Surface effect on the electromelting behavior of nanoconfined water†

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Electric field induced phase transitions of confined water have an important role in cryopreservation and electrocrystallization. In this study, the structural and dynamical properties of nano-confined water in nano-slit pores under the influence of an electric field varying from 0 to 10 V nm⁻¹ are investigated under ambient conditions using molecular dynamics simulations. In order to replicate the nature of different materials, a systematic approach is adopted, including pore-size and lattice constant variations in different lattice arrangements viz., triangular, square and hexagonal, with hydrophilic and hydrophobic surface–fluid interactions. The structural behavior of water is investigated using radial distribution functions, bond order parameters and hydrogen bond calculations; the dynamical properties are analyzed using lateral and rotational diffusivity calculations. The lateral diffusivity with increasing electric field \( E \) increases by order(s) of magnitude during electromelting. The pore-size, lattice constant, lattice arrangement and hydrophobic/hydrophilic nature of the pore surface strongly influence the electromelting behavior for \( E \leq \sim 7 \) V nm⁻¹. Higher values of lattice constants and/or hydrophobic pores enhance the electromelting behavior of nanoconfined water.

1. Introduction

Electric fields play a vital role in many biological, environmental and industrial aspects, such as the cryopreservation of living cells and tissues, the protection of crops, power lines and pipe lines from freezing, electrocrystallization, snow making, various food processing operations, and in making various nanomaterials like graphene.¹⁻³ A recent quasielastic neutron scattering study on water confined in a silica nano-pore⁴ reported that after applying an electric field of 2.5 kV mm⁻¹, the translational diffusivity of the confined water is enhanced due to the dissociation of intermolecular hydrogen bonds. On the other hand, an electric field of around 1 kV mm⁻¹ is observed experimentally to promote the formation of ice in a gold nano-confinement of 0.7 nm pore-size under ambient conditions.⁴ Electric fields of comparable strength are found in nano-confinement of 0.7 nm pore-size under ambient conditions using molecular dynamics simulations. In order to replicate the nature of different materials, a systematic approach is adopted, including pore-size and lattice constant variations in different lattice arrangements viz., triangular, square and hexagonal, with hydrophilic and hydrophobic surface–fluid interactions. The structural behavior of water is investigated using radial distribution functions, bond order parameters and hydrogen bond calculations; the dynamical properties are analyzed using lateral and rotational diffusivity calculations. The lateral diffusivity with increasing electric field \( E \) increases by order(s) of magnitude during electromelting. The pore-size, lattice constant, lattice arrangement and hydrophobic/hydrophilic nature of the pore surface strongly influence the electromelting behavior for \( E \leq \sim 7 \) V nm⁻¹. Higher values of lattice constants and/or hydrophobic pores enhance the electromelting behavior of nanoconfined water.

