

SUPPLEMENTARY INFORMATION

Temperature effects on the hydrophobic force between two graphene-like surfaces in liquid water

TUHIN SAMANTA and BIMAN BAGCHI

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bangalore, Karnataka 560 012, India

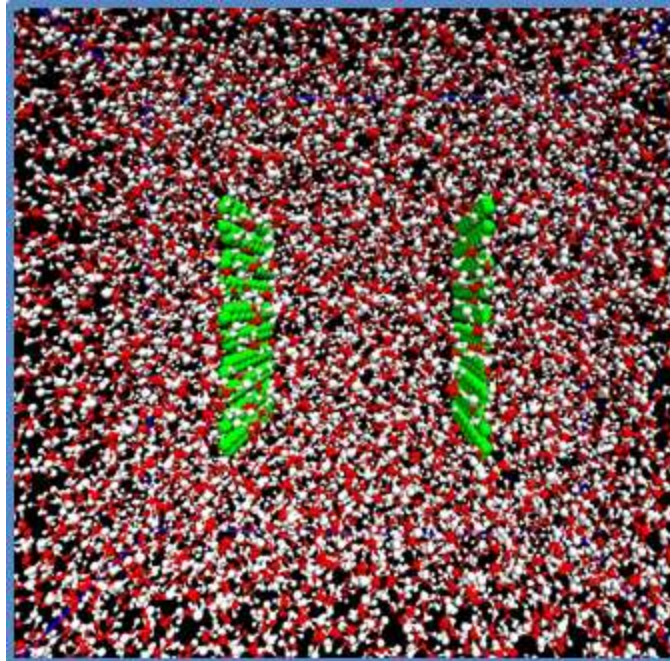
Table of Contents

Figure S1 **Page 2**

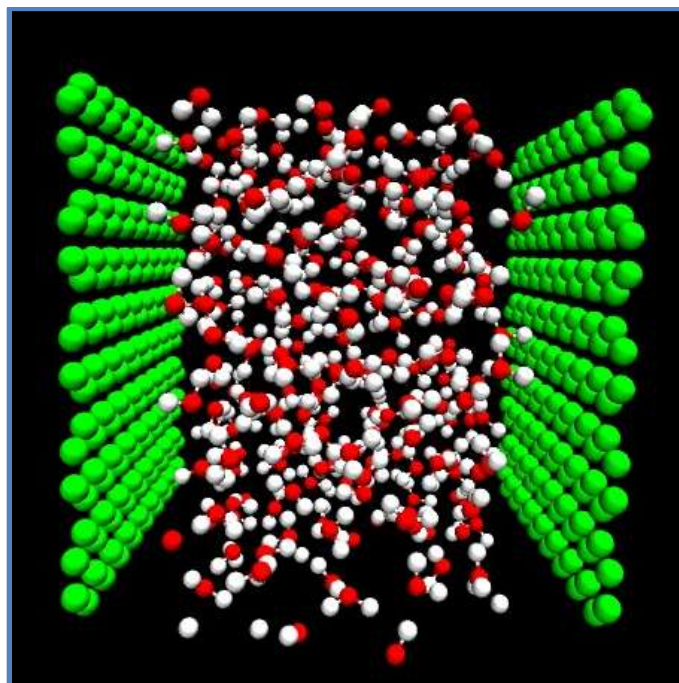
Figure S2-S3 **Page 3**

Figure S4 **Page 4**

Figure S5 **Page 5-6**



(a)



(b)

Figure S1. (a) A representative snapshot of the simulation of the system and (b) representative snapshot of the confined water molecules between two hydrophobic walls are shown for $d = 20 \text{ \AA}$ interwall separations, at $T = 240 \text{ K}$.

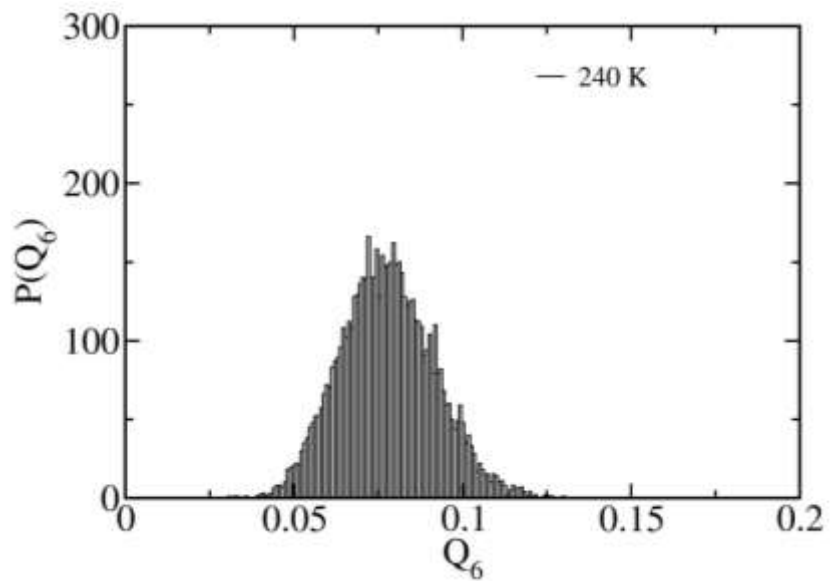


Figure S2. The distribution of local order parameter Q_6 , introduced by Steinhardt *et al.*¹ for water, at $T = 240$ K. The average value (in bulk) of Q_6 (~ 0.078) corresponds that water exists in the liquid phase.

