Supporting Information for
Friction Reduction at a Super-Hydrophilic Surface: Role of Ordered Water

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PS1. Analysis of the friction coefficient in the confined space.

For a steady Couette flow system, the friction force is always equal to that of the pulling force. If we divide the water layer into n (herein without loss of generality $n = 10$) layers and denote the force between every two contacting layers $F_{n,n-1}$, we then have

$$F_{pull} = F_{\mathrm{bs},1} = F_{1,2} = \ldots = F_{9,10} = F_{\mathrm{us},10} \quad (1),$$

where $F_{\mathrm{bs},1}$ is the force between the bottom solid surface and the water layer, $F_{\mathrm{us},10}$ is the force between upper solid surface and the water layer, and $F_{n,n-1}$ is the force between the ($n-1$)th and nth water layers. The friction coefficient can be written as

$$\lambda_{\text{solid-liquid}} = F_{\mathrm{pull}}/(Av_1),$$

$$\lambda_{1,2} = F_{\mathrm{pull}}/(A(v_2-v_1)),$$

$$\ldots$$

$$\lambda_{9,10} = F_{\mathrm{pull}}/(A(v_{10}-v_9)),$$

$$\lambda_{\mathrm{us},10} = F_{\mathrm{pull}}/(A(v_{\mathrm{us}}-v_{10})) \quad (2),$$

where $\lambda_{n-1,n}$ denotes the friction coefficient between the ($n-1$)th and nth water layers, and $\lambda_{\text{solid-liquid}}$ and $\lambda_{\mathrm{us},10}$ denote the bottom and upper solid–liquid friction coefficients.

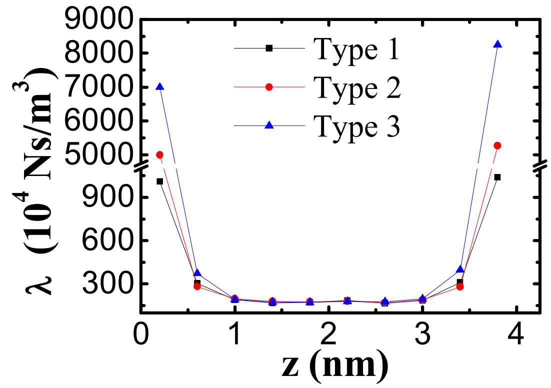

Figure S1. Friction coefficient λ in the confined space versus z for the three types of surfaces.

Thus, we have

$1/\lambda_{\text{solid-liquid}} + 1/\lambda_{1,2} + \ldots + 1/\lambda_{9,10} + 1/\lambda_{\text{us},10} = Av_1/F_{\text{pull}} + A(v_2-v_1)/F_{\text{pull}} + \ldots + A(v_{10}-v_9)/F_{\text{pull}} + A(v_{\text{us}}-v_{10})/F_{\text{pull}} = A(v_{\text{us},10})/F_{\text{pull}} = 1/\lambda_{\text{total}}$ (3).

Here, λ_{total} is the total friction of the system and the forces F_{pull} are 1.30 nN, 0.96 nN, and 1.45 nN for the type 1, 2 and 3 surfaces, respectively. This relationship is similar to the electrical resistance of the parallel circuit. We calculated the friction coefficient as a function of the location of water layers $\lambda_{n-1,n}$. The friction coefficient was almost constant for $3 \leq n \leq 7$: $\lambda_{2,3} = \lambda_{3,4} = \ldots = \lambda_{7,8} = (1.8\pm0.2) \times 10^6$ Ns/m^3 (see Fig S1). In fact, this friction coefficient in bulk water is related to the water viscosity satisfying $\mu = \lambda\Delta z$, and here $\Delta z = 0.4$ nm. The bulk viscosity μ was calculated to be 7.2×10^{-4} Pa·s, which is consistent with previous work [1]. Considering the symmetry of the upper and bottom surfaces in the simulation systems, together with the constant $\lambda_{n-1,n}$ ($3 \leq n \leq 7$), we only focus on the solid/water friction coefficient $\lambda_{\text{solid-liquid}}$ and the first/second water layer friction coefficient $\lambda_{1,2}$ near the bottom surface when we compare the three systems. We thus propose a new parameter λ_{surface} to describe the surface friction coefficient, that combines $\lambda_{\text{solid/liquid}}$ and $\lambda_{1,2}$:

$$1/\lambda_{\text{surface}} = 1/\lambda_{\text{solid/liquid}} + 1/\lambda_{1,2} \quad (4).$$

We also note that this friction reduction effect can be extended to larger systems, even macroscopic systems, because only the solid/liquid friction coefficient $\lambda_{\text{solid-liquid}}$ and first–second layer friction coefficient $\lambda_{1,2}$ contribute to the surface friction.