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range structural order of the ice layer breaks, increasing the lateral diffusivity by many orders of magnitude \((10^{-3} \rightarrow 10^{-5} \text{ cm}^2 \text{s}^{-1})\) during electromelting.\(^{21,23}\) According to a density functional theory study, electric fields beyond a threshold value of \(\sim 3.5 \text{ V nm}^{-1}\) are able to dissociate bulk water with a sustainable ionic current due to a series of proton jumps.\(^{24}\) However, nano-confined water is not seen to dissociate under a higher electric field of \(5 \text{ V nm}^{-1}\) if dense water layers do not allow enough space for the hydrated ions.\(^{23}\) In a recent MD study,\(^{23}\) electric fields \(\langle E \rangle\) in the \(0 \leq E \leq 10 \text{ V nm}^{-1}\) range were able to melt the ice layer in a nano-slit made up of triangularly arranged atoms of a model quartz material under ambient conditions. However, it is not clear if such behavior is feasible for different materials. To address the above query, this work presents a systematic analysis of the structural and dynamical properties of confined water in slit pores over a range of electric fields: \(0 \leq E \leq 10 \text{ V nm}^{-1}\). In order to represent different types of material, various lattice arrangements, namely, triangular, square and hexagonal, have been adopted with the pertinent lattice constant range. Many elements, including copper (Cu), nickel (Ni), gold (Au), silver (Ag), yttrium (Y), rhodium (Rh), scandium (Sc), iridium (Ir), etc., possess 2D triangular lattices with \(0.2-0.3\) nm interatomic distances. Similarly, 2D hexagonal lattice arrangements are also abundant in nature within the \(0.1-0.2\) nm interatomic distance range, such as the basal (0001) planes of magnesium (Mg), cobalt (Co), zinc (Zn), carbon (C), titanium (Ti), zirconium (Zr), hafnium (Hf), etc. On the other hand, the (100) plane of the BCC lattice of alkali-metals (Li, Na, K, Rb, Cs) has a 2D square lattice and their various compounds fall in the \(0.2-0.25\) nm interatomic distance range.\(^{25,26}\) The focus of this molecular dynamics study is to investigate the generality of the behavior of electromelting of nano-confined water in variable slit pores with different lattice geometries under an electric field in the range \(0-10 \text{ V nm}^{-1}\).

2. Models and the methodology

A slit pore is designed by placing two layers of surfaces in parallel separated by a distance \(H\). \(H\) in this work, is in the range \(0.77-0.83\) nm. Surface particles are arranged according to the different lattice arrangements and lattice constants (see Fig. S1–S3, ESI†). To address the characteristics of the various materials available in nature, we have adopted different surface–fluid interactions. Two distinct interactions are considered to model surface particles. In one case, interactions are taken as those of graphene,\(^{27}\) representing hydrophobic interactions. In the other case, quartz (SiO\(_2\)) surface interactions are considered, representing hydrophilic interactions.\(^{21}\) The TIP4P/2005\(^{28}\) model is used for the water–water interaction. The surface–water interaction parameters are considered according to the scheme of Zangi and Mark,\(^{21}\) and are summarized in Table 1. A cutoff distance of 0.9 nm is set for the Lennard–Jones (LJ) interaction.\(^{23}\) The particle–particle–particle–mesh (PPPM) method\(^{29}\) is used for calculating the long-range interactions with a cutoff distance of 1.4 nm. Zangi and Mark\(^{21,22}\) have shown that a bilayer of water forms within the two parallel walls in the range \(0.72 \leq H \leq 0.85\) nm with density variation 0.97–0.87 gm cm\(^{-3}\). Therefore, to investigate the phase transition of water from solid to liquid under an external electric field, we have fixed the number of water molecules at 778, corresponding to an initial density of 0.96 gm cm\(^{-3}\) for \(H = 0.79\) nm, confined between two parallel plates with an area of \(7.2 \times 7.2\) nm\(^2\) along the \(x-y\) plane. The electric field, when applied, is in the \(z\)-direction, perpendicular to the surface.\(^{23}\) The equation of motion of the surface particles is not integrated, i.e., surface particles are kept fixed. To imitate the confinement in between two infinite plates, periodic boundary conditions are applied in the \(x\) and \(y\)-directions, and in the \(z\)-direction, a 5 nm vacuum is applied on top of the upper plate and in the \(-z\) direction a 5 nm vacuum is used beneath the lower plate to avoid unrealistic interactions.

| Surface-type | Oxygen-surface | Hydrogen-surface |
|--------------|----------------|-----------------|
|              | \(\varepsilon\) (kcal mol\(^{-1}\)) | \(\sigma\) (nm) | \(\varepsilon\) (kcal mol\(^{-1}\)) | \(\sigma\) (nm) |
| Hydrophilic  | 0.1986         | 0.3160          | 0.0992          | 0.2840          |
| Hydrophobic  | 0.1139         | 0.3352          | 0.0569          | 0.2647          |

All MD simulations are conducted using the LAMMPS package.\(^{30}\) An N\(_{T}\) ensemble is utilized. Time integration of the equations of motion is performed at a 300 K temperature and at 1 bar lateral pressure, using the Nosé-Hoover thermostat and a barostat with 1 ps and 2.5 ps relaxation times, respectively.\(^{31,32}\) All of the systems under study have been equilibrated for 5 ns, followed by an additional 10 ns to evaluate structural and dynamic properties, with a time step of 2 fs.

