Supporting Information

Possible formation of H_2-hydrate in different nanotubes and surfaces using molecular dynamic simulation

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Table S1. The lateral and perpendicular components of the pressures tensor of the confined water molecules in the different systems. The x-direction is parallel to the nanotubes and surfaces. The z-direction is perpendicular to the nanotube and surfaces.

System		$P\parallel:(P_{xx}+P_{yy})/2$ (katm)	$P^{\perp}: P_{zz}$ (katm)
126 H_2O and 18 H_2 in Nanotubes	Carbon	0.1967	0.3149
	BN	-0.1845	-0.1052
	SiC	0.7565	0.8209
210 H_2O and 38 H_2 between Surfaces	Carbon	0.9024	3.3812
	BN	8.2469	21.800
	SiC	9.8643	25.462

Table S2. The lateral and perpendicular components of the pressures tensor of the confined water molecules in the different systems

System		$P\parallel:(P_{xx}+P_{yy})/2$ (katm)	$P\perp: P_{zz}$ (katm)
210 H_2O and 38 H_2 between Surfaces	Carbon	0.9024	3.3812
	new BN	1.4189	5.6005
	new SiC	1.2073	5.0366

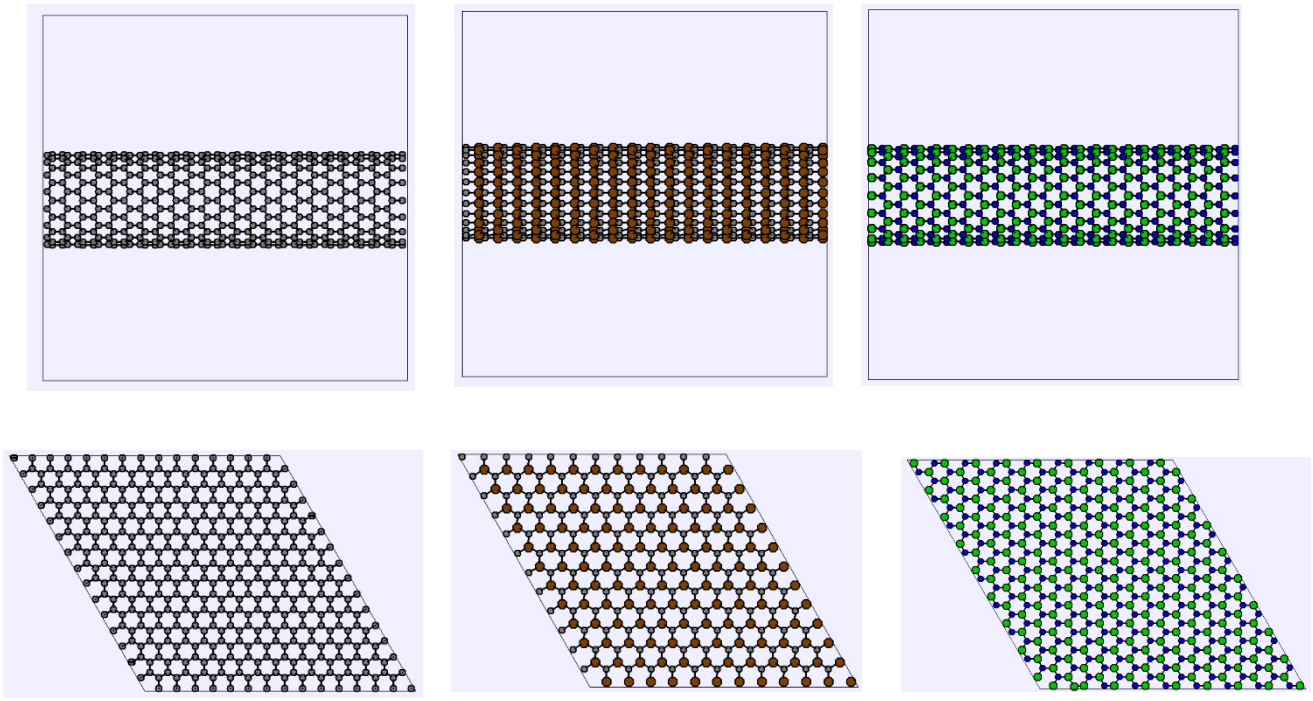
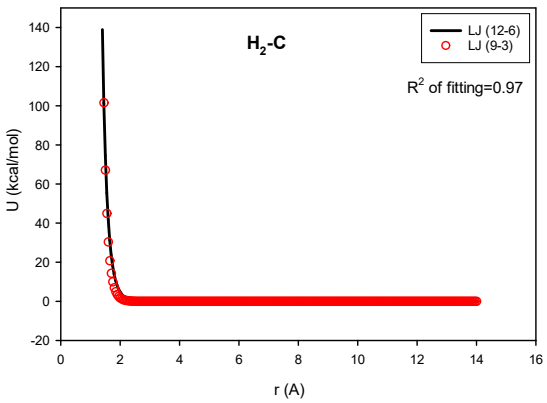
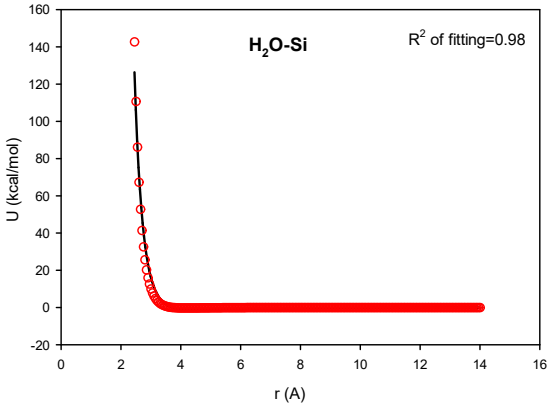
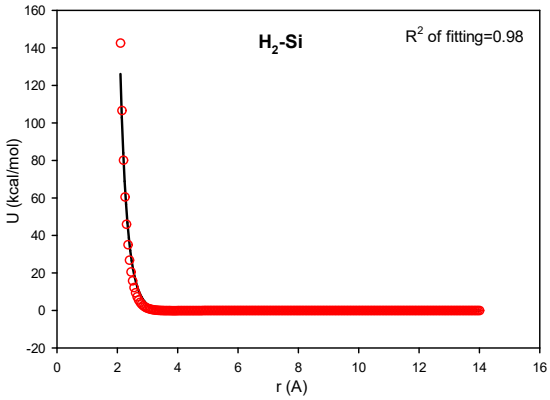
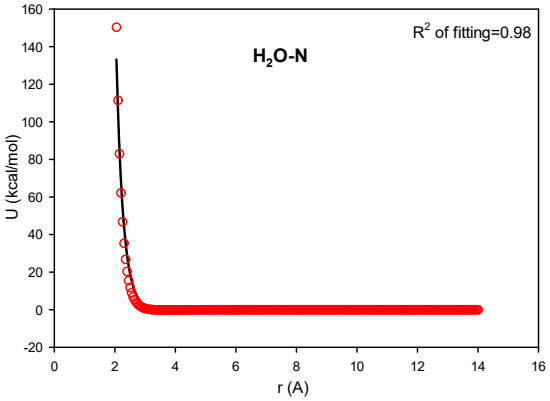


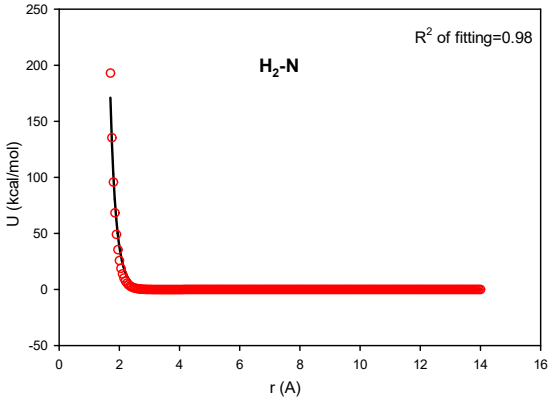
Fig. S1. The snapshots of all nanotubes and surfaces used in this work.

