Abnormal in-plane permittivity and ferroelectricity of confined water: from sub-nanometer channels to bulk

Reference:
Hamid Ilyar, Jalali Hossein, Peeters François, Neek-Amal Mehdi.- Abnormal in-plane permittivity and ferroelectricity of confined water: from sub-nanometer channels to bulk
The journal of chemical physics - ISSN 0021-9606 - 154:11(2021), 114503
Full text (Publisher's DOI): https://doi.org/10.1063/5.0038359
To cite this reference: https://hdl.handle.net/10067/1775790151162165141
Abnormal in-plane permittivity and ferroelectricity of confined water: from sub-nanometer channels to bulk

Ilyar Hamid,1 Hossein Jalali,2,3 Francois. M. Peeters,1 and Mehdi Neek-Amal1,3, a)
1)Department of Physics, Universiteit Antwerpen, Groenenborgerlaan 171, B-2020 Antwerpen, Belgium.
2)Department of Physics, University of Zanjan, 45195-313, Zanjan, Iran.
3)Department of Physics, Shahid Rajaee Teacher Training University, 16875-163 Lavizan, Tehran, Iran.

(Dated: 24 February 2021)

Dielectric properties of nano-confined water are important in several areas of science, i.e. it is relevant in dielectric double layer that exist in practically all heterogeneous fluid-based system. Molecular dynamics simulations are used to predict the in-plane dielectric properties of confined water in planar channels of width ranging from sub-nanometer to bulk. Because of suppressed rotational degrees of freedom near the confining walls the dipole of the water molecules tend to be aligned parallel to the walls which results in a strongly enhanced in-plane dielectric constant ($\varepsilon_{||}$) reaching values of about 120 for channels with height $8\text{Å} < h < 10\text{Å}$. With increasing width of the channel, we predict that $\varepsilon_{||}$ decreases nonlinearly and reaches the bulk value for $h > 70\text{Å}$. A stratified continuum model is proposed that reproduces the $h > 10\text{Å}$ dependence of $\varepsilon_{||}$. For sub-nanometer height channels an abnormal behaviour of $\varepsilon_{||}$ is found with two orders of magnitude reduction of $\varepsilon_{||}$ around $h \sim 7.5\text{Å}$ which is attributed to the formation of a particular ice phase which exhibits long-time ($\sim \mu\text{s}$) stable ferroelectricity. This is of particular importance for the understanding of the influence of confined water on the functioning of biological systems.

INTRODUCTION

Adsorbed water in nanopores and its anomalous properties are a subject of recent theoretical and experimental interest, which is poorly understood. Several of its physical properties are strongly modified, e.g. its thermodynamics, mass transport, flow dynamics, heat transfer, melting and energy transport. The study of nanoconfined fluids (fluids confined in nanoscale geometries) has developed rapidly over the past few years. For example, the thermal conductivity of nanoconfined water was found to be anisotropic and when the confining walls are made of graphene oxide membranes, nanoconfined water showed remarkable fast permeation. Recently, in a review paper Kavokine et al. discuss how basic equations that govern fluid behavior in the continuum limit break down and new properties emerge in molecular-scale confinement. It was shown that a large number of analytical estimates and physical arguments are needed to organize various properties of confined water at channels with different heights.

Determining the dielectric constant of nanoconfined water is a recent subject of research with conflicting predictions. Generally, the dielectric constant of a material has three main contributions: i) electronic, ii) ionic, and iii) dipolar. The dipolar contribution can be found using molecular dynamics simulations (MDS) or Monte Carlo simulations (MCS). In the past few years, MDS or MCS were used to examine water’s unique properties employing a variety of classical force fields under both normal and critical conditions. For example, using MCS the variation of the dielectric constant of water with temperature and pressure were obtained by Aragones et al. for both proton ordered and proton disordered structures of different ices using several water models. The dielectric constant of proton disordered ices (e.g. ice Ih at low temperatures) were predicted to be larger than 100 while the proton ordered structures have a much smaller dielectric constant of the order $\sim 3-4$. The latter is due to the decrease of the rotational degree of freedom and/or decrease of the number of H-bonds.