PS2. Discussion of the effect of the pulling velocity on surface friction

We also investigated the effect of the pulling velocity on friction reduction. Here, without loss of generality, we investigated the friction force stress and friction coefficient when the pulling velocity was 50 m/s. The results are shown in Fig S2(A). We still found the relationship $\sigma_1 \approx \sigma_2 < \sigma_3$, where $\sigma_1 = (1.06\pm 0.03) \times 10^7$ Pa, $\sigma_2 = (1.06\pm0.02) \times 10^7$ Pa and $\sigma_3 = (1.12\pm0.03)\times 10^7$ Pa. Because of the lower pulling velocity, the friction stress at v = 50 m/s is less than that at v = 100 m/s. However, the friction coefficient when v = 50 m/s is quite close to that when v = 100 m/s. As shown in Fig S2(B), the $\lambda_{solid/liquid}$ values on the type 1, 2, and 3 surfaces were $(8.7\pm1.1) \times 10^6$ Ns/m^3, $(3.1\pm1.1) \times 10^7$ Ns/m^3, and $(4.2\pm1.2) \times 10^7$ Ns/m^3, respectively. The $\lambda_{1,2}$ values for the type 1, 2, and 3 surfaces were $(3.2\pm0.2) \times 10^6$ Ns/m^3, $(2.5\pm0.2) \times 10^6$ Ns/m^3, and $(3.7\pm0.1) \times 10^6$ Ns/m^3, respectively. By combining $\lambda_{solid/liquid}$ and $\lambda_{1,2}$, we obtained $\lambda_{surface}$ values of $(2.3\pm0.2) \times 10^6$ Ns/m^3, $(2.3\pm0.3) \times 10^6$ Ns/m^3, and $(3.7\pm0.2) \times 10^6$ Ns/m^3 for the type 1, 2, and 3 surfaces, respectively, as shown in Fig S2(B). We still obtained friction reduction of 36% on the super-hydrophilic surface when comparing type 2 and type 3 surfaces. Remarkably, the friction coefficient on the type 2 surface is the almost the same as that of the more hydrophobic type 1 surface, which agrees very well with the results in the main text when the pull velocity was v = 100 m/s.

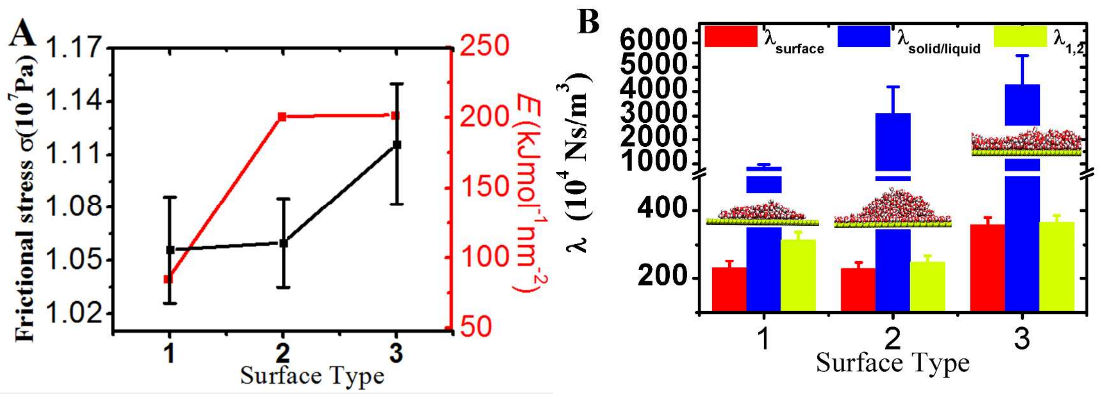

Figure S2. (A) Frictional stress σ in Couette fluid systems and surface–water interactions of unit area E on type 1–3 surfaces when the pulling velocity was 50 m/s. (B) Friction coefficient λ and apparent contact angles 44°, 74°, and 0° of the three types of surface when the pulling velocity was 50 m/s.