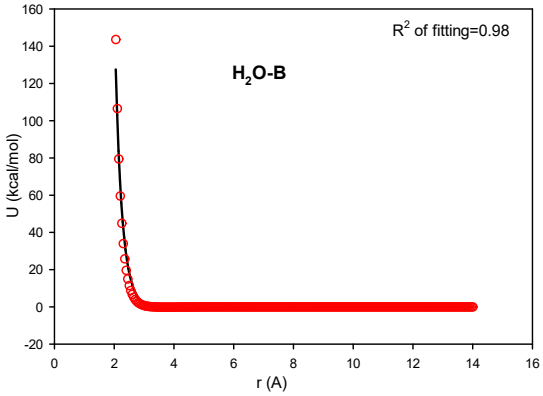

H2-C
LJ (12-6)
LJ (9-3)
R2 of fitting=0.97
U (kcal/mol)
r (A)


H2O-Si
R2 of fitting=0.98
U (kcal/mol)
r (A)


H2-Si
R2 of fitting=0.98
U (kcal/mol)
r (A)


H2O-N
R2 of fitting=0.98
U (kcal/mol)
r (A)


H2-N
R2 of fitting=0.98
U (kcal/mol)
r (A)


H2O-B
R2 of fitting=0.98
U (kcal/mol)
r (A)

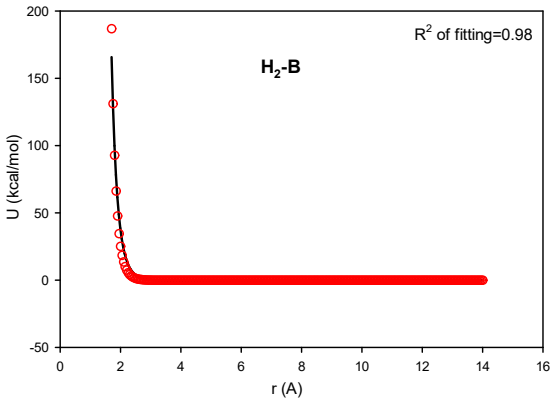


Fig. S2. The fitted (9-3) LJ potential to the (12-6) potential for different interactions.

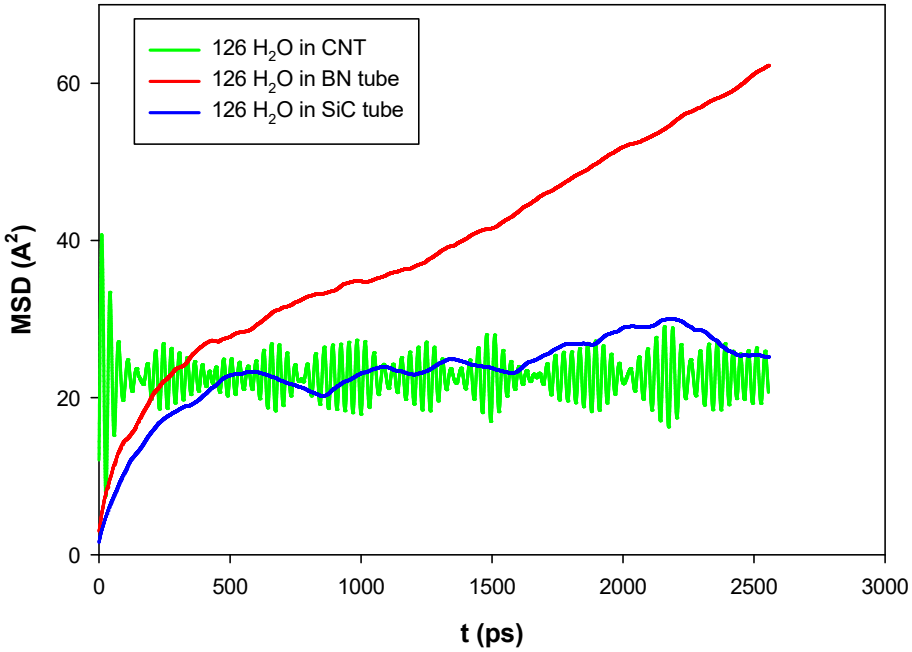


Fig. S3. The MSD curves of the confined H_2 molecules in the different nanotubes.