In the literature conflicting reports can be found on the value of the in-plane dielectric constant of confined water. For instance by applying a large external electric field $E_0 = 0.01 \text{V/Å}$, Itoh et al. found a nonlinear increase in the dielectric constant of confined water (for channels wider than 10Å) for both lateral and perpendicular fields. On the other hand, the in-plane dielectric constant of water as a function of the distance between hydrophobic confining surfaces (graphene) for nano-scale size channels was found to be fluctuating around the bulk dielectric constant when $h > 10\text{Å}$ and larger than the bulk value for $h \approx 10\text{Å}$, i.e. 105. Gekle et al. reported a small difference (up to 5%) between the in-plane dielectric constant of confined water in channels with size $h=11$, 31, and 61Å and bulk water. In addition, Ruiz-Barragan et al. disclose stark dependences of the tensor profile for parallel dielectric response of confined water within planar graphene slit pores as a function of the confinement length. Also, Schlaich et al. studied the dielectric constant of confined water in channels made of flexible polar head-groups of walls for channels with height $h>10\text{Å}$ and found the bulk dielectric constant of water for channels with height $h > 10\text{Å}$ and 85 for channel $h \sim 10\text{Å}$. For channels smaller than $h < 10\text{Å}$ there is no experimental data so far. Moreover, recently, by using electrostatic force detection with an atomic force microscope (AFM), unexpected variation in the out-of-plane permittivity of confined water between graphene and hexagonal boron nitride (h-BN) was observed.

---

Electronic mail: mehdi.neekamal@gmail.com
The presence of a surface layer with vanishing small polarization is the reason for such small out-of-plane permittivity \( \varepsilon_{\perp} \) for channels with size of \( h < 20 \text{ Å} \). Beyond 20 Å a nonlinear increase in the permittivity was observed. Despite several studies that determined the out-of-plane component of the dielectric constant of confined water, there is currently no experimental data for the in-plane component.

Up to now ferroelectricity in nanoconfined water is controversial and is expected to influence the functioning of biological systems. The timescale of proton vibration is beyond experimentally accessible timescales, thus observing proton ordering (ferroelectricity) in cubic and hexagonal ice XI is infeasible and controversial\(^{25,26}\). In bulk water the hydrogen bonds screen the dipole-dipole coupling resulting in the suppression of ferroelectric order. However, in confined water ordering of molecular dipoles trapped in beryl crystal lattices was detected\(^{27}\). A ferroelectric soft mode that causes a Curie-Weiss behaviour of the static permittivity was also observed\(^{27}\). Nakamura et al.\(^{28}\) reported spontaneous step-wise changes in the net polarization at the transition of immobile to mobile water when confined inside a carbon nanotube, which was understood as due to the transformation to single-domain ferroelectric water.

In this paper we performed extensive MDS to simulate water confined between graphene and h-BN layers. We calculate the in-plane component of the dielectric constant (dipolar part) of confined water as a function of the channel size \( h \). Since the dielectric constant is a second rank tensor, the variation of \( \varepsilon_{||} = (\varepsilon_{xx} + \varepsilon_{yy})/2 \) with the slab size from \( h = 6.4 \text{ Å} \) to \( h = 100 \text{ Å} \) was obtained by calculating the fluctuation of the total dipole moment of water. We present a continuum model where we include some of the microscopic details of confined water which is able to reproduce like decreasing behaviors of \( \varepsilon_{||} \) results for \( h > 10 \text{ Å} \). Furthermore, we predict long time stable ferroelectricity (\( \approx 1 \mu s \)) of confined water in channels with \( h = 7.4 \pm 0.5 \text{ Å} \).

### THE MOLECULAR DYNAMICS SIMULATIONS

Equilibrium molecular dynamics simulations with the large scale atomic/molecular massively parallel simulator LAMMPS\(^{29}\) was used to investigate the impact of the confining walls on the relative permissivity of water confined inside graphene (and hexagonal boron nitride) capillaries. Our simulated system (see Fig. 1(b)) contains two layers of graphene each with 680 carbon atoms, i.e. our configuration unit cell has a planar geometry with dimensions \( A = l_y \times l_z = 42 \text{ Å} \times 43 \text{ Å} \).