PS 3. Role of the first water layer in surface–water interactions

The strength of surface–water interactions are important in determining surface–water friction [2]. In the simulations, the first water layer (thickness 0.4 nm) near the hydrophilic surface is important to understand surface friction and surface wetting behavior, as described in the main text. To further verify this point, we calculated the interactions (van der Waals and electrostatic interactions) between each water molecule in the water layers and the solid surface. As shown in Fig S3, the interactions between each molecule in the first water layer and the surface were −11.0 kJ/mol, −20.7 kJ/mol, and −22.7 kJ/mol, while the interactions between each molecule in the second water layer (0.4 nm < $z \leq 0.8$ nm) and the surface were −1.0 kJ/mol, −1.3 kJ/mol, and −1.4 kJ/mol for type 1, 2, and 3 surfaces, respectively. Clearly, the interaction between the first water layer and the surface make up over 90% of the surface–water interaction. Thus, we conclude that the friction of the solid surface and the first water layer is the key in determining surface–water friction. Thus we used the friction coefficient $\lambda_{solid/liquid}$ between the surface and first water layer to characterize the friction coefficient between the surface and all the water molecules.

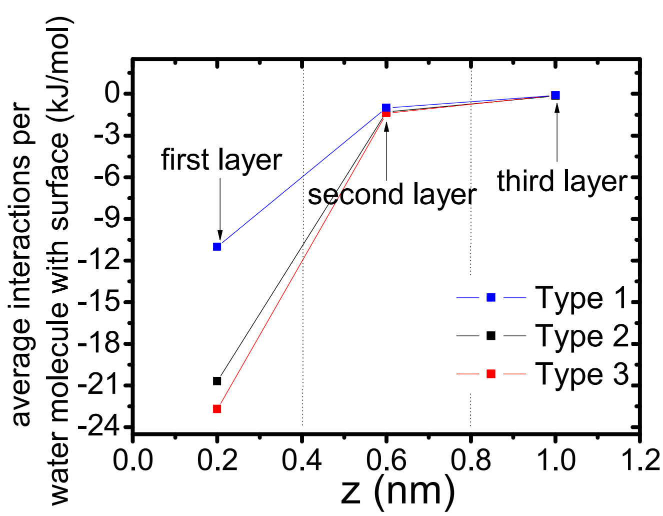

Figure S3. Interactions between the water molecules in the first, second, and third water layers with the solid surface for the three surface types.

PS 4. Density profiles of water confined in the space

Density profiles of water confined in the space are shown in Figure S3.

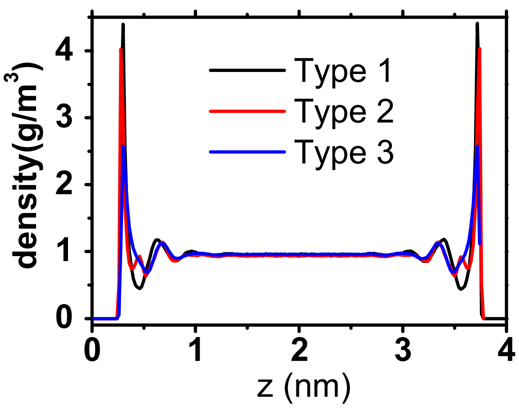

Figure S4. Density profiles of water molecules in the nanoconfined space.

PS 5. Velocity profiles near the solid surface types 1-3.

Velocity profiles near the solid surface types 1-3, where a non-linear effect can be found near the solid surfaces, consistent with the previous work by Netz et al.[3]. This effect should be attributed to that the friction coefficient between the first water layer and the second water layer is different from that between water layers in the bulk water. It should be noted that, this no-linear effect is more obvious when the shear rate is large.

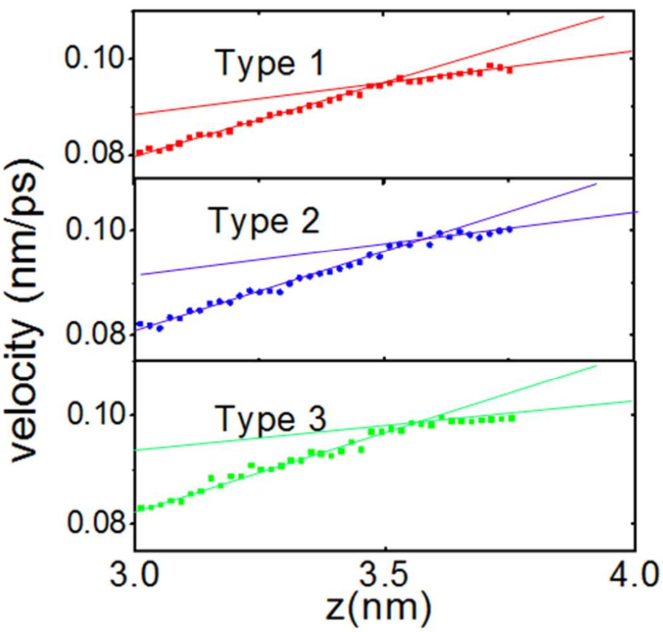

Figure S5. Velocity profiles near the solid surface types 1-3.

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