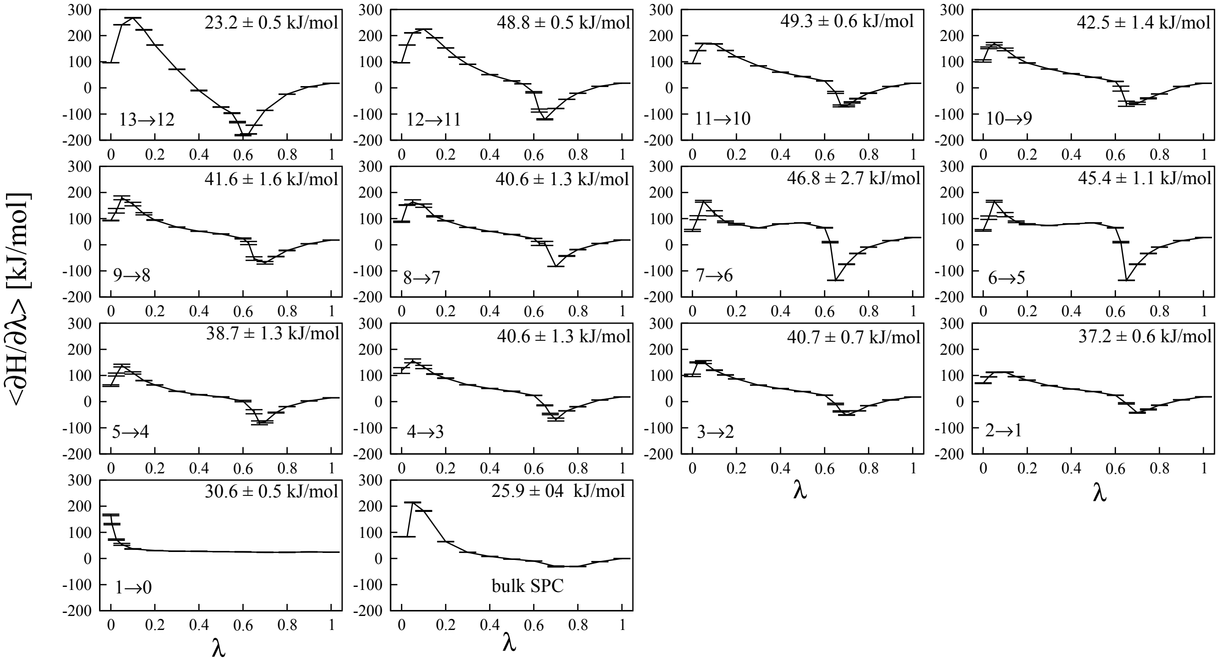
Chris Oostenbrink*
Institute of Molecular Modelling and Simulation.
University of Natural Resources and Life Sciences.
Vienna, Austria.