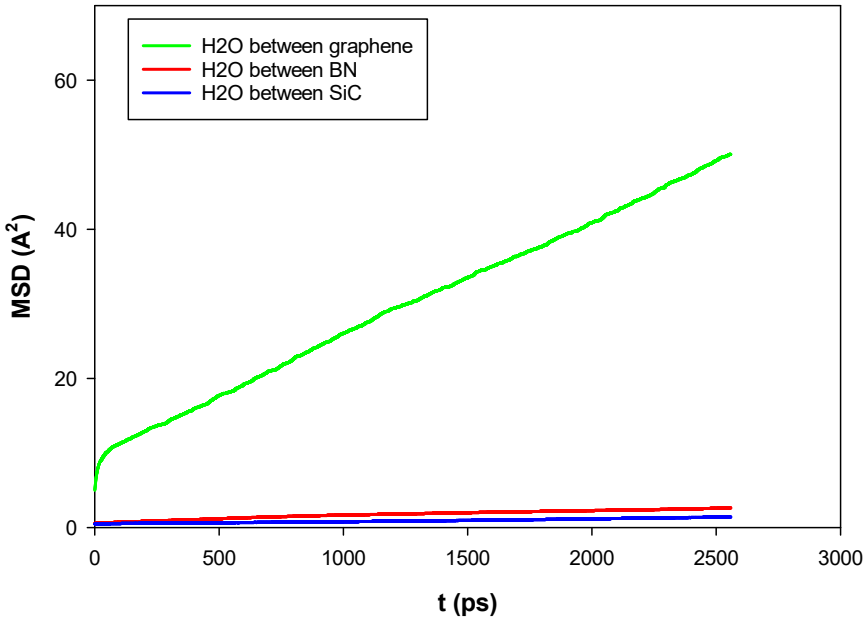


Fig. S4. The MSD curves of the confined H_2 molecules between the different surfaces.

