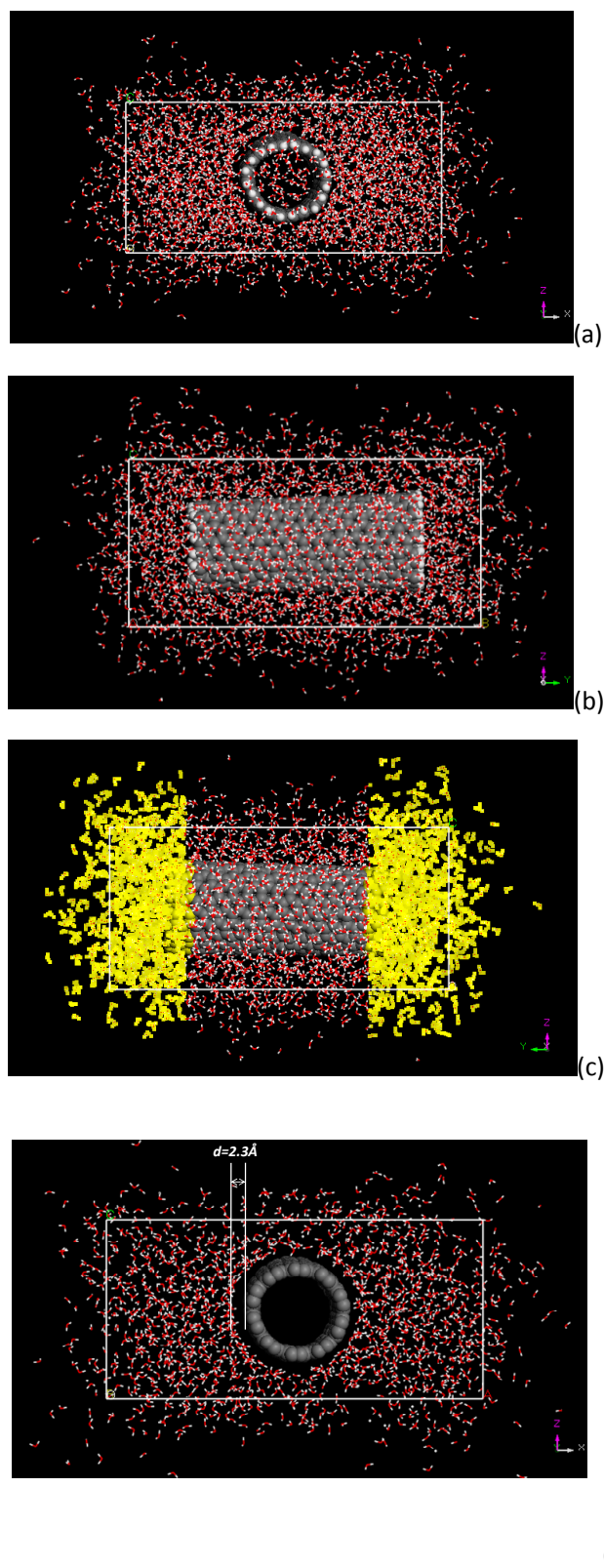
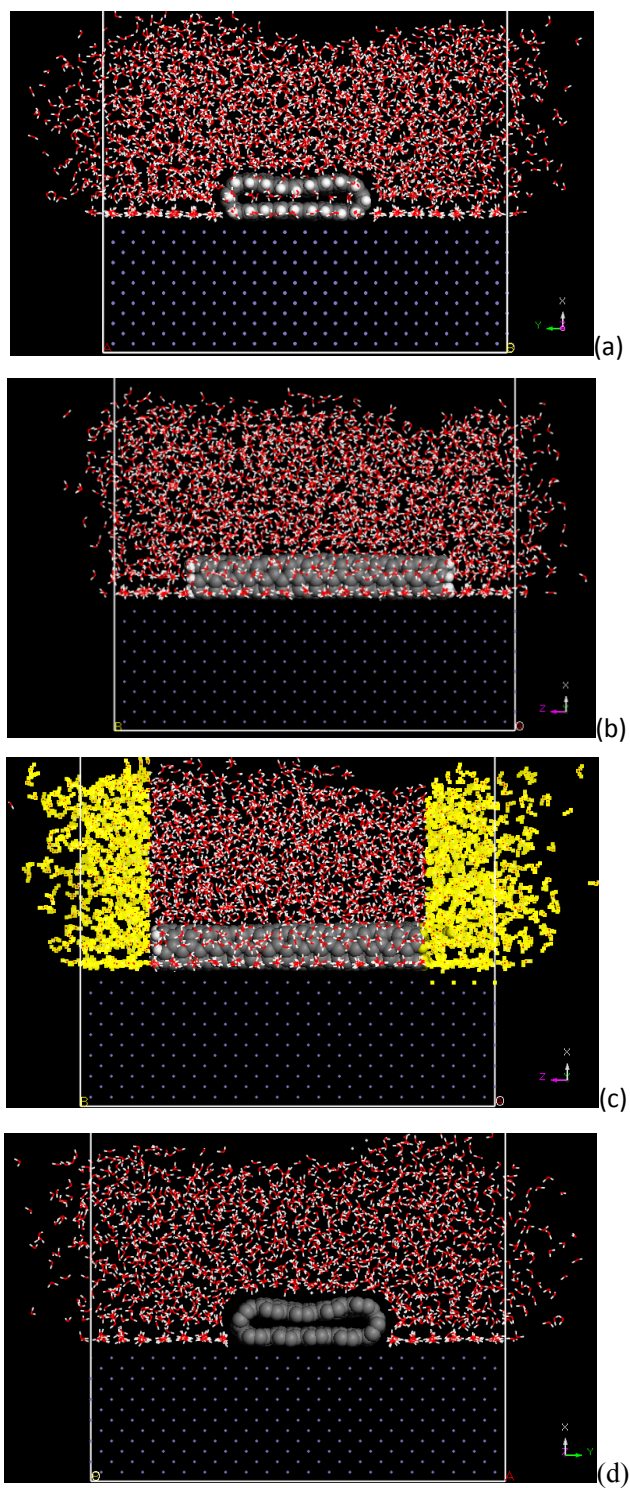