The confining walls were fixed at their \( z \)-positions. The SPC/E model was used to describe the water molecules\(^{30}\). The number of water molecules inside channels have been chosen to provide bulk density, i.e. \( \rho_w \approx 1 \text{ g.cm}^{-3} \). For example the number of water molecules in the channel with heights of 6.5 and 10 Å are 175 and 410, respectively. Other number of molecules for other channels can be found using \( N = \int |[\text{A}h^{2/3}] \rho_w N_A|/m \), where \( N_A \) is the Avogadros number, \( m \) is the mass of one water molecule and \( Ah^{2/3} \) is the effective volume that is introduced in next section. Notice that, the density of nanoconfined water might not be determined experimentally because different setups have different conditions such as size and confining walls and etc. Rather than the density, the chemical potential of water inside the channel should agree with the bulk value which can either be set by attached reservoir (as done in experiments) or by measuring the chemical potential\(^{31–33}\). The driving force of water flow into graphene channel arises from lower chemical potential of nanoconfined water molecules to bulk water where the chemical potential difference is proportional to the logarithm of relative water density\(^{31,34,35}\). The water molecules interact with the graphene sheet via Lennard-Jones (LJ) pair potentials using \( \varepsilon_C = 71.224 \text{ cal mol}^{-1} \), \( \sigma_C = 3.41 \text{ Å} \) and the cross LJ potential parameters were obtained using the Lorentz-Berthelot combining rules. The cut-off radius for the LJ potential was chosen at 10 Å. The NVT ensemble (Nose-Hoover thermostat) was used to keep the temperature at 300 K.

Periodic boundary conditions are employed along all directions and the confinement was along the \( z \)-direction. The vacuum space between two periodic images in the \( z \)-direction is taken to be \( l_z = 100 \text{ Å} \). This number is large enough to minimize the long range electrostatic interaction between periodic images along the \( z \)-axis. The particle-particle particle-mesh method was used to compute the long-range Coulomb interaction with a relative accuracy of \( 10^{-4} \). Water bonds and angle were fixed by the SHAKE algorithm\(^{36}\). This condition resulted in densities close to the bulk density when \( h \geq 10 \text{ Å} \) and slightly larger than the bulk density for \( h < 10 \text{ Å} \). A time step of 2 fs was taken. After relaxing the system for 1 ns, the thermodynamical sampling was done up to 16 ns to ensure that the permittivity was converged.

### THE MICROSCOPIC MODEL

By defining parallel polarization correlation function\(^{23,24,37,38}\):

\[
C_{||}(z) = \langle m_{||} M_{||} \rangle - \langle m_{||} \rangle \langle M_{||} \rangle,
\]

where \( m_{||}(z) \) is the laterally averaged polarization density at position \( z \). Also \( \langle \rangle \) is the average over many uncorrelated realizations (MD snapshots) having equal \( z \). Here, \( M_{||} = A \int m_{||}(z) dz \) is the total in-plane polarization. Note that the symbol \( \parallel \) refers to either \( x \) or \( y \) directions. Using

![FIG. 1. (a) Continuum model and the atomistic model for confined water between two graphene or h-BN sheets (black balls) which are separated by distance \( h \). In (a) the surface water layers and middle bulk water are shown by different colors and in (b) white (red) balls are hydrogen (oxygen) atoms.](Image: Figure 1)
the fluctuation-dissipation theorem the local in-plane dielectric constant is given by\textsuperscript{23}:
\[
\varepsilon_{||}(z) = 1 + \frac{C_{||}(z)}{\varepsilon_0 k_B T},
\]

(2)

In Fig. 2, as a typical case, we depict the variation of \(\varepsilon_{||}(z)\) with \(z\) for confined water between two graphene sheets which are separated by \(h=10\text{Å}\). Our result is in good agreement with those reported in Ref. \[24\].

Next, by assuming an effective dielectric constant \(\varepsilon_{||}^{\text{eff}}\) in a box with effective height \(h_{\text{eff}}\) and using Eq. (2)\textsuperscript{23} one finds:
\[
\varepsilon_{||}^{\text{eff}} = 1 + \frac{\int_{-h/2}^{h/2} \varepsilon_{||}(z) dz - h}{h_{\text{eff}}},
\]

(3)

Because of uniform charge distribution\textsuperscript{23} in a plane located at height \(z\), one can approximate Eq. (3) by\textsuperscript{22}:
\[
\varepsilon_{||}^{\text{eff}} = 1 + \frac{\sigma_{||}^2}{\varepsilon_0 k_B T V_{\text{eff}}},
\]

