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Original
Water filling in carbon nanotubes with different wettability and implications on nanotube/water heat transfer via atomistic simulations / Casto, Alessandro; Bellussi, Francesco Maria; Diego, Michele; Del Fatti, Natalia; Banfi, Francesco; Maioli, Paolo; Fasano, Matteo. - In: INTERNATIONAL JOURNAL OF HEAT AND MASS TRANSFER. - ISSN 0017-9310. - ELETTRONICO. - 205:(2023), pp. 1-10. [10.1016/j.ijheatmasstransfer.2023.123868]

Availability:
This version is available at: 11583/2975768 since: 2023-05-29T11:08:32Z

Publisher:
Elsevier

Published
DOI:10.1016/j.ijheatmasstransfer.2023.123868

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12 June 2023

Water filling in carbon nanotubes with different wettability and implications on nanotube/water heat transfer via atomistic simulations: supporting information

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This supporting information document includes additional Notes, Figures and Tables detailing the methods and results presented in the main text.

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1. Supporting Note S1: Details on the Molecular Dynamics setup for the Free Energy Perturbation approach

A snapshot of the simulation for the FEP with the calculation of the work of adhesion and the corresponding CA is given in Figure S1.

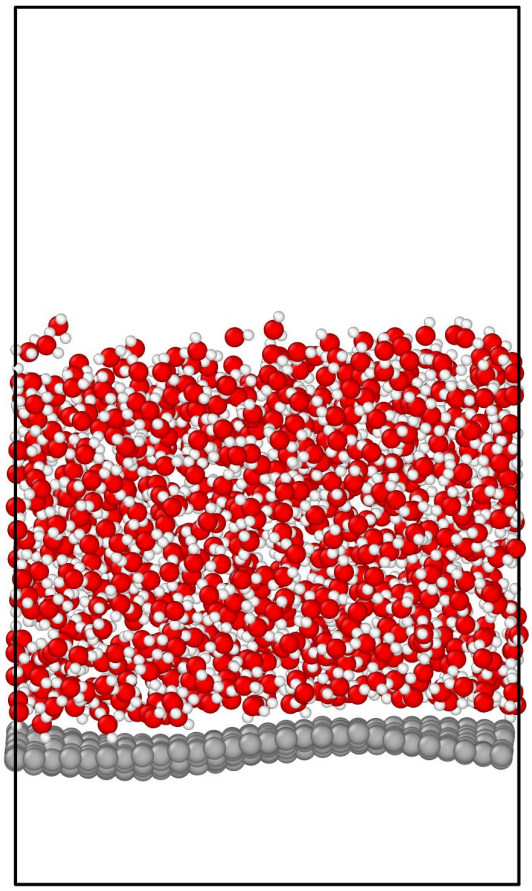

Figure S1: Snapshot of the simulation to calculate the work of adhesion between the graphene sheet and water.

2. Supporting Note S2: Details on the Lennard-Jones parameters mixing

We report the mixing rules used to calculate Lennard-Jones parameters for carbon-oxygen interaction combining SPC/E model for water [1] and OPLS-AA force field for aromatic carbon atoms [2]: $\sigma_{OO} = 0.3166$ nm, $\epsilon_{OO} = 0.1553$ kcal/mol for oxygen and, $\sigma_{CC} = 0.355$ nm, $\epsilon_{CC} = 0.07$ kcal/mol for carbon atoms. The values of $\sigma_{CO} = 0.3358$ nm, $\epsilon_{CO} = 0.10426$ kcal/mol correspond to geometric mixing rule (Equation S1), $\sigma_{CO} = 0.33525$ nm, $\epsilon_{CO} = 0.10426$ kcal/mol correspond to arithmetic mixing (Equation S2) while $\sigma_{CO} = 0.385$ nm, $\epsilon_{CO} = 0.0984$ kcal/mol are calculated by the six power mixing rule (Equation S3).

$$\epsilon_{CO} = \sqrt{\epsilon_{CC}\epsilon_{OO}} \qquad \sigma_{CO} = \frac{1}{2}\left(\sigma_{CC} + \sigma_{OO}\right) \tag{S1}$$

$$\epsilon_{CO} = \sqrt{\epsilon_{CC}\epsilon_{OO}} \qquad \sigma_{CO} = \sqrt{\sigma_{CC}\sigma_{OO}} \tag{S2}$$

$$\epsilon_{CO} = \frac{2\sqrt{\epsilon_{CC}\epsilon_{OO}}\sigma_{OO}^3\sigma_{CC}^3}{\sigma_{OO}^6 + \sigma_{CC}^6} \qquad \sigma_{CO} = \sqrt[6]{\frac{1}{2}\left(\sigma_{OO}^6 + \sigma_{CC}^6\right)} \tag{S3}$$

3. Supporting Note S3: Summary of the setups

In Figure S2 are shown snapshots of the MD setup.