S1: The complete equilibrium snapshot of the CNT-water system. (a-b) The snapshot of the system in z-x and z-y plane; (c) The yellow parts represent the checked H₂O molecules outside two ends of CNT in y-z plane; (d) The sectional view after deleting the checked H₂O molecules in x-z plane.

A model of the composite system is embedded by the intrinsic CNT, which is consisted of a supercell in the range of $57 \times 57 \times 27 \text{ \AA}^3$. The initial density of water is 1 g/cm^3 at 300K. The model is put into a NVT ensemble simulation with a temperature of 300K for 500ps at a time step of 1 fs. The S1 shows that the complete equilibrium snapshot of the CNT-water system. We can observe that the CNT doesn't deform in water solvent; we calculate the binding energy ($199.037327 \text{ kcal/mol}$) between CNT and water, which shows that there exists the repulsive interaction force between CNT and water. Moreover, the space (d) between the water molecular and the CNT is about $2.3 \text{ \AA}$, which shows that the water moleculars don't contact the CNT. In addition, as shown in S1 (d), we can observe that there doesn't exist the water molecular in the interior of the CNT. The results show the hydrophobicity of the CNT. The video S1 shows the equilibrium process of the CNT-water system.



S2: The complete equilibrium snapshot of the collapsed CNT/Fe-water system. (a-b) The snapshot of the system in x-y and x-z plane; (c) The yellow parts represent the checked H₂O moleculars outside two ends of CNT in x-z plane; (d) The sectional view after deleting the checked H₂O moleculars in x-y plane.

We construct the model of the collapsed CNT/Fe in water solvent. The initial density of water is 1 g/cm^3 at 300 K. The model is put into a NVT ensemble simulation with a temperature of 300 K for 500 ps at a time step of 1 fs. The S2 shows that the complete equilibrium snapshot of the collapsed CNT-water system. As shown in S1(d), we can observe that the collapsed CNT can isolate the Fe surface from water solution due to the hydrophobicity of the CNT indeed. Moreover, because the interface adhesion is very strong between the collapsed CNT and Fe surface, the collapsed CNT isn't be removed from the Fe surface in water solvent. Therefore, the CNTs collapsed onto Fe surface have potential application in corrosion protection and scale inhibition fields.