Supporting Information

Curious characteristics of polar and non-polar molecules confined within carbon nanotubes (CNT) of varied diameter: Insights from Molecular Dynamics simulation

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Table S1. Bonded forcefield parameters

Molecules/Ions	bonds	K (kcal/mol)	r_{eq}
CNT	C-C	938	1.42
SPC (H_2O)	H-O	345000	0.10
CH_3OH	C-H	553	1.03
	C-O	300	1.26
	O-H	300	1.54
CH_4	C-H	525	1.48
	Angles	K (kcal/mol)	θ_{eq}
CNT	C-C-C	126	120.0
SPC (H_2O)	H-O-H	383	109.5
CH_3OH	H-C-H	45	105.3
	O-C-H	150	120.0
	C-O-H	125	114.0
CH_4	H-C-H	100	108.2

Table S2. Nonbonded forcefield parameters

molecules/ions	site	σ (Å)	ε (kcal/mol)
CNT	C	3.40	1.224
SPC (H_2O)	O	3.17	0.650
	H	1.00	0.000
CH_3OH	C	3.5	0.276
	H	2.5	0.126
	O	3.12	0.711
	H	1.00	0.000
CH_4	C	3.5	0.276
	H	2.5	0.126

Table S3. Charge parameters

molecules/ions	site	q (coul)
CNT	C	0.0
SPC (H_2O)	O	-0.82
	H	0.41
CH_3OH	C	0.145
	HC	0.04
	O	-0.683
	HO	0.418
CH_4	C	-0.240
	H	0.060

Table S4. Bond order parameter for CNT confined water molecules

CNT	Bond order value
CNT(6,6)	0.506
CNT(7,7)	0.426
CNT(8,8)	0.197
CNT(9,9)	0.159
CNT(10,10)	0.127
CNT(12,12)	0.094

Orientation of confined water molecules w.r.t. nanotube axis was evaluated using the order parameter, given as equation S1. $S = \left\langle 0.5(3\cos^2\theta - 1) \right\rangle$ --- (S1)

where θ is the angle between nanotube-axis and dipole moment of water molecules. S vector is averaged over time and over all water molecules, confined inside the CNT.