Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

Pressure induced phase diagram of double-layer ice under confinement: A first-principles study

M. V. Jyothirmai[1], B. Moses Abraham[1] and Jayant K. Singh[1,2]*

[1]*Department of Chemical Engineering, Indian Institute of Technology Kanpur, Kanpur-208016, India.*

[2]Prescience Insilico Private Limited, Bangalore 560049, India.

*E-mail: jayantks@iitk.ac.in

Table S1: Computed lattice cohesive energy per water molecule (E_{latt}) using various DFT functionals.

	Buckled	**HCP**	**Hexagonal**	**Pentagonal**	**Square**	**Square-tube**
LDA	0.86	0.85	0.93	0.89	0.85	0.87
PBE	0.45	0.48	0.57	0.51	0.48	0.49
TS	0.55	0.58	0.63	0.59	0.57	0.58
D3	0.55	0.57	0.64	0.59	0.56	0.58
optB88	0.56	0.58	0.61	1.14	0.56	0.58
optB86B	0.55	0.58	0.61	0.58	0.56	0.58

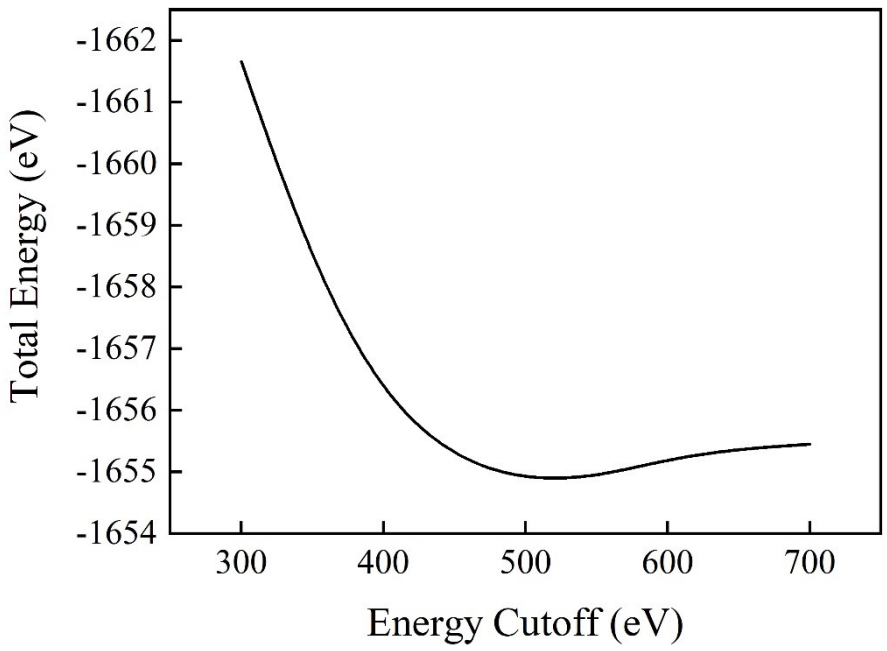

Figure S1: Relative energies of carbon nanotube as a function of cutoff values by using DFT-D3 dispersion correction method.

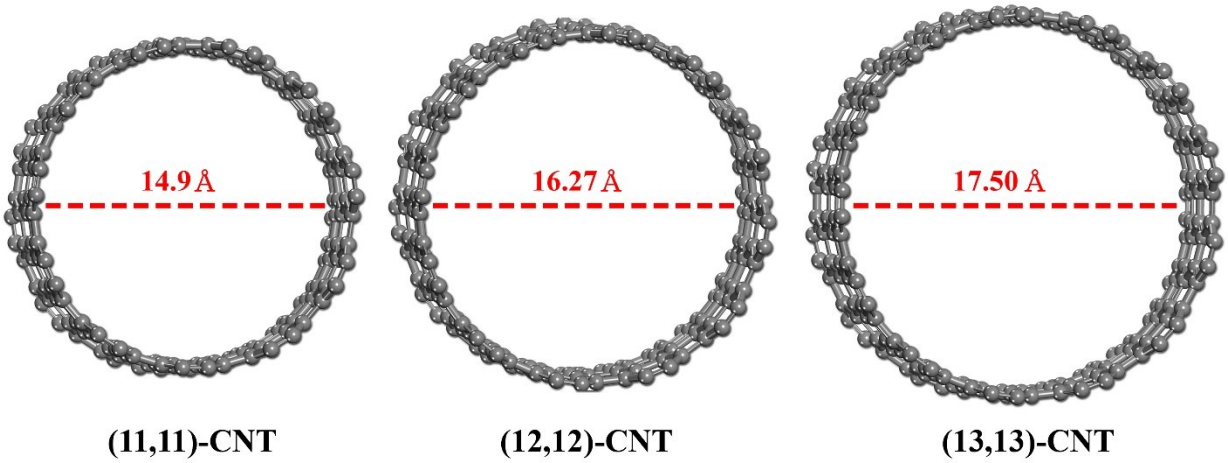

Figure S2: Optimized structures of (11,11)-CNT, (12,12)-CNT and (13,13)-CNT with a diameter of 14.9, 16.27 and 17.50 Å, respectively. The grey color balls represent carbon atoms.