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Surface Effect on Electromelting Behavior of Nanoconfined Water

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Electronic Supplementary Information:

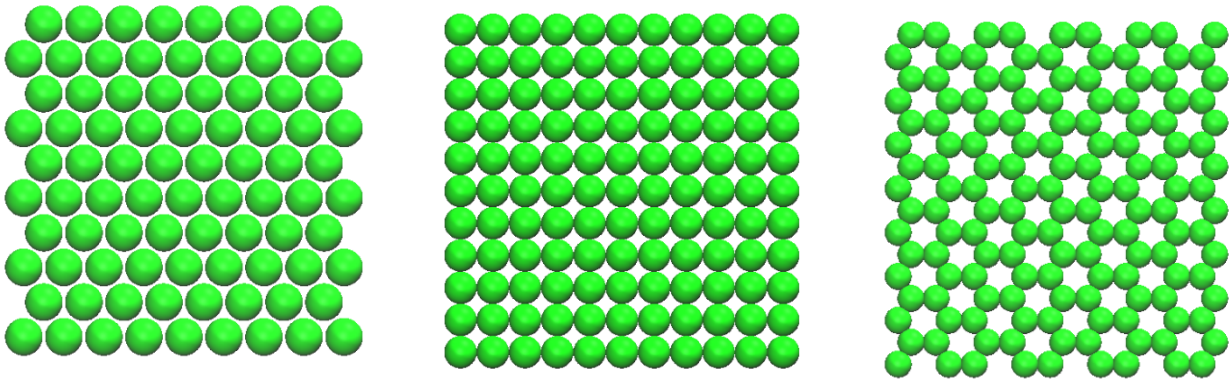

Fig. S1: Different types of lattices, i.e., triangle (left), square (middle) and hexagon (right), used for the study.

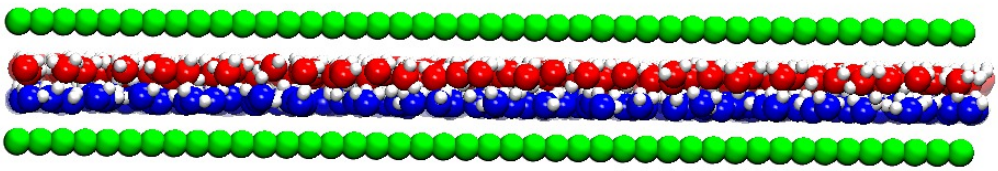

Fig. S2: The side view of the hydrophilic confinement (H = 0.79 nm) having triangular lattice arrangement with lattice constant, a = 0.23 nm in absence of electric field. Green colour particles represent the surface of the confinement. White colour denotes the hydrogen atoms of water

molecules. Red and blue colours denote the oxygen atoms of water molecules in top and bottom layers respectively.

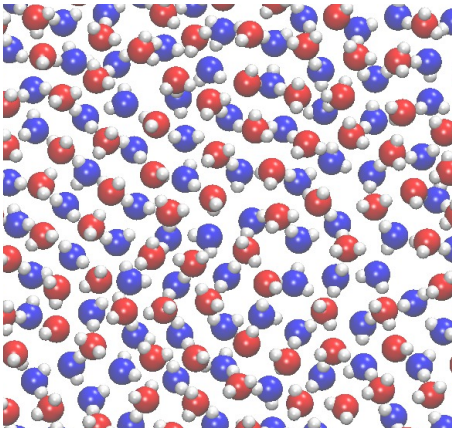

Fig. S3: The arrangement of the water molecules (top view) in the top (red) and bottom (blue) layers within hydrophilic confinement, H = 0.79 nm, with triangular lattice arrangement with lattice constant, a = 0.23 nm, in absence of electric field. The surface particles are not shown in the schematic.