2.1 Analysis

In-plane oxygen–oxygen radial distribution function (RDF). The in-plane oxygen–oxygen radial distribution function is typically used to analyze the structures of a layer of oxygen atoms of water molecules in a plane (here, \(x-y\) plane) to see whether the confined water is ordered or disordered. It is calculated in the following manner: \(^{24}\)

\[
g_{OO}^{xy}(r) = \left\langle \frac{A(z_{i-1} - z_j)\left\langle N(r; z_{i-1}, z_j) \right\rangle}{2\pi \Delta r \Gamma_i} \right\rangle = \left\langle \frac{N(r; z_{i-1}, z_j)}{2\pi \Delta r \Gamma_i} \right\rangle, \tag{1}
\]

where \(A(z_{i-1} - z_j)\) is the cross sectional area and \(N(r; z_{i-1}, z_i)\) denotes the total number of oxygen atoms in the distance band of \(r - \Delta r/2\) and \(r + \Delta r/2\) in the \(i\)th layer between \(z_{i-1}\) and \(z_i\). \(\Gamma_i\) denotes the two dimensional density. As two layers of confined water show no significant differences structurally and dynamically, the averages of the properties are reported here, such as 2D RDF: \(g_{OO}^{xy}\).

In-plane bond order parameters. The structure of a monolayer of oxygen atoms of confined water molecules is scrutinized using the in-plane bond order parameters, which are defined as: \(^{33,36}\)

\[
\psi_b = \left\langle \frac{1}{N_0} \sum_{j=1}^{N_0} \exp(ik\theta_j) \right\rangle, \tag{2}
\]
where $N_b$ is the total number of neighbours within a distance cutoff of 1.5\AA \space \text{in each layer}; \theta_j$ is the angle formed by an oxygen atom with its nearest neighbours with reference to a fixed reference frame. $\psi_k$ indicates that there is complete $k$-times symmetry in that layer, where $\psi_k = 0$ signifies that there is no $k$-times symmetry. In order to estimate the square and triangular symmetries of the water molecules, $\psi_4$ and $\psi_6$ of the oxygen atoms are calculated.

**Lateral diffusion.** The lateral diffusion coefficient, $D_{xy}$, is a dynamical property that is directly related to molecules' mobility in the solid (ordered) phase and liquid (disordered) phase of the confined water. In solid phase, the value of the lateral diffusion coefficient ($D_{xy}$) is much smaller than that in the liquid phase. Thus, mobility can serve as a good estimate for the solid–liquid phase transition.\(^{37}\) It can be estimated for two dimensions (in the $x$-$y$ plane) by the following mathematical formula:\(^{22,38}\)

\[
\langle \Delta x_i^2 + \Delta y_i^2 \rangle = 4D_{xy} t,
\]

where $\langle \Delta x_i^2 \rangle$ and $\langle \Delta y_i^2 \rangle$ denote the ensemble average of the displacement of a water molecule, $i$, from its initial position at time $t = 0$ in the $x$- and $y$- directions, respectively.

**Rotational diffusion.** The rotational diffusion coefficient, $D_{rot}$, is a measure of the degree of rotation. In this study, the rotational diffusion coefficient is calculated using the following expression:\(^{39}\)

\[
\langle \Delta \phi^2 \rangle = 2D_{rot} t,
\]

where $\phi_i$ is the angle between the dipole of a water molecule $i$ and the direction of the applied electric field ($z$-axis). $\langle \Delta \phi^2 \rangle$ denotes the ensemble average of the square value of angular displacement of a water molecule $i$.

