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Enhanced Wettability of Long Narrow Carbon Nanotubes in a Double-walled Hetero-structure: Unraveling the Effects of Boron Nitride Nanotube as the Exterior

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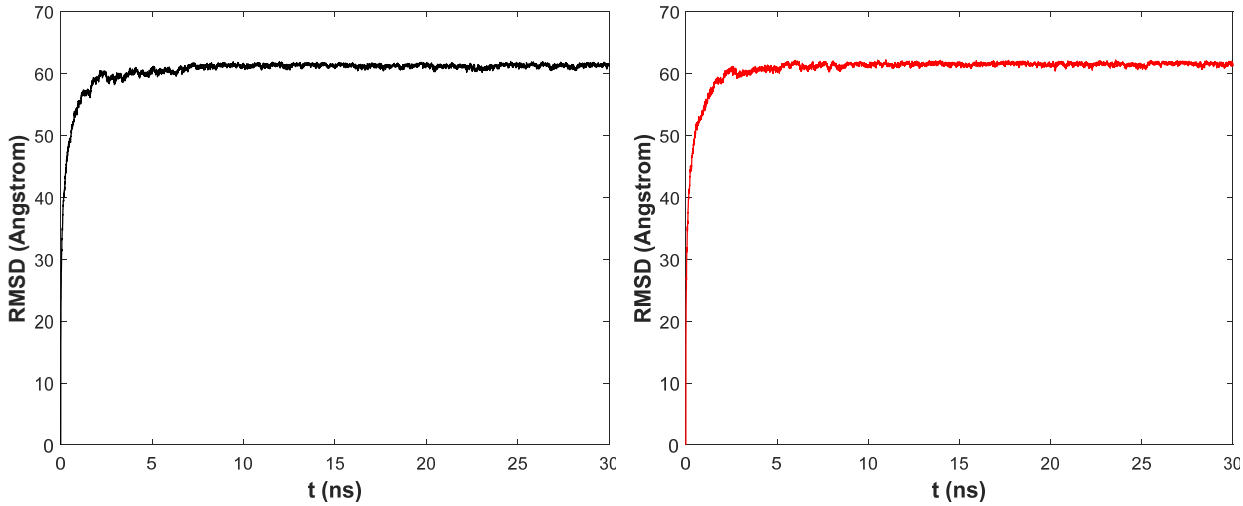
Equilibration of water in the system

In order to ensure the equilibrium of water, the root mean square deviation (RMSD) for water molecules was evaluated. As illustrated in Figure S1, the RMSD diagram for both systems fluctuates around a constant level in a restricted way after 7 ns.



(a) (b)

Figure S1. RMS deviation for water molecules. Panels (a) and (b) demonstrate the RMS deviation of water in SWNT and DWHNT systems respectively.

The average electrostatic potential map

The electrostatic potential map is evaluated by VMD plugin PMEpot. NAMD computes long-range electrostatic forces controlled by particle-mesh Ewald (PME) factors. In this algorithm, each point charges are assumed as spherical Gaussian:

$$\rho_i(r) = q_i\left(\frac{\beta}{\sqrt{\pi}}\right)^3 e^{-\beta^2|r-r_i|^2}$$

The potential electrostatic is calculated by solving Poisson equation:

$$\nabla^2\varphi(r) = 4\pi\sum_i \rho_i(r)$$

Finally, the instantaneous electrostatic potential φ(r) is averaged over the entire MD trajectories to obtain the mean electrostatic potential. Averaging the potential electrostatic over the nano-channel dimensions and depicting in the X-Y plane results an electrostatic potential map [1].

Water permeability

The number of water molecules permeating through the nano-channels along the both direction of the Z axis per simulation time was obtained in terms of water permeability calculation. The following equation was used to calculate the water permeability (P_W);

$$P_W = \frac{R_t\, v_w}{N_A} \qquad \text{S1}$$

In the equation S1, v_w and N_A represent average volume of a single water molecule and, Avogadro's number, respectively. Furthermore, R_t is the rate of water permeating through the nano-channels [2,3].

References

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