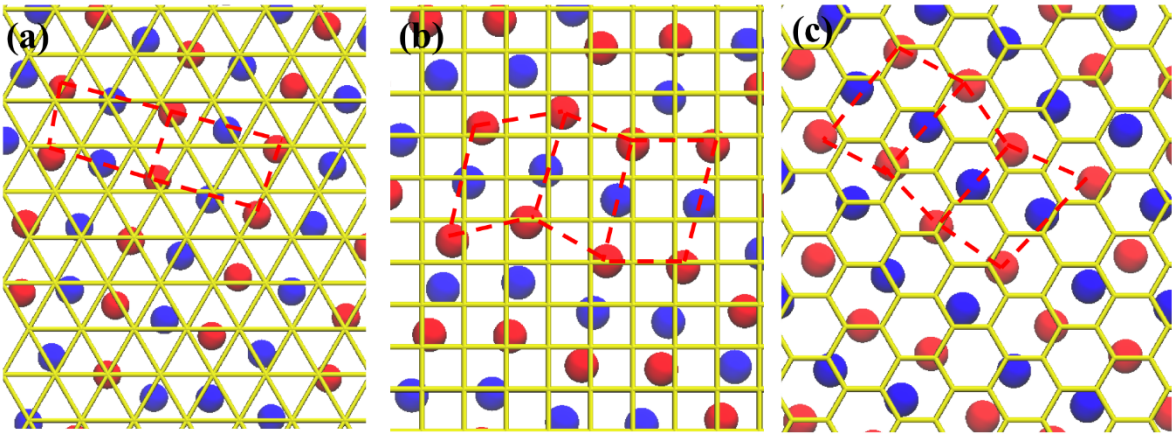

Fig. S4: Top view of a hydrophilic confinement of (a) triangular, a = 0.23 nm, (b) square, a = 0.17 nm and (c) hexagonal, a = 0.142 nm lattice properties, respectively. The red and blue spheres are the oxygen atoms of the top and bottom water layers, respectively. Yellow mesh represents top view of the confining substrate. The red lines are connecting lines for neighboring oxygen atoms in the top water layer.

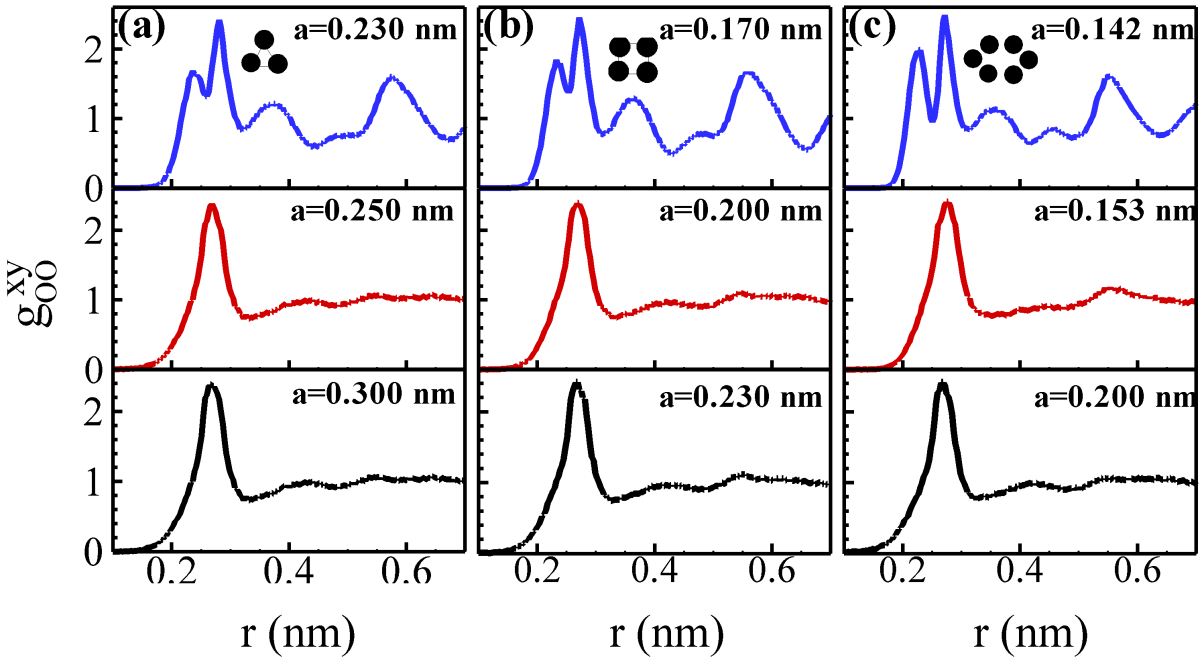

Fig. S5: Variation of in-plane oxygen-oxygen radial distribution function at various lattice constants at a fixed pore-size, H = 0.79 nm, in (a) triangle, (b) square and (c) hexagonal lattice arrangements under hydrophobic surface-fluid interactions in the absence of electric field.

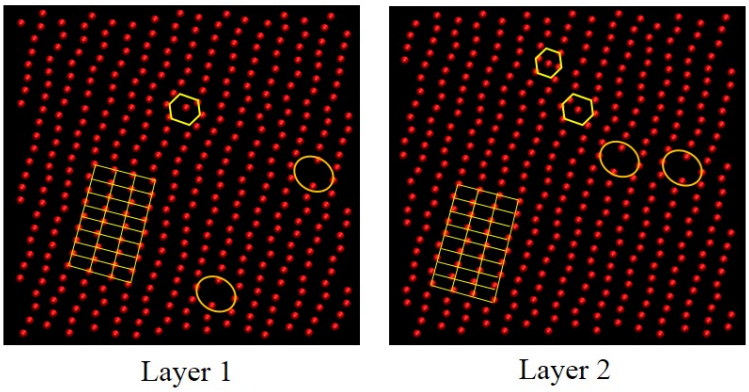

Fig. S6: Snapshot of different layers of water molecules in triangular hydrophilic nanopore at 15 ns. The red dots are the oxygen atoms. The yellow ellipses, hexagon and rectangular meshes denote vacant sites, triangular and square symmetries, respectively.

