Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supplementary Information

Coupling Solute Interactions with Functionalized Graphene Membranes: Towards Facile Membrane-Level Engineering

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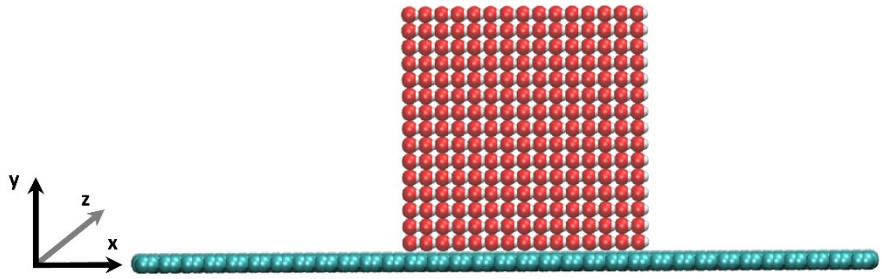

Fig. S1 Initial configuration for the droplet simulation where water molecules are arranged in a cubic lattice structure over the graphene membrane with similar wetting characteristic with the nanoporous graphene membrane.

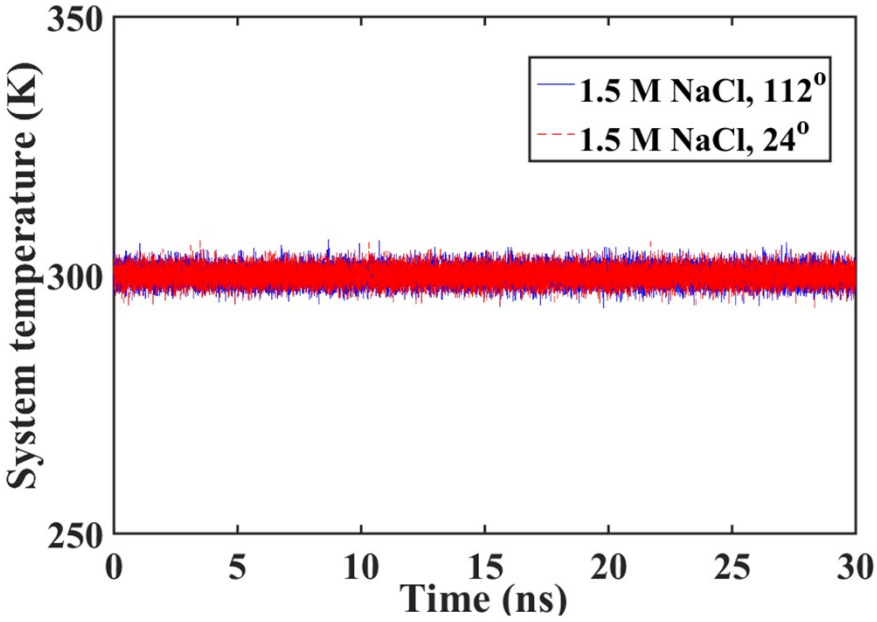

Fig. S2 Time evolution of average system temperature for $\theta_e = 112°$ and $\theta_e = 24°$ at $1.5M$ $NaCl$ concentration. Steady temperature is achieved for both the cases with minor fluctuation of temperature around the mean.

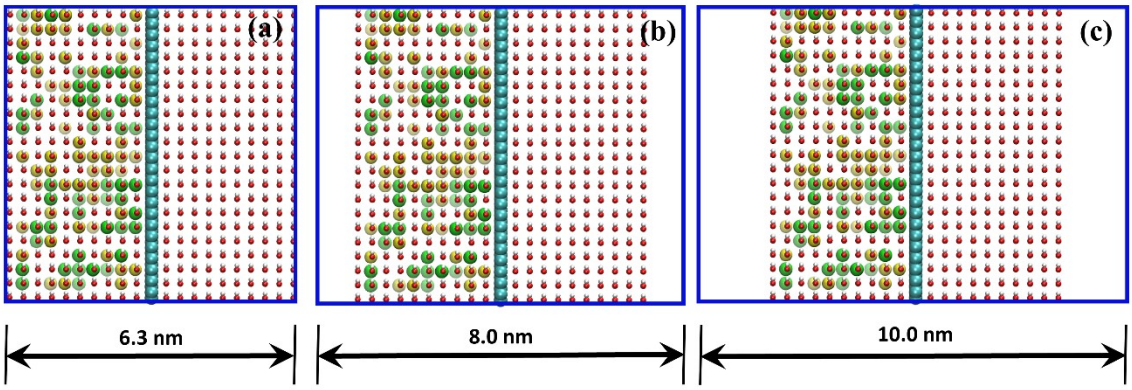

Fig. S3 Initial configurations of the simulation domain with three different box sizes being considered where the axial direction was varied from $6.3-10nm$.

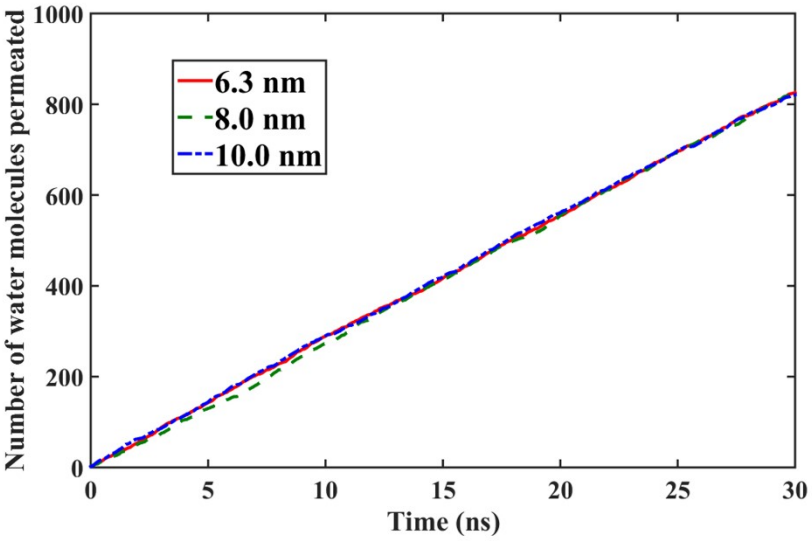

Fig. S4 Permeation of water molecules as a function of simulation time for equilibrium contact angle of 41° and $NaCl$ concentration of $1.5M$ for box sizes of $6.3nm$, $8nm$ and $10nm$.The permeation behaviour of water molecules almost coincides with each other signifying negligible effect of box size on the simulation dynamics.