(4)

where the effective volume is \(V_{\text{eff}} = Ah_{\text{eff}}, h_{\text{eff}} = (h - \sigma_{C-O}), \) and \(\sigma_{||}^2 = \langle M_{||}M_{||} \rangle - \langle M_{||} \rangle \langle M_{||} \rangle\). Here \(\sigma_{C-O} = 3.2\) is subtracted from \(h\) in order to use the actual height of channels in the calculations, i.e. the excluded volume effect\textsuperscript{21}. Notice that when the confining walls are h-BN layers the \(h_{\text{eff}} = h - \frac{1}{2} (\sigma_{N-O} + \sigma_{B-N})\) where \(\sigma_{N-O} = 3.26\text{Å}\) and \(\sigma_{B-N} = 3.31\text{Å}\textsuperscript{39}\).

To prove that the results of direct integration using Eq. (3) and that of Eq. (4) are equal, for channel with \(h=10\text{Å}\), we directly integrate over Eq. (2) and found \(\varepsilon_{||}^{\text{eff}} \approx 124.5\) which is an agreement with the number that we found by using Eq. (4), i.e. 120. Notice that the results for \(\varepsilon_{||}^{\text{eff}}\) do not change remarkably by changing slightly the effective height of channel. Note that Eq. (4) can be reformatted\textsuperscript{23} to have the usual form of the fluctuation dissipation theorem. Hereafter for simplicity, we use the \(\varepsilon_{||}\) instead \(\varepsilon_{||}^{\text{eff}}\). In fact, Eq. (4) has the linear response theory form with thermal averaging of the dipole of confined water when the external electric field is zero. This allows us to determine \(\varepsilon_{||}\) using an equilibrium correlation function. By calculating \(M_{\chi}\) and \(M_{\chi}\) and corresponding variance using Eq. (4), we were able to compute \(\varepsilon_{||} = (\varepsilon_{xx} + \varepsilon_{yy})/2\) as a function of \(h\).

In addition, one can find \(\sigma_{||}^2\)
\[
\sigma_{||}^2(h) = \lambda(h) k_B T,
\]

(5)

where \(\lambda(h) = \left(\frac{2d}{3}(\varepsilon_{||} - \varepsilon_b) - (\varepsilon_b - 1)\varepsilon_0 V\right)\). This equation relates the macroscopic parameters of confined water to a microscopic parameter \(\sigma_{||}^2\) which has the usual form of the fluctuation dissipation theorem\textsuperscript{40}.

**DENSITY PROFILE**

The number of water molecules across the channels significantly influences the physical properties of confined water. The variation of local mass density \(\rho(z)\) was depicted in