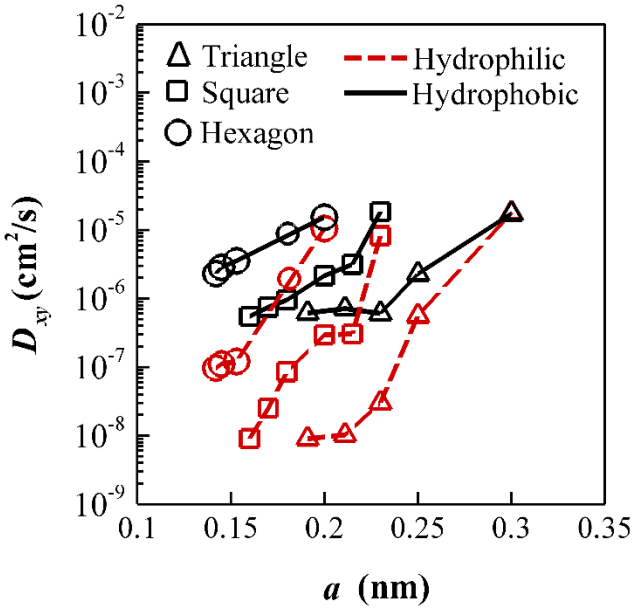

Fig. S7: Variation of lateral diffusion coefficient with lattice constants at three different lattice arrangements with H = 0.79 nm in the absence of electric field.

The surface-atom-density of the simulation system with different arrangement of the surface particles arrangement

The table S1 clearly shows that for the lattice constant, a = 0.23 nm, surface-atom-density decreases from triangle (~ 22 /nm^2) to square (~ 19/nm^2) lattice arrangement. Furthermore, the surface-atom-density again decreases at a lattice constant a = 0.200 nm, from square (~ 25/nm^2) to hexagon (~ 20/nm^2) lattice arrangement. Hence, for a given lattice constant, the surface-atom-density decreases in the order: triangular $\rightarrow$ square $\rightarrow$ hexagon. Moreover, the configurational energy per water molecule starts to increase when surface-atom-density decreases. Thus, the water network becomes less prominent in the same order: triangular $\rightarrow$ square $\rightarrow$ hexagon. We have calculated the average distance of nearest O-O of water molecules. The nearest distances are 0.278, 0.276 and 0.274 nm for triangle, square and hexagonal having lattices constants 0.23, 0.17 and 0.142 nm, respectively. Moreover, the order parameter analysis (Figure 4) shows that water layers possess square symmetry ($\Psi_4 \geq 0.5$) irrespective of the arrangement of the surface-particles in slit pores. This fact indicates that the hydrogen bond network does not commensurate with the lattice constants.

Table S1: Dependence of configurational energy of confined water on the surface-particle density of different confinements in the absence of electric field.

Lattice properties		**Surface-particle-density (per nm^2)**	Configurational energy of water (kcal/mol)	
Arrangement	Lattice constant (a nm)		Hydrophilic	Hydrophobic
Triangle	0.230	22	-13.21±0.18	-10.43±0.09
	0.250	18	-12.89±0.24	-9.82±0.11
	0.300	13	-12.76±0.16	-9.02±0.04
Square	0.170	38	-18.54±0.01	-11.75±0.05
	0.200	25	-13.23±0.07	-10.84±0.04
	0.230	19	-12.95±0.20	-9.62±0.14
Hexagon	0.142	35	-16.52±0.09	-11.34±0.09
	0.153	31	-14.71±0.09	-11.06±0.09
	0.200	20	-13.08±0.12	-10.28±0.25

Calculated lattice constant of the simulation system as a function of electric fields

The structure of the substrate undergoes modification during the simulation. Hence, we analyzed the lattice constant of the system under applied electric fields. We found that the lattice constant increases up to ~8% with increasing electric field. As an example, table S2 summarizes the lattice constant for triangular lattice arrangement (a = 0.23 nm) of the surface particles under hydrophilic surface fluid interaction.

Table S2: Effect of electric fields on lattice constant of the surface particle under hydrophilic surface-fluid interaction with triangular lattice arrangement (a=0.23nm).