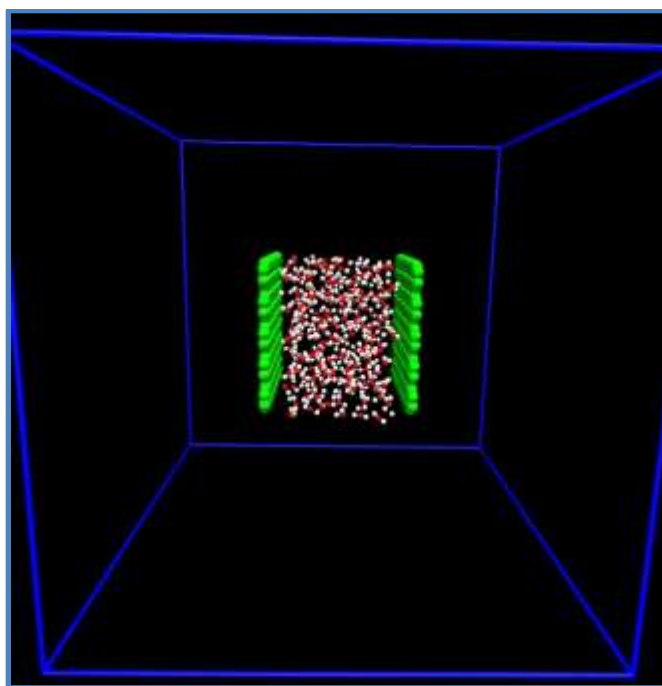


Figure S3. Representative snapshot of the simulation of the confined water molecules, for $d = 30$ Å interwall separations, at $T = 270$ K.