---

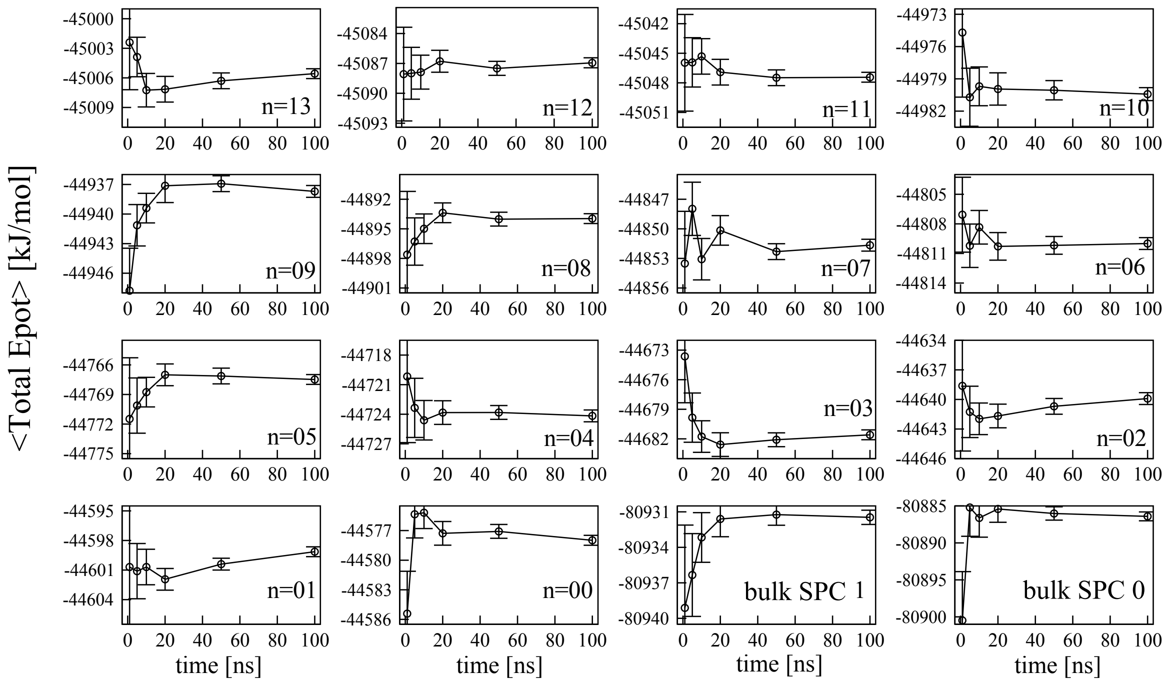
*Correspondig Author Address: Muthgasse 18 - 6/58, Tel:+43 1 476548302, E-mail: chris.oostenbrink@boku.ac.at,



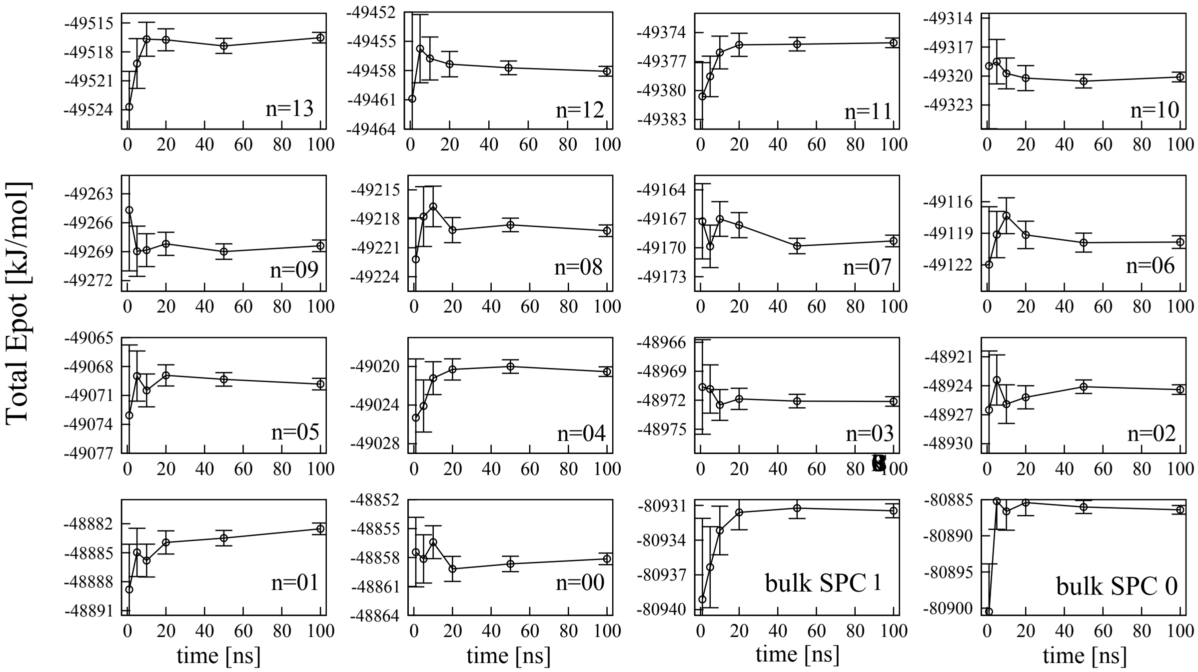
Supp. Fig. 1: Thermodynamic integration perturbing a SPC water into dummy atoms at every load state of the (5.5) carbon nanotube. The numerical value of the integral, employing the trapezoidal rule, is shown for each curve.