Electric filed (V/nm)	Lattice constant (nm)
0	0.227 ± 0.005
1	0.228 ± 0.003
3	0.231 ± 0.001
5	0.235 ± 0.002
7	0.248 ± 0.003
10	0.250 ± 0.002

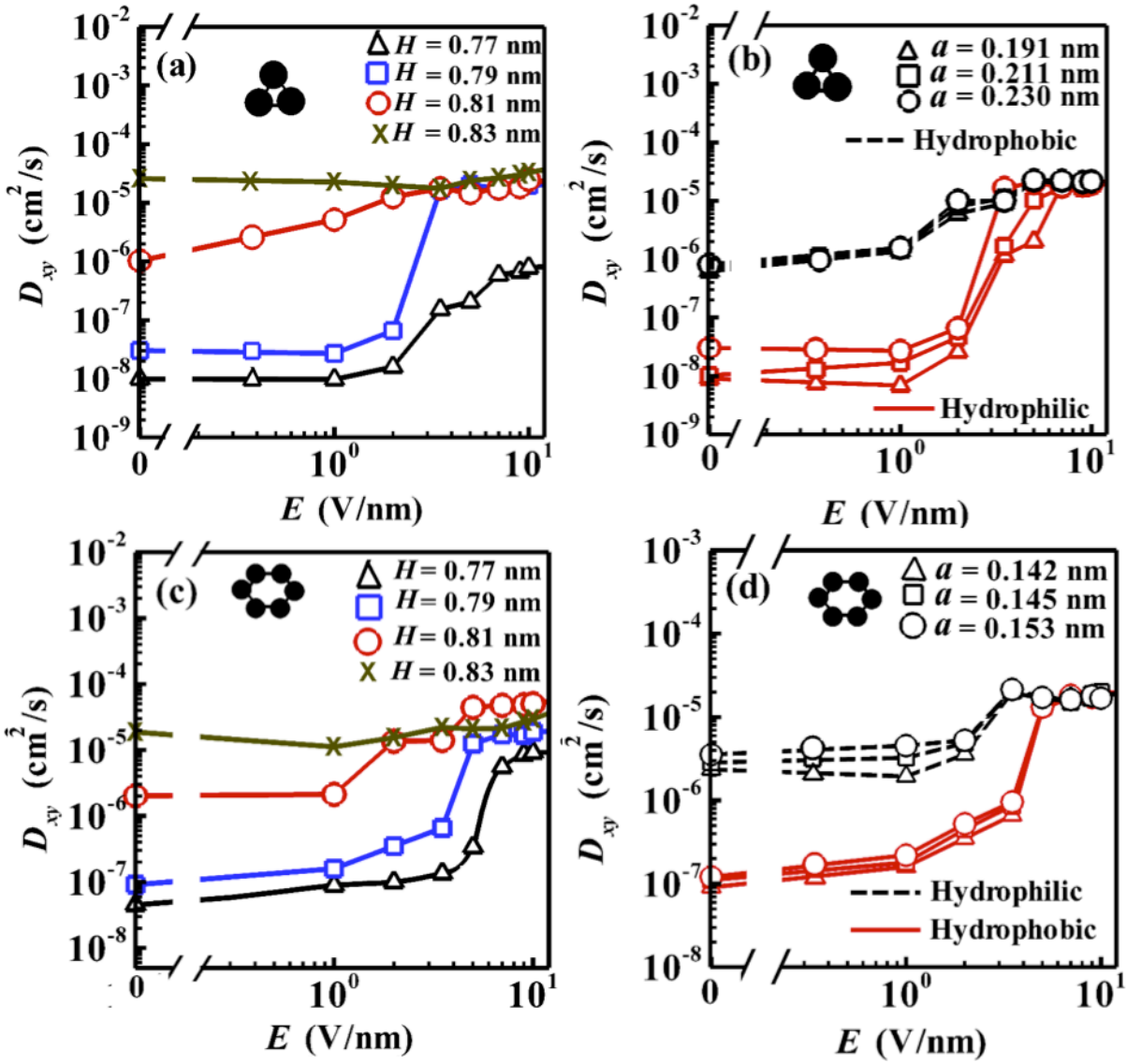

Fig. S8: Lateral diffusivity as a function of applied electric field (a) at various pore-sizes, with lattice constant a = 0.23 nm in triangular lattice arrangement under hydrophilic surface-fluid interaction, (b) at various lattice constants, with pore-size, H = 0.79 nm in triangular lattice arrangement, (c) at various pore-sizes, with lattice constant a = 0.142 nm in hexagon lattice arrangement under hydrophilic surface-fluid interaction, (d) at various lattice constants, with pore-size, H = 0.79 nm in hexagon lattice arrangement.