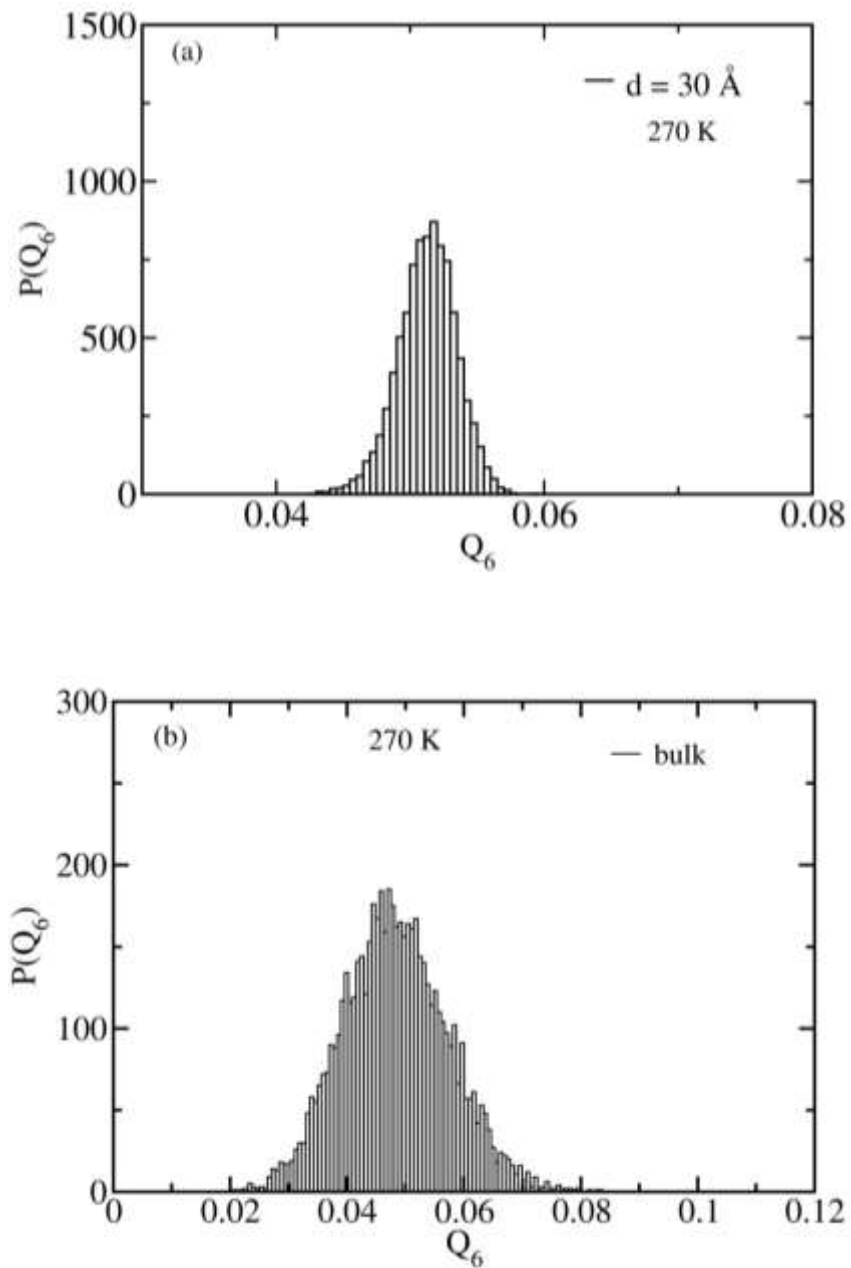
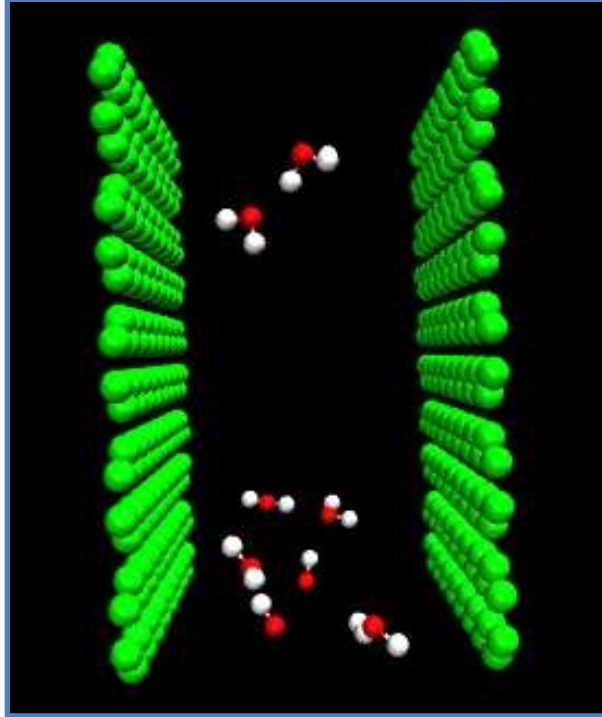
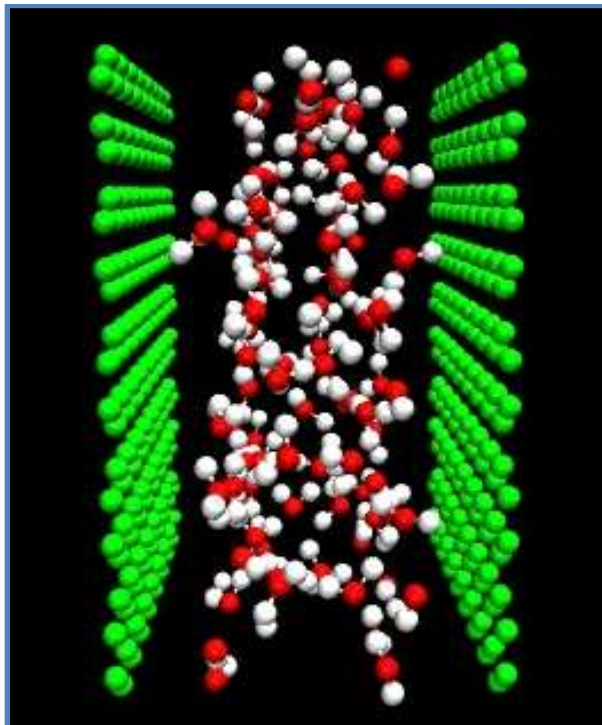


Figure S4. Distributions of local order parameter Q_6 , introduced by Steinhardt *et al.*¹ for water, (a) within the cavity ($d = 30 \text{ \AA}$) and (b) in the outside (bulk) of the hydrophobic walls, at $T = 270$ K. The average values of Q_6 are (a) 0.053 (with in the cavity) (b) 0.051 (in bulk). These values correspond that water exists in the liquid phase.



(a)



(b)

Figure S5. Representative snapshots of the simulation of the confined water at (a) $d = 10 \text{ \AA}$ and (b) $d = 12 \text{ \AA}$, at $T = 300 \text{ K}$.

Reference

1. Steinhardt P J, Nelson D R and Ronchetti M 1983 Bond-orientational order in liquids and glasses. *Phys. Rev. B* 28 784