**Hydrogen bond (HB) calculation criteria.** The average number of hydrogen bonds per water molecule ($n_{HB}$) is calculated to obtain information about the structures of the water layers in the confinement. Two water molecules are hydrogen bonded if the following conditions are satisfied:\(^{23}\) $R_{OO} < 0.35$ nm, and OH · · · O angle $> 150^\circ$.

### 3. Results and discussion

We first present the effects of pore-size and surface lattice arrangement on the structure of water in extremely narrow pores, in the absence of an electric field. Fig. 1 presents the 2D radial distribution function of oxygen–oxygen for different pore-sizes for different lattice arrangements.

In the case of a triangular lattice arrangement, multiple peaks in the RDF are observed for $H = 0.77–0.81$ nm. Similar behaviors are seen for square (Fig. 1b) and hexagonal arrangements of surface particles (Fig. 1c), though ordered behavior is slightly suppressed for $H = 0.81$ nm. The RDF curves, for pore-size less than 0.81 nm, consist of a split-peak, which is an indication of crystalline phase. As the pore-size increases, the split-peak vanishes, and a dominant single peak appears. The location of the prominent first peak is at 0.28 nm for all cases.

We estimate the 2D oxygen–oxygen coordination number (CN) by integrating the RDF up to the minimum of the prominent first peak. For pore-size $H = 0.77–0.81$ nm, the average coordination number is within the range 4.1 to 4.4 for all surface arrangements. At $H = 0.83$ nm, the coordination number is high at 4.8, indicating liquid-like behavior. This nature is observed for all of the surface arrangements. The diffusivity plots, shown in Fig. 2a, further corroborate the above findings.

The lateral diffusivity in the hydrophilic pores increases from $\sim 10^{-8}$ to $\sim 10^{-4}$ cm$^2$ s$^{-1}$ with increasing pore-size. The lateral diffusivity ($D_{xy}$) of water is on the order of $10^{-8}$ for $H = 0.77–0.79$ nm. The diffusivity is enhanced by 2 to 3 orders with a slight increase in the pore-size, as evident for $H = 0.81$ and 0.83 nm. The low mobility of water molecules at lower pore-sizes, along with the RDF plots, clearly indicates that there is an ordered network structure among the confined water molecules for low values of $H = 0.77–0.79$ nm. At higher $H$ values, the MSD starts to diverge, as can be seen for the pore-size $H = 0.83$ (see Fig. 2b), indicating liquid-like behavior. In contrast to the hydrophilic surface, the hydrophobic surface (graphitic pore)
of a triangular surface (see Fig. S5, ESI†) an increase in \( a \) (in nm) from 0.23 to 0.25 or 0.30 decreases the RDF peaks significantly, leading to a disordered structure, as indicated by the single peak in the RDF plot. Therefore, the lower values of lattice constant allow the confined water molecules to stay in an ordered network, whereas the higher values promote disorderliness.