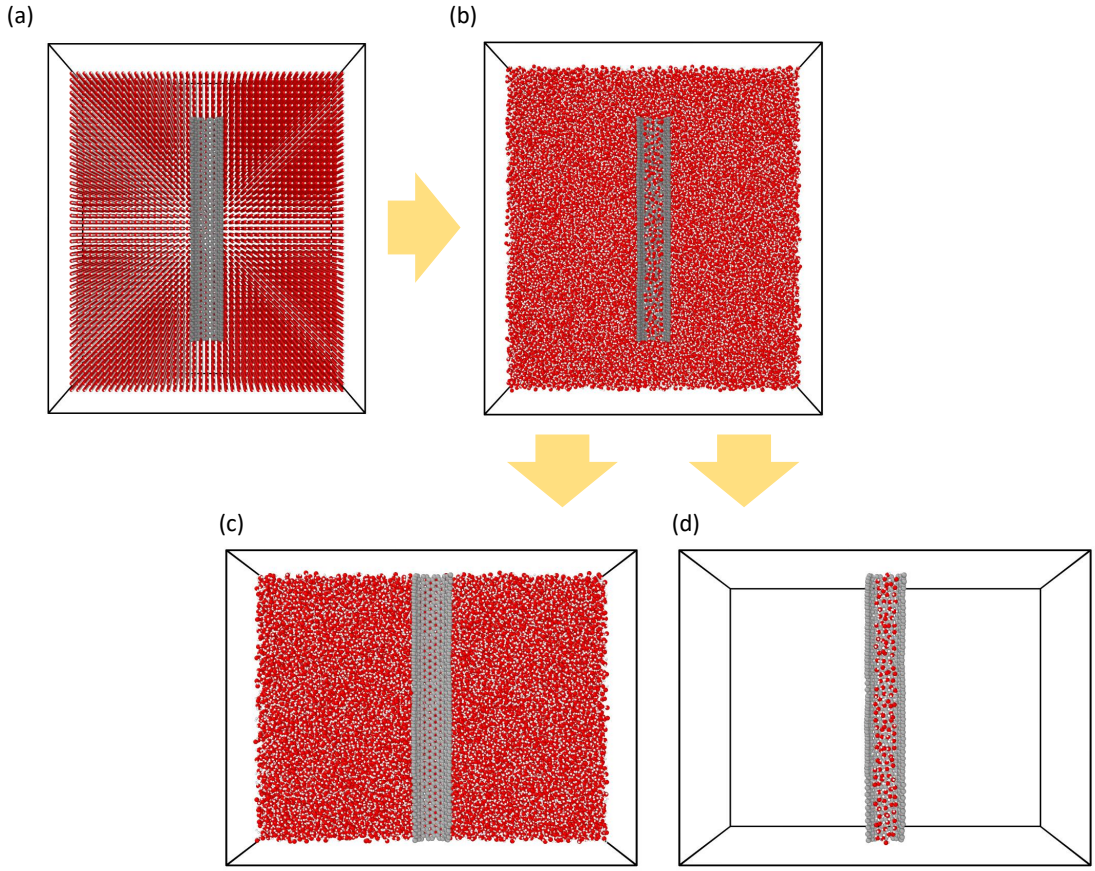

Figure S2: (a) Initial Molecular Dynamics setup with water molecules outside the nanotube. (b) Water molecules are let entering inside the CNT. The top and bottom parts of the simulation domain are then removed and periodic conditions are applied. Water molecules inside (outside) the CNT are then removed to compute TBR at the outer (inner) CNT/water interface, as in panels (c) and (d) respectively.