Supp. Fig. 2: Thermodynamic integration perturbing a SPC water into dummy atoms at every load state of the (6.6) carbon nanotube. The numerical value of the integral, employing the trapezoidal rule, is shown for each curve.



Supp. Fig. 3: Total potential energy as a function of simulated time for each load state of the (5,5) CNT and Bulk SPC water.



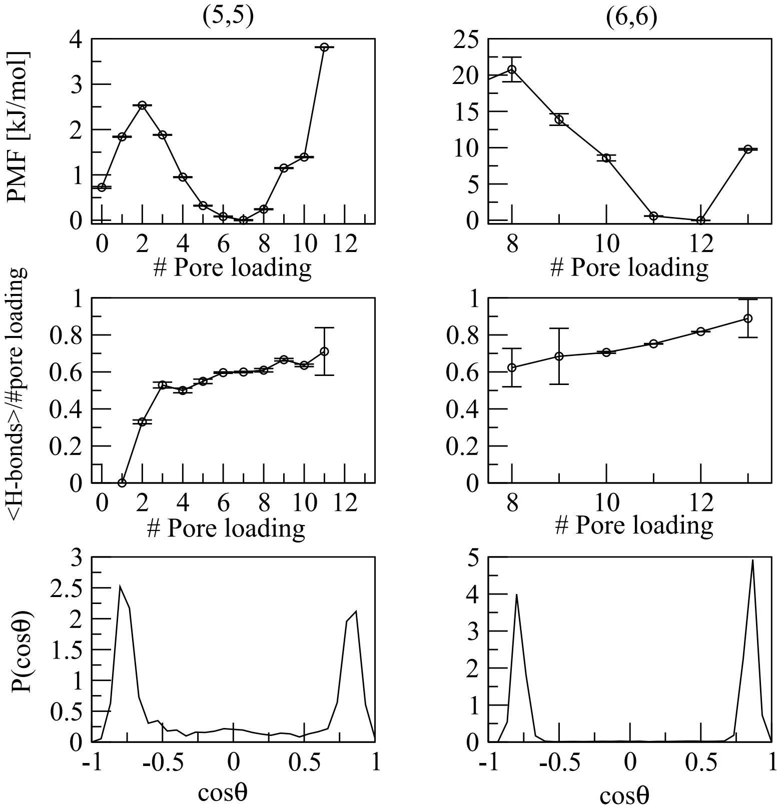
Supp. Fig. 4: Total potential energy as a function of simulated time for each load state of the (6,6) CNT and Bulk SPC water.

Supp. Table 1: Total potential energies of all simulated systems.

# Pore loading	E [kJ/mol]	
	SWCNT	
	System (6,6)	System (5,5)
13	-49516.5 ± 0.5	-45005.6 ± 0.5
12	-49458.0 ± 0.5	-45086.9 ± 0.6
11	-49375.1 ± 0.5	-45047.4 ± 0.5
10	-49320.0 ± 0.5	-44980.4 ± 0.6
9	-49268.4 ± 0.6	-44937.7 ± 0.5
8	-49219.3 ± 0.6	-44894.0 ± 0.5
7	-49169.3 ± 0.6	-44851.7± 0.6
6	-49119.8 ± 0.6	-44810.0 ± 0.6
5	-49069.8 ± 0.5	-44767.5 ± 0.5
4	-49020.6 ± 0.5	-44724.2 ± 0.5
3	-48972.3 ± 0.5	-44681.6 ± 0.5
2	-48924.4 ± 0.5	-44639.9 ± 0.6
1	-48882.5 ± 0.6	-44639.9 ± 0.5
Bulk SPC 1	-80931.2 ± 0.6	-
Bulk SPC 0	-80886.4 ± 0.6	-

---

[1] Errors are obtained by calculating block averages, extrapolating to infinite block length.