While lattice constant plays an important role, the lattice arrangement can also affect the properties significantly. For example, in the case of a square arrangement with \( a = 0.23 \) nm (Fig. 3b), for hydrophilic interactions, the RDF has considerably fewer peaks compared to the number seen for the triangular arrangement (Fig. 3a), signifying a disordered water network. Similar behavior is seen for hydrophobic surfaces (see Fig. S5, ESI†), which is well supported by the lateral diffusivity behavior (see Fig. S7, ESI†). The low mobility of water molecules at the lower lattice constant clearly indicates that there is an ordered network structure among the confined water molecules for low values of the lattice constant. Furthermore, the ordered water network becomes more prominent at lower values of lattice constant when the lattice arrangement varies in the order: triangular \( \rightarrow \) square \( \rightarrow \) hexagonal. These observations are due to the number of interaction sites (i.e., the number of surface-particles), which is directly related to the lattice constant and arrangement of the surface atoms. Since, for a given lattice constant, the surface-atom-density decreases in the order: triangular \( \rightarrow \) square \( \rightarrow \) hexagonal, the water network becomes less prominent in the same order, which affects accordingly the configuration energy of water in the same order (see Table S1, ESI†). Furthermore, for a fixed lattice constant (\( a = 0.2 \) nm), in the case of square lattice surfaces, the ordered structure is conspicuous under hydrophilic confinement, whereas it is less prominent in the case of hydrophobic confinement. Therefore, it is important to note that the ordered network of water under confinement in the absence of an electric field depends on the lattice properties, as well as on the surface–fluid interaction. From the RDF and diffusivity results, we conclude that the ordered network of water exists for a narrow range of lattice constants. To this end, we have taken \( a = 0.23, 0.17 \) and 0.142 nm for triangular, square and hexagonal, respectively, as representative lattice constants for our electric field-induced phase transition studies.

Now, we turn our attention to explore the effects of the electric field on the structural and dynamic properties of water under nano-confinement. To explore the effect of electric field on the arrangement of the water molecules under various nano-confinements, we have calculated the structural properties such as the in-plane bond order parameters and the radial distribution function. Fig. 4 presents the bond order parameters with the variation of electric field (0–10 V nm\(^{-1}\)) for different lattice properties and surface–fluid interactions.

In the case of the triangular arrangement (\( a = 0.23 \) nm), at \( E = 0 \) V nm\(^{-1}\), the values of \( \Psi_4 \) and \( \Psi_6 \) are 0.53 and 0.36, respectively, under hydrophilic confinement. The in-plane order parameter value clearly indicates that the water molecules have a propensity to remain in the square symmetry, though some water molecules remain in triangular symmetry in
the confinement of the triangular lattice arrangement. The corresponding snapshots (Fig. 4d) also show the existence of symmetries within a water layer for the triangular lattice. On the other hand, for the square (a = 0.17 nm) and hexagonal (a = 0.142 nm) hydrophilic confinements, the higher values of $\Psi_4 > 0.5$ compared to $\Psi_6 < 0.05$ indicate that the water molecules prefer to remain in the square symmetry. The existence of such ordered structures is corroborated by the RDF plots as shown in Fig. 4d-f. Furthermore, analysis of the peak locations suggests that the lattice constant of the surface is not commensurate with the structure of the water layer. We observed both the square and hexatic symmetry for the triangular substrate at lower electric field. This result implies that the triangular confined system might have some kind of geometric preference for both symmetries. The snapshots shown in Fig. S6 (ESI†) clearly depict oxygen atoms in square and hexatic symmetries. To address this conjecture, we evaluate the average configuration energy for different confined systems. The average configurational energy of confined water is approximately $-18.54$ kcal mol$^{-1}$ and $-16.52$ kcal mol$^{-1}$ for the square and hexagonal arrangements, respectively (see Table S1, ESI†), in the absence of an electric field. Whereas for the triangular arrangement, the energy value is approximately $-13.21$ kcal mol$^{-1}$, which is closer to the configurational energy values of the bulk water under ambient conditions. The higher configuration energy, due to the large oxygen–oxygen distance in triangular confinement, arises due to the low surface density of the surface particles. This allows defects in the system (see Fig. S6, ESI†), and thus promotes both forms of water symmetry. This is also evident from the RDF plots in Fig. 4d-f, which show the location of the first peak at 0.398 nm, 0.375 nm, 0.375 nm for triangular (a = 0.23 nm), square (a = 0.17 nm) and hexagonal (a = 0.142 nm), respectively.

