

SUPPORTING INFORMATION

Water Flow through Interlayer Channels of 2D Materials with Various Hydrophilicities

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1. Contact angle of a water droplet on walls with various partial charges

Due to scale limitations, MD simulations generally adopt nanometer-sized water droplets, which leads to a nonnegligible line tension force at the tri-phase junction. Therefore, the apparent contact angle is usually system-size-dependent.¹ Thus, we utilize the method proposed by Rafiee *et al.*², which eliminates the system-size effect on the contact angle once the size of the droplet is larger than 2000 molecules.

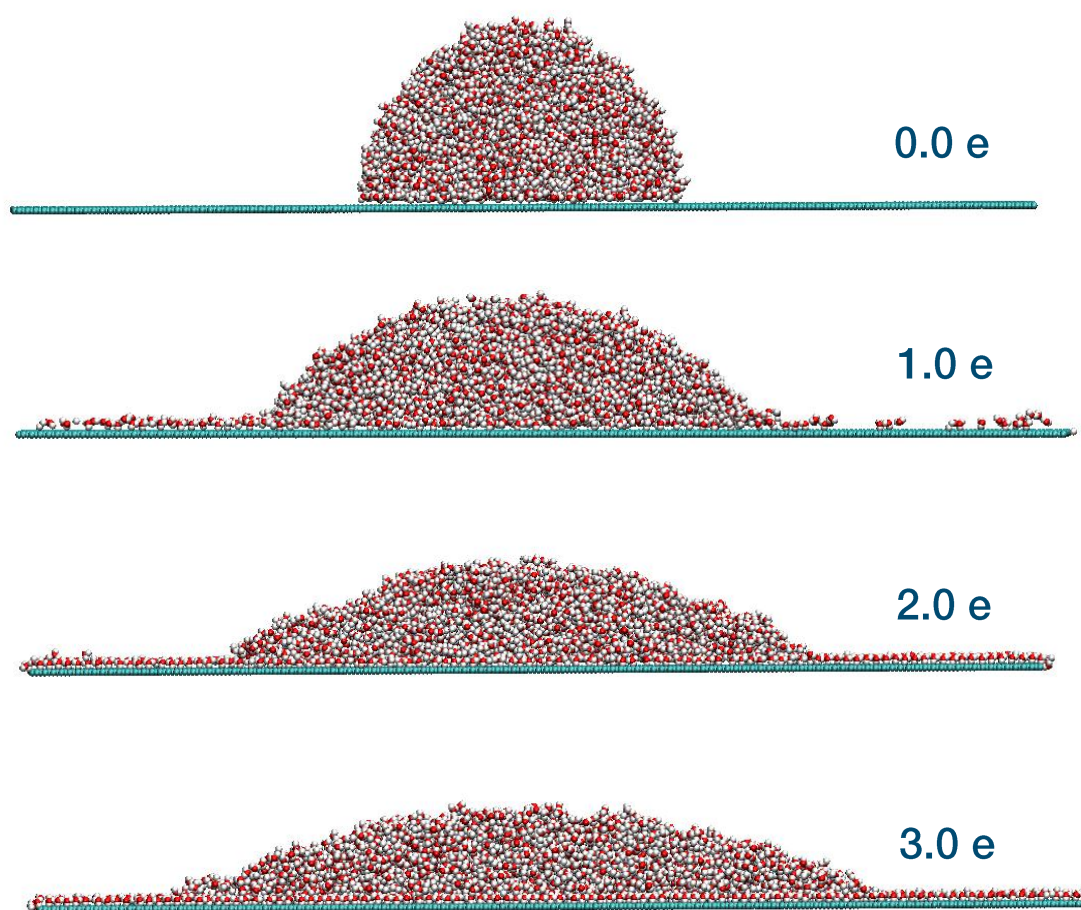


Figure S1. Contact angles of water droplets on four interfaces

2. Methodology used to calculate the slip length based on the friction coefficient

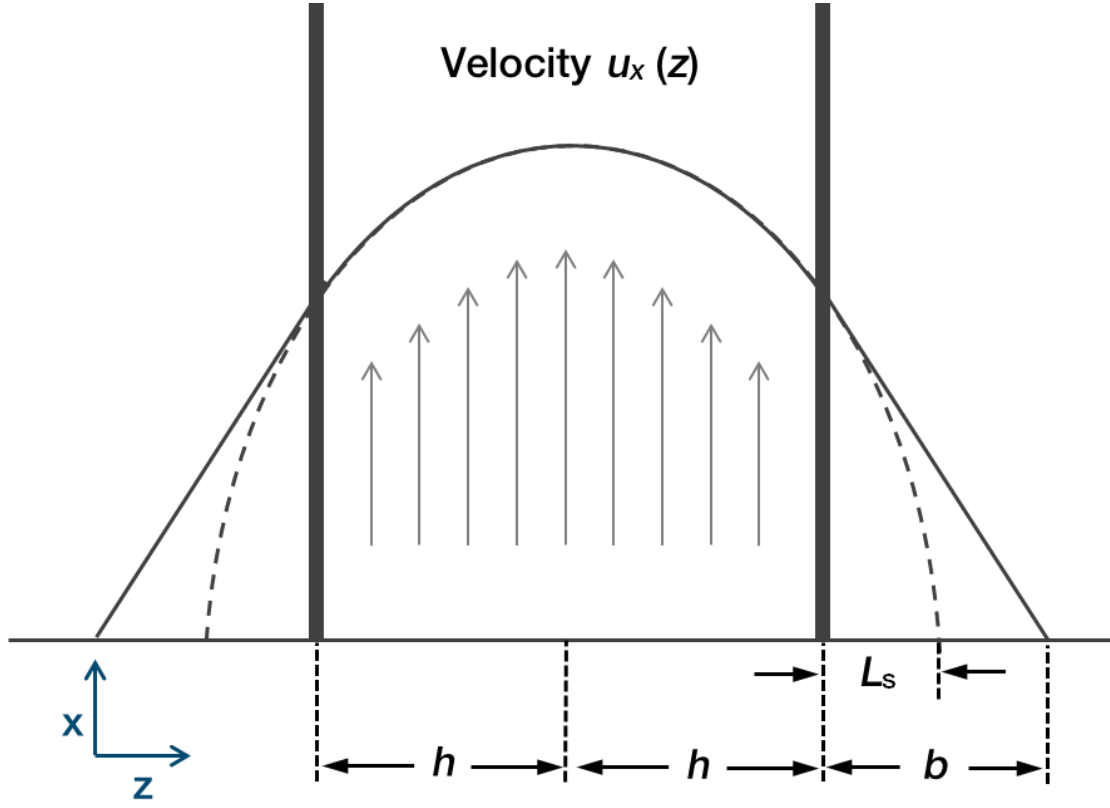


Figure S2. Schematic of fluid flow in the channel and the fluid slip length