4. Supporting Note S4: Computation of the Thermal Boundary Resistance

The thermal boundary resistance is calculated following the method used by Jabbari et al. [3]. The time-dependent temperature profiles of the two carbon nanotubes geometries with water molecules outside the tube are shown in Figure S3. The slope of the curves in Figure (c) and (d), displaying the energy as a function of the integral of temperature difference, allows direct extraction of the TBR using equation S4.

$$\frac{S}{R_K} = -\frac{E_t - E_0}{\int_0^t (T_p - T_a)\, dt} \tag{S4}$$

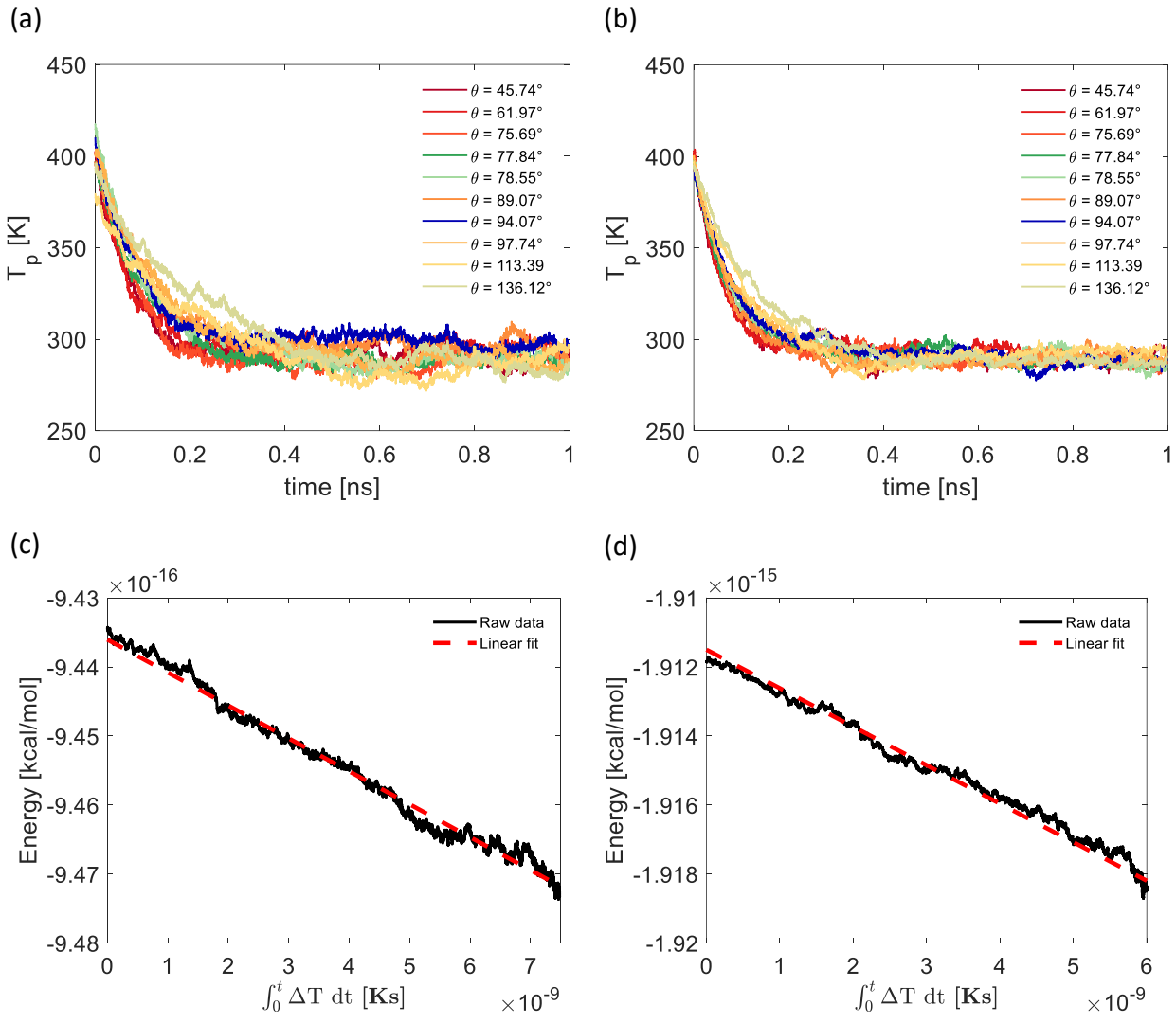

Figure S3: (a) and (b) temperature decays of the CNT for empty (5,5) and (10,10) CNTs with water molecules outside. (c) and (d) energy decays for $\theta = 45.74°$ and their linear fit leading to determination of TBR.