**CHANNELS WITH HEIGHT SMALLER THAN 10Å**

It is seen from Fig. 4 that for channels with size smaller than 6.7Å the total in-plane dielectric constant \(\varepsilon_{||}^{\text{eff}}\) is larger than 120, and for channels with height within the range 6.7Å < \(h < 8\text{Å}\) there is a deep minimum at \(h=7.4\text{Å}\) with \(\varepsilon_{||}^{\text{eff}} \approx 1.93\). The latter is about a factor 40 smaller than the bulk value. This is
FIG. 4. The variation of the in-plane dielectric constant $\varepsilon_||$ with height of the channel for confined water between graphene sheets for channels with size $h \leq 10 \text{Å}$. The inset shows the corresponding results for confined water between two h-BN sheets. Due to the formation of an unusual amorphous ice structure of confined water\footnote{Due to the formation of an unusual amorphous ice structure of confined water between the two confining walls when they are separated by $h \approx 7.4 \pm 0.5 \text{Å}$. Because of the obtained structure, one can categorize this as a proton-disordered ice phase of water. Previously it was found that the proton-disorder phase of ice (e.g. ice Ih) can have a dielectric constant of 100 and larger\ifnum\@footnotemark\setcounter{footnote}{0}}\else\footnote{Previously it was found that the proton-disorder phase of ice (e.g. ice Ih) can have a dielectric constant of 100 and larger.}\fi.\footnote{The radial distribution function (RDF) of the oxygen atoms confirms the mentioned ordered structure of confined water (see Fig. 5). The two dimensional RDF (RDF$_{||}$) of systems with size $h=6.5 \text{Å}$ and $h=7.4 \text{Å}$ are shown in Fig. 5 where the horizontal axis is $r = \sqrt{x^2 + y^2}$. In these RDFs significant second and third peaks appear only for $h=7-8 \text{Å}$. On the one hand, the results for $h=7.4 \text{Å}$ and $h=6.5 \text{Å}$ indicate a very different planar microscopic structure of confined water. When evaluating the time series of the total dipole moment, we discovered that confined water in channels with size $h=7.4 \pm 0.5 \text{Å}$ exhibits ferroelectricity. In Fig. 6(a), we depict the time evolution of $P_{x,y,z}$ for water in a channel with height $h=7.4 \text{Å}$. Notice that $P_z = 0$ while $P_x \neq 0$ and $P_y \neq 0$ for very long time simulation (we ran the simulation up to $\sim 1 \mu\text{s}$ and found $P_z$ is nonzero), i.e. non-zero net macroscopic electrical polarization. We found that when we repeat our simulations with new seed points, $P_x$ and $P_y$ showed other patterns but still $P_z \neq 0$ and $P_t \neq 0$. This led us to conclude that confined water in channels with height $h = 7.4 \pm 0.5 \text{Å}$ exhibits ferroelectricity. This effect profoundly influence water permittivity and transport inside either one dimensional or two-dimensional channels.\footnote{For other values of $h$ we did not find any net dipole moment. To gain more insights, we calculated the time average of the polarization vectors ($< M_{x,y} >$) of confined water for channels $h<10 \text{ Å}$. The results are shown in Fig. 5(b). It is seen that the confined water in channels $h = 7.4 \pm 0.5 \text{Å}$ exhibits ferroelectricity. The latter is due to the particular local ordered structure of confined water at these channels. Note that $< M_z >$ almost equal zero for all channel heights.} \footnote{By increasing the channel height further $\varepsilon_||$ approaches the bulk value $\simeq 75$, see Fig. 7. Notice that the scattering in the data of $\varepsilon_||$ for confined water between two h-BN sheets (the inset of Fig. 7) is due to the ionic nature of the h-BN sheet, i.e. the N and B atoms have local charges of -0.3e and 0.3e, respectively. In other words, in addition to the vdW interactions between water molecules and N and B atoms, the Coulomb interaction is also involved in the simulations. The latter causes a competition between thermal motion of the water molecules and the Coulomb (and vdW) interaction resulting in an enhanced variance of the dipoles of water i.e. $\sigma^2$. The results for h-BN were obtained by using the water-h-BN potential introduced by Wu et al.\footnote{Therefore we conclude that independent of the strength of the interaction between the water and the confining walls, there is a universal behavior in $\varepsilon_||$ with $h$ in case of hydrophobic confining walls.}} \section*{THE CONTINUUM MODEL} The capacitors-in-series model can explain the channel size dependence of the out-of-plane dielectric constant. It was first proposed by Zhang\cite{ZHANG201950}. Here, we extend this idea and to find the in-plane dielectric constant of nanoconfined water. It has
also been used to explain experimental results in Ref. [7]. Confined water can be considered as a continuum media consisting of three regions, i.e. two surface water layers (SL) and bulk water (b) between them (see Fig. 1(a)). One naturally expects, because of the isotropy in the (x,y)-plane in the absence of external field, that the net in-plane polarization of the system is zero. For a given channel with height \( h \), the boundary conditions on the in-plane components of the electric field \( \mathbf{E}_{||} \) at the interfaces of the aforementioned regions are \( \mathbf{E}_{||}^{SL} = \mathbf{E}_{||}^{b} \) where || refers to the planar component. Moreover, the total in-plane dipole moment \( P_{||}^{T} \) of the system is given by

\[
P_{||}^{T} = 2P_{||}^{SL} + P_{||}^{b},
\]

where \( P_{||}^{SL} \) and \( P_{||}^{b} \) are the dipole moments at the SL and bulk region of the system (see the small box in Fig. 1(a) which indicates the interface between bulk and SL regions). The factor 2 in Eq. 6 is added because there are two SLs at the top and bottom of the system (see Fig. 1(a)). Here, \( P_{||}^{SL,b} = E_{||}^{SL,b} - 1 \) and \( V_{SL,b} = \sqrt{dA} \) where \( V_{SL} = dA \) and \( V_{b} = (h - 2d)A \) are the volume of SL and bulk region, respectively. Also, \( A \) is the area of the interface and \( h(d) \) is the height of the channel (SL). Notice, \( \epsilon_{||}^{SL} \) and \( \epsilon_{||}^{b} \) are the parallel (in-plane) component of the dielectric constant of SL and bulk water, respectively. Substituting the polarization in Eq. 6, one finds the following in-plane component of dielectric constant

\[
\epsilon_{||}^{T}(h) = \frac{2d(\epsilon_{||}^{SL} - \epsilon_{||}^{b})}{h} + \epsilon_{||}^{b}.
\]