With increase in the electric field, both the $\Psi_4$ and $\Psi_6$ values for the triangular arrangement, and only the $\Psi_4$ values for the square and hexagonal arrangements decrease sharply, indicative of electromelting behavior. At $E = 10$ V nm$^{-1}$, the height of the dominant peak decreases, and the RDF approaches unity, as shown in Fig. 4g–i. It should be noted that there is a small variation in the lattice constant under the influence of the electric field (see Table S2, ESI†). In addition, to check the sensitivity of the LJ parameters, $\varepsilon$ and $\sigma$ of substrate–oxygen interactions, towards the order parameters, we have varied $\varepsilon$ and $\sigma$ by ±5%. Typically, the sensitivity of $\sigma$ is greater than that of $\varepsilon$ at lower electric field, whereas at higher electric field the order parameters are insensitive to both LJ parameters.

Fig. 5 presents the lateral diffusivity of water under different arrangements of surface particles and surface–fluid interactions with the electric field varying from 0 to 10 V nm$^{-1}$. The figure clearly indicates a lower value of diffusivity of $\sim 10^{-8}$ cm$^2$ s$^{-1}$ for the hydrophilic surface and $\sim 10^{-6}$ cm$^2$ s$^{-1}$ for the hydrophobic surface, representing the order-like structures when the applied electric field is in the range 0 to $\sim 3.5$ V nm$^{-1}$. Further increase in the electric field increases the diffusivity to $\sim 10^{-5}$ cm$^2$ s$^{-1}$, indicative of the electromelting or disordered state. In the lower range of electric field, the lateral diffusivity is higher in hydrophilic pores in comparison to hydrophilic pores. During electromelting, the effect of electric field on the diffusivity of water in a hydrophilic nano-pore displays interesting behavior, where the electromelted state ($D_{xy} \sim 10^{-5}$ cm$^2$ s$^{-1}$) is achieved much earlier for the triangular ($E = 3.5$ V nm$^{-1}$) and hexagonal ($E = 5$ V nm$^{-1}$) lattice surface in comparison to that of the square ($E = 7$ V nm$^{-1}$) lattice surface. It is noted that once the confined water is electromelted, the overall behavior of diffusivity with further increase in electric field is similar for both the hydrophilic and hydrophobic nano-pores. Furthermore, at low electric field, the variation in the lateral diffusivity ($\sim 10^{-8}$ → $\sim 10^{-7}$ cm$^2$ s$^{-1}$) demonstrates that the surface particle arrangement can have a drastic influence on the diffusivity in the hydrophilic or hydrophobic confinements. Importantly, our results are also
in various lattice arrangements. At ambient conditions, 40
ments is less than the reported value for bulk water under
hydrogen bonds (intralayer HB + interlayer HB) in all confine-
nanopores of various lattice arrangements. The total number of
the effect of electric field on the intralayer and interlayer
water molecule ($n$)

With further increase in the electric field, the rotational diffu-
sivity is of the same order ($\sim 10^{-5}$ rad$^2$ ps$^{-1}$) in all three
cases. The values of the rotational diffusivity are of the order
$10^{-5}$ rad$^2$ ps$^{-1}$ when the electric field is in the range 0–1 V nm$^{-1}$.
With further increase in the electric field, the rotational diffu-
sivity values decrease from $\sim 10^{-5}$ rad$^2$ ps$^{-1}$ to $\sim 10^{-7}$ rad$^2$ ps$^{-1}$,
which are independent of the surface-fluid interactions and
the lattice properties (rotational diffusivity for the hydrophobic
surface is not shown). The drop in the rotational diffusivity is
due to the reorientation of water molecules in a fashion such
that their dipoles are aligned in the direction of the applied
electric field. It should be noted that the rotational diffusivity
decreases monotonously with increasing electric field, which is
in contrast to the behavior seen for the lateral diffusivity, where
lateral diffusivity first increases and remains constant for a range
of $E$. On the other hand, the rotational diffusivity continuously
decreases even during the electromelting stage.