5. Supporting Note S5: β parameters for the carbon nanotubes

β parameter for the two CNT geometries are reported in Table S1.

	σ **[nm]**	ϵ **[kcal/mol]**	$\beta_{(5,5)}$ **[kcal/mol]**	$\beta_{(10,10)}$ **[kcal/mol]**
	0.3190	0.1498	-0.1928	-0.6800
	0.3190	0.1348	-0.1736	-0.6122
	0.3190	0.1199	-0.1546	-0.5442
	0.3352	0.1043	-0.0784	-0.5273
	0.3358	0.1043	-0.0765	-0.5291
	0.3190	0.1049	-0.1350	-0.4762
	0.3385	0.0984	-0.0635	-0.5080
	0.3190	0.0937	-0.1206	-0.4253
	0.3190	0.0749	-0.0964	-0.3401
	0.3190	0.0445	-0.0578	-0.2040

Table S1: β parameter in [kcal/mol] for different interaction parameters.

6. Supporting Note S6: Stable number of water molecules as a function of Contact Angle

The number of water molecules at equilibrium is represented as a function of CA in Figure S4. Comparison of this figure and Figure 3 in the main text (with β in the horizontal axis) indicates that β seems to better predict the filling of water molecules inside CNTs, especially around the hydrophilic/hydrophobic transition. Differences are more prominent for the (10,10) CNT.

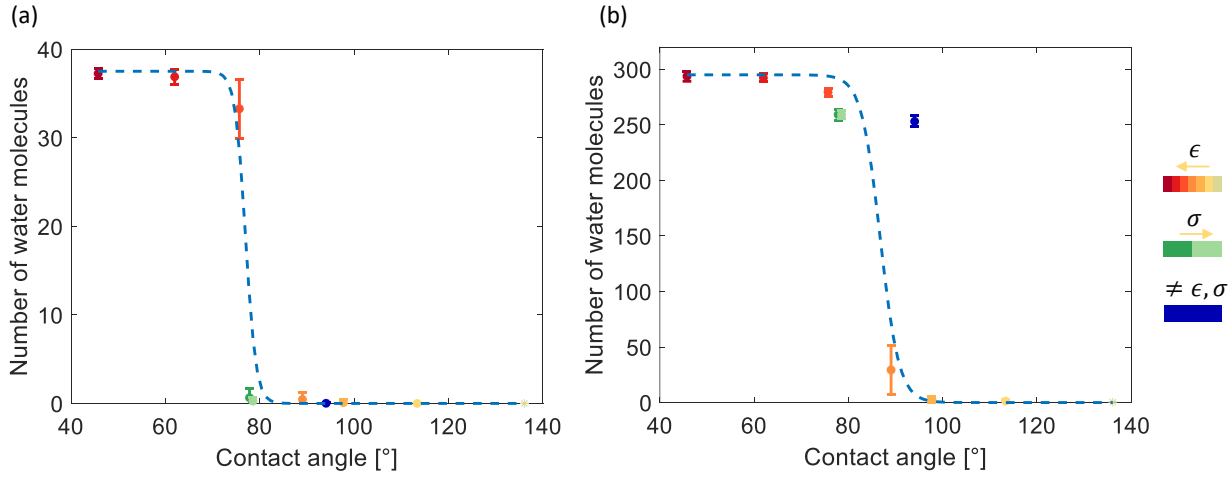

Figure S4: Stable number of water molecules in the CNT for the (5,5) (a) and (10,10) (b) cases.