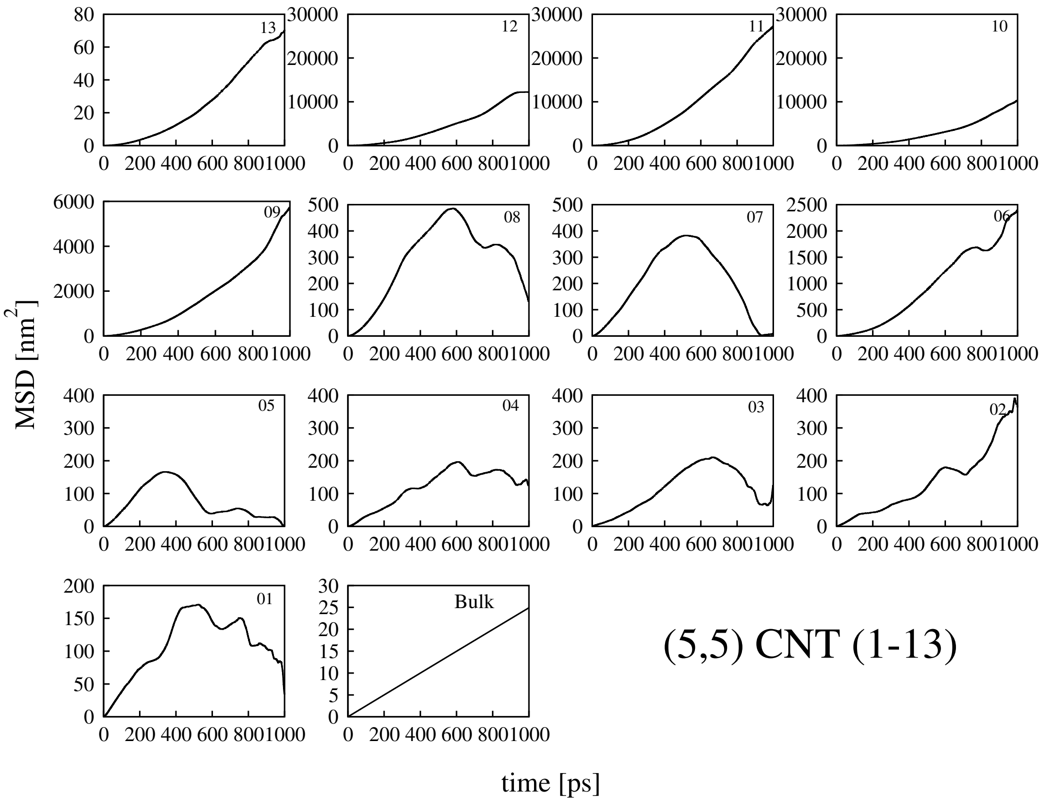


Supp. Fig. 5: Potential of mean force as a function of the load state (first row) and average number of hydrogen bonds per water molecule as a function of the load state (second row) for the (5,5) and (6,6) open tubes systems); Distributions of $\cos\theta$ (third row), for the (6,6) and (5,5) open tube systems. θ is the angle between the water dipole μ and the z axis. $\cos\theta$ was calculated for loadings equal or higher to 2, due to the noise added by lower loadings, as they shown no dipolar orientation preference.