To explore the variation of ordering in the water-layers, we
have evaluated the average number of hydrogen bonds (HBs)
per water molecule ($n_{HB}$) under different confinements with the
electric field varying in the range 0–10 V nm$^{-1}$. Fig. 7 presents
the effect of electric field on the intralayer and interlayer
hydrogen bond network within hydrophilic and hydrophobic
nanopores of various lattice arrangements. The total number of
hydrogen bonds (intralayer HB + interlayer HB) in all confine-
ments is less than the reported value for bulk water under
ambient conditions.40

In hydrophilic confinement, the average number of hydrogen
bonds within a single layer (intralayer HBs) is $\sim 2.5$, indicating the presence of an in-plane ordered network of water
in the 0 to $\sim 3.5$ V nm$^{-1}$ electric field range. With further
increase in the electric field, intralayer HBs decrease due to
disruption of the HB network within the plane. However, the
average number of interlayer HBs increases. This suggests that
the intralayer HBs of the ordered water layer are largely inter-
rupted with increasing electric field, leading to electromelting.
At higher values of electric field ($E = 10$ V nm$^{-1}$), the dipoles of
the water molecules become oriented in the direction of the
applied electric field. Thus, the average number of intralayer
hydrogen bonds decreases, whereas the interlayer hydrogen
bonds increase, signifying a stronger interlayer connectivity at
high $E$ values. Furthermore, to see the onset of the melting
behavior with increasing electric field, we have estimated the
average number of intralayer and interlayer HBs within a 0 ps
to 50 ps time scale. Fig. 8 represents the variation of the average
number of intralayer and interlayer HBs with respect to time at
different electric fields ($E = 1, 5$ and 7 V nm$^{-1}$) for triangular,
hydrophilic ($a = 0.23$ nm and $H = 0.79$ nm) confinement.

The intralayer and interlayer HBs do not change much at low
values of the electric field ($E = 1$ V nm$^{-1}$), which indicates strong
order in the system. On the other hand, at higher electric field
values ($E = 5$ and 7 V nm$^{-1}$), the number of intralayer HBs drops
sharply within 10 ps, as evident from Fig. 8a. Thus, the breaking
of the intra-layer HB network indicates that melting has started
at the solid–liquid interface with increasing electric field. Inter-
layer hydrogen bonding, on the other hand, increases slightly at

![Fig. 6](image1.png) Variation of rotational diffusivity with electric field in various hydrophilic nanopores. Error bars are calculated by the block average method.

![Fig. 7](image2.png) Variation of average number of intralayer and interlayer hydrogen bonds per water molecule as a function of electric field for triangular, square and hexagonal lattices with $a = 0.23, 0.17$ and 0.142 nm, respectively. Panels (a) and (b) are for hydrophilic and hydrophobic surface–fluid interac-
tions, respectively. Solid lines are average intralayer HBs and dashed lines are average interlayer HBs. Error bars are smaller than the symbol size.

![Fig. 8](image3.png) Instantaneous number of hydrogen bonds per water molecule as a function of time at different electric fields for (a) intralayer HBs and (b) interlayer HBs.
4. Conclusions

We have reported the electric field-induced phase transition of water in various confinements with different lattice properties and surface-fluid interactions. Electromelting is attributed to the success of electric field induced disordering over surface induced ordering. A strong influence of pore-size, lattice constants, lattice arrangements and interaction nature on the electromelting ($E \leq 7 \text{ V nm}^{-1}$) behavior has been observed. The electromelted region (higher lateral diffusivity regions in the presence of an electric field) shrinks with decreasing pore-size. We note that the lattice constant from 0.1 to 0.3 nm with various surface-particle arrangements closely resembles many metals and non-metal surfaces. However, based on the current results the electromelting of nanoconfined fluids may vary in the case of polar or charged surfaces due to the simplified model considered in this work. Hence, the precise nature of electromelting behavior depends strongly on the lattice properties, pore-size and the strength and nature of the substrate-fluid interactions.

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