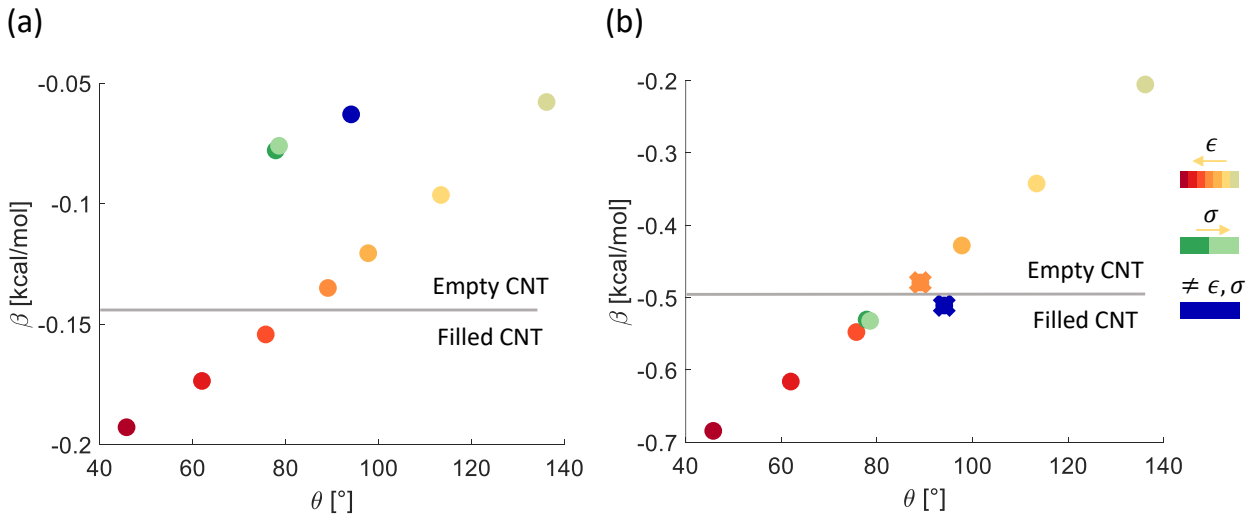

Figure S5: β parameter is plotted as a function of CA for the (5,5) (a) and (10,10) (b) CNTs. The grey line indicates the limit of spontaneous filling of the nanotube.

7. Supporting Note S7: Shape of the potential in the outer region of CNT

In Figure S6 it is displayed the $U(r)$ as calculated in Equation 8 of one oxygen atom along the radius of the CNTs in the mid cross-section.

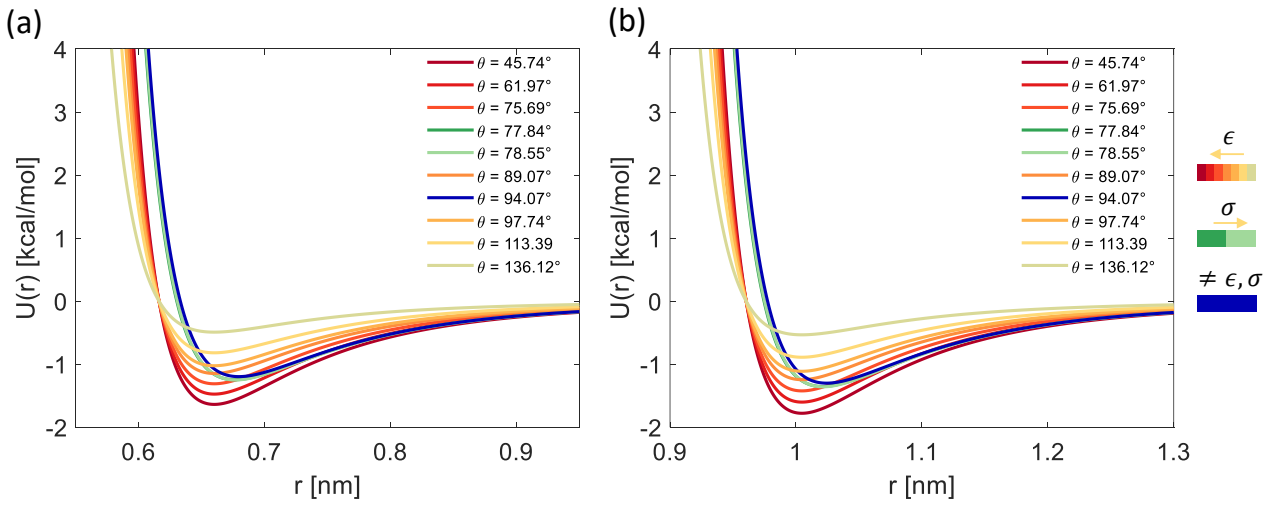

Figure S6: a) Interaction potentials between all the C atoms of a (5,5) CNT and an O atom at position r in the mid-length cross-section. b) Same for a (10,10) CNT.

References

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