The friction of water on a solid surface is usually discussed in terms of the partial slip hydrodynamic boundary condition, which relates the water boundary velocity v_{slip} at the interface to its gradient $\partial_n v$ in the direction normal to it as $b\partial_n v = v_{slip}$, where b is the slip length based on the gradient at the interface.³ Then, the “bulk” viscous stress is $\sigma_f = \eta\partial_n v = -F/A = \lambda v_{slip}$, in which η is the shear viscosity, λ is the water/solid friction coefficient and A is the contact area; the slip length is accordingly deduced from the water/solid friction coefficient λ by the relation $b = \eta/\lambda$.⁴ However, according to Equation 1 (velocity distribution of the Navier-Stokes equation), we proposed that the definition of

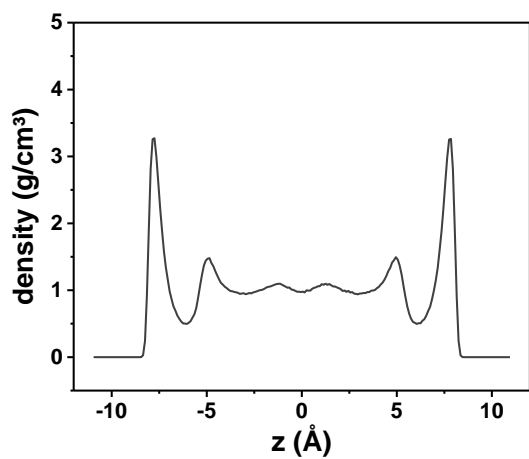
slip lengths should be based on an extension of the velocity profile. Thus, according to the quantitative relationship between b and L_s , the slip length calculated based on the friction coefficient is:

$$L_{s-\lambda} = \sqrt{h^2 + 2h\frac{\eta}{\lambda}} - h \quad (S1)$$

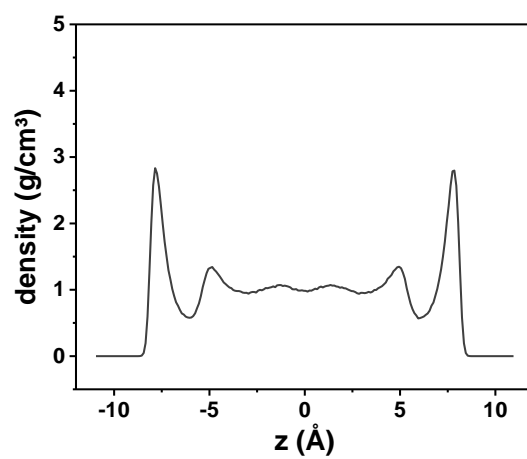
3. Detailed water structure in channels with varying hydrophilicity

Water flow in nanochannels is related to the corresponding water structure configuration. To further characterize the water behavior in channels with different hydrophilicity, in Figure S3, we show the density profile along the z direction of water molecules confined in channels with four different degrees of hydrophilicity. In our work, the structure of water inside each channel remains considerably stable when steady flow is reached and is not associated with external pressure differences, which suggests that this structure is only dependent on the hydrophilicity of the interface. The bulk phase appears at the middle of each channel, where the density of water approaches 1 g/cm^3 .

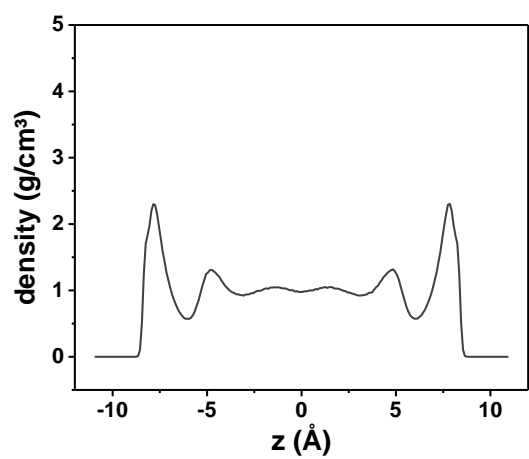
However, the degree of hydrophilicity exerts a strong influence on the structure of water molecules within the first layer adjacent to the channel wall. It is clear from Figure S3 that the first layer adjacent to the wall becomes increasingly wider and the peak becomes increasingly lower when the channel is modified with charges from 0.0 e to 2.0 e. In addition, when the assigned charge increases, the water molecules in the channel are closer to the wall. It appears that there are similar density distributions in the 1.0 e and 2.0 e channels compared with the pristine channel, which is consistent with the similar low-curvature curves in the corresponding velocity profiles (shown in Figure 5). However, when the assigned charge increases to 3.0 e, the peak contradicts this trend, appearing sharper and higher than in other conditions, corresponding to a zero velocity in the boundary layer in the velocity profile.



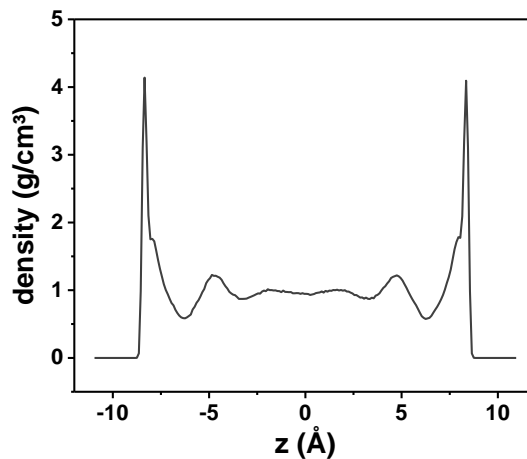
(a)



(b)



(c)



(d)

Figure S3. Density profiles of water in four channels with various hydrophilicities, (a) 0.0 e, (b) 1.0 e, (c) 2.0 e, (d) 3.0 e.

References

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