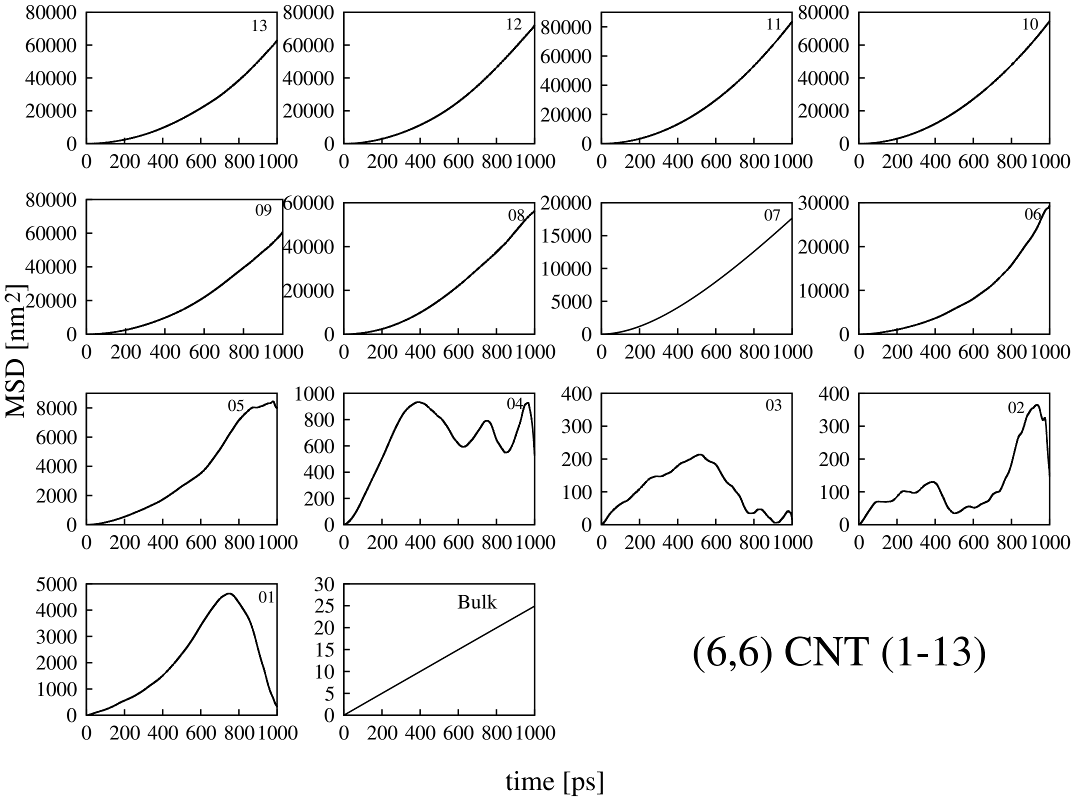
Supp. Table 2: Average velocity ($\langle V_z \rangle$), average absolute velocities ($\langle \sqrt{V_z{}^2} \rangle$) and diffusion coeficients (D_z) along the pore axis of the water oxygens within the pore

	SWCNT					
# Pore loading	System (6,6)			System (5,5)		
	< V_z> [nm/ps]	<sqrt V_z^2> [nm/ps]	D_z [nm^2/ps]	< V_z> [nm/ps]	<sqrt V_z^2> [nm/ps]	D_z [nm^2/ps]
13	-0.251 ± 0.008	0.424 ± 0.003	-	-0.008 ± 0.001	0.365 ± 0.001	-
12	-0.269 ± 0.005	0.432 ± 0.002	-	-0.110 ± 0.010	0.381 ± 0.001	-
11	-0.288 ± 0.003	0.437 ± 0.073	-	-0.165 ± 0.011	0.392 ± 0.003	-
10	-0.270 ± 0.004	0.429 ± 0.002	-	-0.102 ± 0.012	0.374 ± 0.004	-
9	-0.247 ± 0.008	0.420 ± 0.003	-	-0.076 ± 0.014	0.372 ± 0.002	-
8	-0.238 ± 0.009	0.415 ± 0.003	-	0.011 ± 0.018	0.364 ± 0.003	-
7	-0.022 ± 0.050	0.398 ± 0.005	-	-0.003 ± 0.020	0.371 ± 0.003	-
6	-0.171 ± 0.017	0.395 ± 0.005	-	-0.049 ± 0.014	0.371 ± 0.003	-
5	0.089 ± 0.022	0.381 ± 0.004	-	0.001 ± 0.019	0.352 ± 0.004	-
4	0.023 ± 0.03	0.390 ± 0.005	-	-0.011 ± 0.014	0.352 ± 0.003	0.172
3	0.004 ± 0.024	0.366 ± 0.005	0.290	-0.011 ± 0.013	0.349 ± 0.005	0.095
2	0.012 ± 0.025	0.333 ± 0.007	0.427	-0.019 ± 0.014	0.321 ± 0.007	0.156
1	0.0178 ± 0.044	0.279 ± 0.016	1.535	0.006 ± 0.019	0.246 ± 0.009	0.160

Bulk SPC D_{xyz} [nm^2/ps] = 0.004



Supp. Fig. 6: Mean-square displacement (MSD) of the water oxygens at every load state for the (5,5) systems and for bulk water as function of time.



Supp. Fig. 7: Mean-square displacement (MSD) of of the water oxygens at every load state for the (6,6) systems and for bulk water as function of time.