The water molecules in SLs are weakly bound to the graphene walls due to the van der Waals interaction between the water molecules and graphene, therefore, they are less mobile as compared to the water molecules in the bulk region. In order to determine \( \epsilon_{||}^{T}(h) \) one needs to know \( d, \epsilon_{||}^{SL} \) and \( \epsilon_{||}^{b} \). It is known that in bulk water \( \epsilon_{||}^{b} = \epsilon_{||}^{b} = \epsilon_{||}^{b} \) \( \approx 80 \). Moreover, in Ref. [6], it was found that the SLs have: i) an effective width of about \( d = 5-10 \AA \), ii) an amorphous ice structure, and iii) small out-of-plane dielectric constant \( \epsilon_{\perp}^{SL} \sim 2-3 \). From our MD simulations we found that \( \epsilon_{||}^{SL} \ll \epsilon_{||}^{SL} \) which results in a nonlinear decrease in \( \epsilon_{||}^{T} \) versus \( h \), i.e. \( d\epsilon_{||}^{T} / dh < 0 \). In addition, Eq. (4) is a capacitors based model as previously introduced by Zhang for determining the out-of-plane dielectric constant of nanoconfined water [49].

The solid curve in Fig. 7 and corresponding inset figure are the results of Eq. 7. With \( d = 5 \AA, \epsilon_{||}^{SL} = 115 \) and \( \epsilon_{||}^{b} = \epsilon_{||}^{b} = 72 \) (the bulk value as obtained from the SPC/E model). For h-BN walls we used \( d = 6 \AA \). In fact, there is a weak van der Waals adhesion between the graphene (and h-BN) walls and the water molecules resulting in a weak bonding of water to the walls. A typical length scale of this attraction is \( 5 \AA \) for SLs near graphene and \( 6 \AA \) for that near h-BN. Notice that this simplest model is able to describe the \( h > 10 \AA \) behavior of \( \epsilon_{||} \) very well.

**CONCLUSION**

In summary, we performed extensive atomistic simulations
to determine the in-plane component of the dielectric constant of confined water in two regimes, i.e. \( h < 10 \text{Å} \) and \( h \geq 10 \text{Å} \). The atomically smooth graphene and h-BN interfaces were used as confining walls. The correlation between the height of the channels and the physical properties of the trapped water was studied. We constructed continuum model that is able to fit our atomistic simulations for channels with \( h \geq 10 \text{Å} \) where there is a strong enhancement of \( \varepsilon_{||} \). Our results verify the final conclusions of the review paper by Kavokine et al.\(^{5}\) about different theoretical approach that one needs to study confined water at slits with size smaller or larger than 10Å. For channels with \( h = 7.4 \pm 0.5 \text{Å} \) we obtained values for \( \varepsilon_{||}(\varepsilon_{||}(\infty)) \) up to almost two orders of magnitude smaller (the same order of magnitude) as compared to the bulk value \( \sim 80 (\sim 3)\)\(^{45}\). This was explained as due to the formation of a crystalline phase of water. Furthermore, we predict ferroelectricity in the experimentally accessible timescales (1µs) and temperature (300 K) in water confined in channels with height \( h = 7.4 \pm 0.5 \text{Å} \). We found that while the diffusion coefficient reaches its bulk value for channels of \( h > 15 \text{Å} \) (i.e. diffusion is governed by short range effects), the effects of graphene (or h-BN) sheets on the fluctuation of \( M_{x,y} \) is long range, i.e. channels with height of 50Å have still suppressed fluctuations of \( M_{x,y} \). The abnormal decrease in the dielectric constant of confined water in channels with height \( h = 7.4 \pm 0.5 \text{Å} \) is related to the emergence of ferroelectricity. Our results provide insights into the dielectric properties of nanoconfined water gives a consistent physical picture of \( \varepsilon_{||} \) as function of the water layer thickness.

**DATA AVAILABILITY**

The data that support the findings of this study are available from the corresponding author upon reasonable request.

**REFERENCES**


