Electronic Supplementary Material (ESI) for Nanoscale Advances.

Strength, Number, and Kinetics of Hydrogen Bonds for Water Confined inside Boron Nitride Nanotubes: Supplementary Material

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S1. Hydrogen Bond Potential of Mean Forces for Water Molecules Supported by hexagonal Boron Nitride (h-BN) Sheet

We performed a ReaxFF MD simulation of a water slab on a hexagonal Boron Nitride (h-BN) sheet [see Fig. S1(a)] in the NVT ensemble at a temperature of 300 K. The h-BN sheet was parallel to the XY plane, and the water slab was approximately 4 nm tall in the Z dimension. Periodic boundary conditions were used in all the three dimensions, and to inhibit interactions between periodic images in the Z direction, we left a vacuum slab of ~ 150 Å. The simulations lasted 5 ns and we used the last 3 ns as the production trajectory. We sampled r and θ every 500 fs for the analysis. To study the hydrogen bond (HB) PMF of the interfacial water, we considered the water molecules within 2 nm from the h-BN sheet [see Fig. S1(b)]. We used the same procedure described in the **Methods** section (see the main paper) to obtain the HB PMF. Figure S1(c) shows the HB PMF for the h-BN-sheet-supported interfacial water molecules along with the HB basin boundary (solid black line). As the radius of the boron nitride nanotube (BNNT) increases and a BNNT transitions to a h-BN sheet at the limit of infinite radius, the HB PMF shows a near identical behavior to that of bulk water. As the confinement effect completely disappears, the second solvation basin is found to be situated close to the HB basin and is separated by a saddle region as seen in Fig. S1(c). While similar behavior was also seen in the (12, 12) BNNT system, we see a much closer resemblance between the bulk water and BN sheet interfacial water (in terms of the water HB PMF), despite the same interfacial interactions imparted by the BNNT and the BN sheet on nearby water molecules.

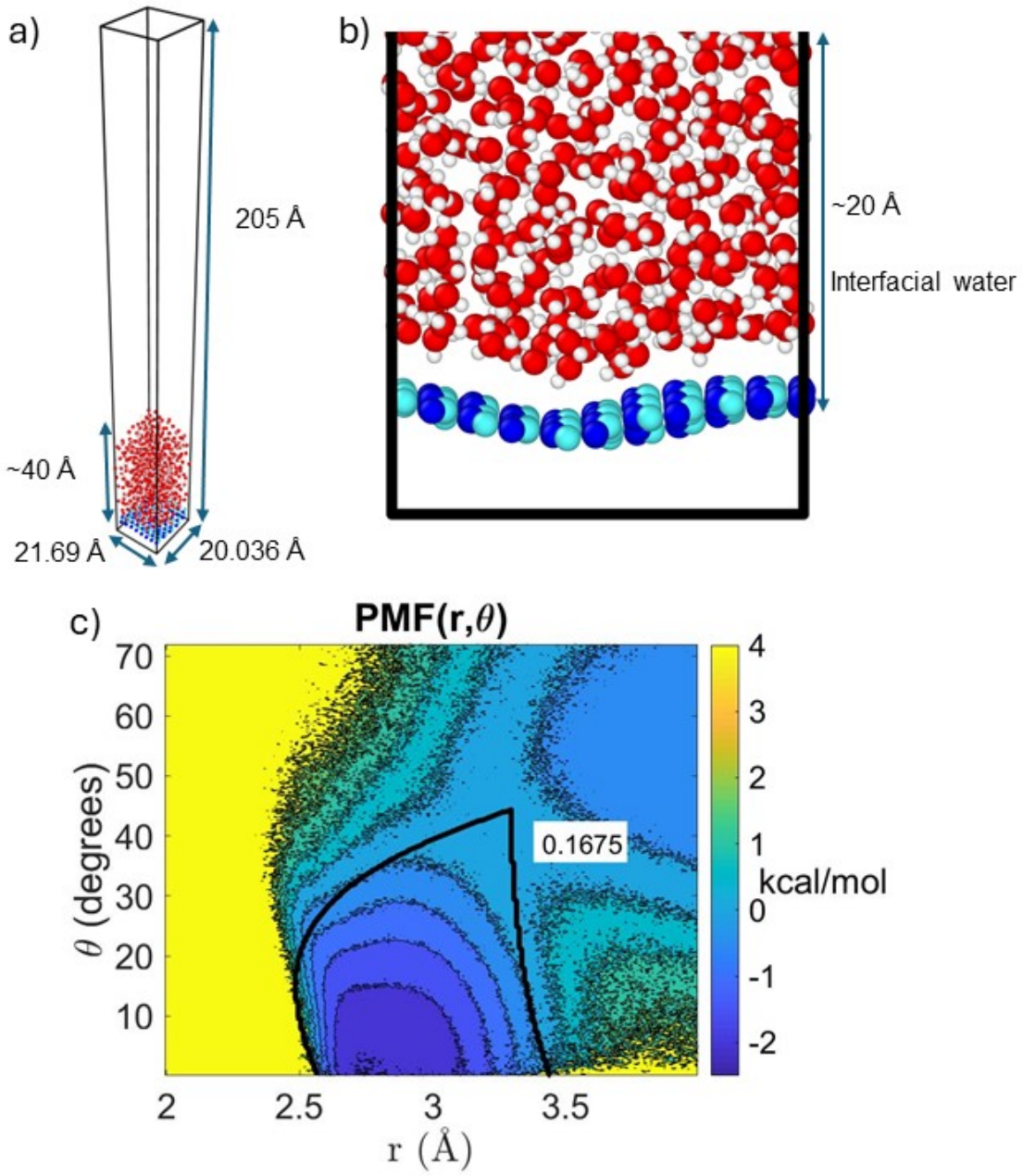

Figure S1: (a) MD simulation snapshot showing a water slab on a Boron Nitride (BN) sheet. (b) Identification of the interfacial water layer that is used to obtain the hydrogen bond PMF for the BN-sheet-supported interfacial water molecules. (c) Two dimensional potentials of mean force (2D PMF) as functions of r and θ for the BN-sheet-supported interfacial water molecules. In this figure, the continuous black contour line and the adjacent label indicate the iso-surface separating the HB basin and the corresponding PMF value at this iso-surface, respectively.