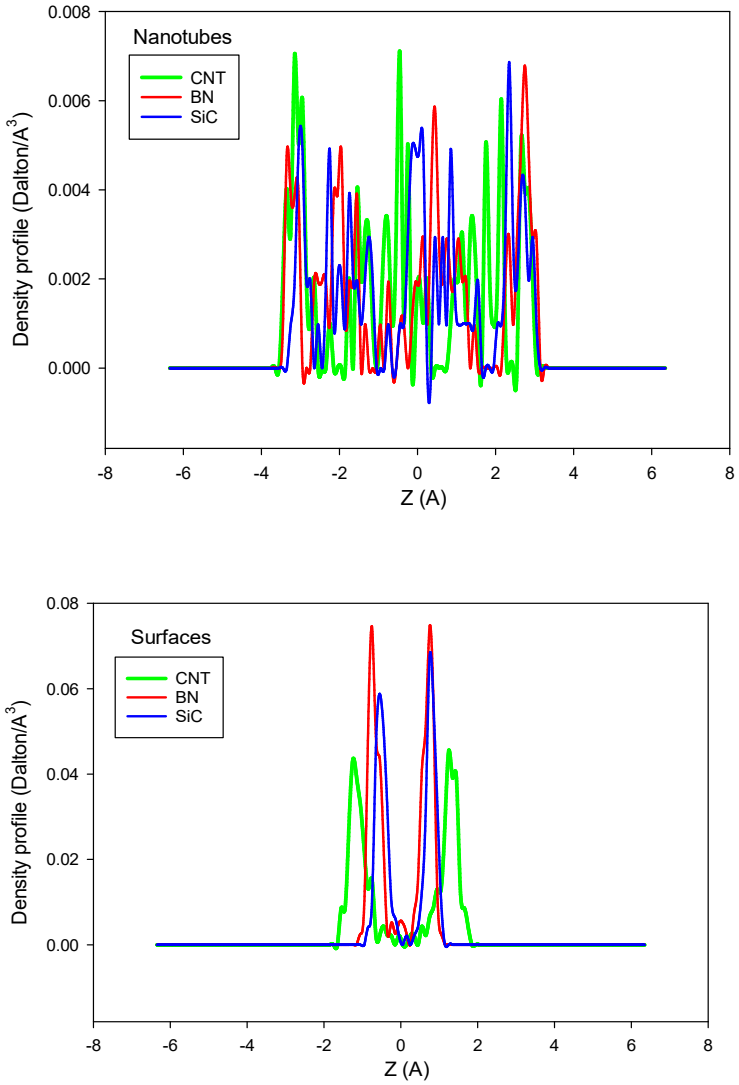


Fig. S5. The density profiles of the confined water molecules in the different nanotubes and surface.

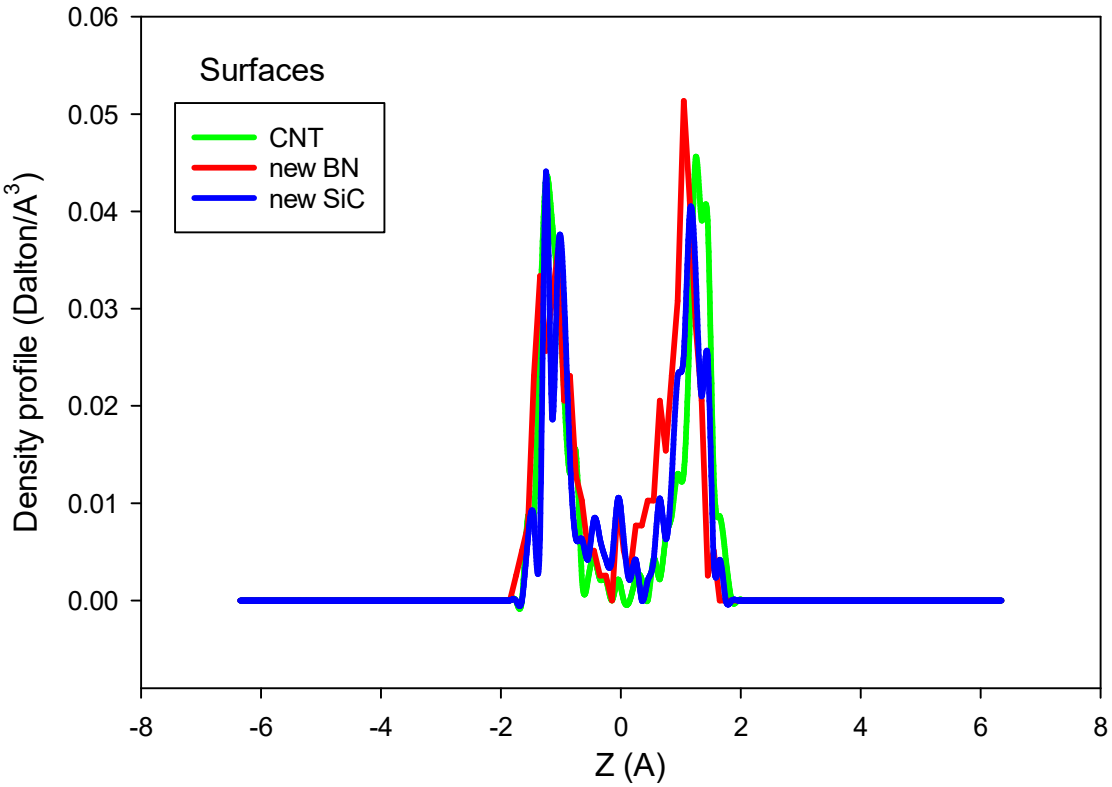


Fig. S6. The density profiles of the confined water molecules in the different surfaces.