Supporting Information for "Evaporation of Tiny Water Aggregation on Uniformly Complete Wetting Surface with Different Temperatures"

Yuwei Guo^{1,2}, Rongzheng Wan^{1*}

¹Division of Interfacial Water and Key Laboratory of Interfacial Physics and

Technology, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, P.O.

Box 800-204, Shanghai 201800, China

²University of Chinese Academy of Sciences, Beijing 100049, China

*E-mail address: wanrongzheng@sinap.ac.cn

*Tel.: 021-5955478

The evaporation rate of 0.41 nm thickness liquid water on the substrate with charge distance of 0.426 nm.

We have performed the MD simulations for the different substrate with the 0.426 nm distance between the positive and negative charges. Fig. S1(a) shows the structure of the hydrophilic substrate with the same size in our work, positive and negative charges of the same magnitude q = 0.6 e were assigned to the atoms at a distance of 0.426 nm, and the water molecules can spread on the substrate. 10614 TIP4P/2005 water molecules were placed 0.5 nm above the substrate in a box shape. With the same conditions of the MD simulation in our work, the evaporation rates of nanoscale water molecules with different temperatures are shown in Fig. S1(b). As Fig. S1(b) shows, for the different lattice parameter of the substrate, the growth of nanoscale water evaporation rates still has a slow trend in high temperature range.



Fig.S1 The evaporation rate of 0.41 nm thickness water on the substrate with charge distance of 0.426 nm. (a) Detailed geometry of the solid substrate model. The blue and red spheres represent the atoms of solid with positive charges and negative charges of 0.6 e, respectively. The cyan spheres represent the neutral atoms. (b) The evaporation rate R of nanoscale water on the surface shown in (a) with different temperature T.

Fitting method of the evaporation rate with different temperatures.

We choose the data of temperature range 280 K \sim 340 K for exponential fitting in Fig. 2(a). Fig. S2 shows the evaporation rate with different temperatures and the fitting curves. The fitting curves in Fig. S2 derives from the fitting range of temperature 280 K to 360 K. In Fig. S2, there are also deviations at high temperatures. When the temperature is roughly below 340 K, the exponential fitting is in good agreement. Thus, we choose the temperature range of 280 K \sim 340 K for fitting.



Fig. S2 The evaporation rate R versus temperature T. The red squares with error bars represent the evaporation rates R of water film with thickness of 0.41 nm. The dark cyan circle and the orange triangle with error bars represent the evaporation rates R of water film with thickness 0.64 nm and 2.12 nm respectively. The red, dark cyan and orange dash lines are the exponential fits using the fitting range of temperature 280 K to 360 K.

The selection of outermost water.

The outermost water molecules in the simulations are defined as follows:

We divided the 30 nm * 30 nm substrate into x-y small cell with 3.5 Å * 3.5 Å side length. And all the water molecules was considered under the accelerating region. If there is only one water molecule in the unit, and there are more than 3 water molecules within 6 Å around the water molecule, we will regard this water molecule as the outermost water molecule in the unit. If there are multiple water molecules in the unit, we choose the water molecule which is largest in the Z coordinate and still belongs to the bulk water on the surface as the outermost water. Then the outermost water molecules in all units will make up the outermost water layer.

The autocorrelation functions of H-bond and molecular orientation.



Fig. S3 (a) (b) (c) Autocorrelation functions of the H-bond of the water thickness 0.41 nm, 0.64 nm, 2.12 nm respectively with different temperatures. (d) (e) (f) Autocorrelation functions of the water molecular orientation of water thickness 0.41 nm, 0.64 nm, 2.12 nm respectively with different temperatures.

Fig. S3 shows the autocorrelation functions of H-bond and molecular orientation with time *t* for different water thicknesses and different temperatures. By fitting the autocorrelation function of H-bond for t = 0 ps to t = 50 ps with the exponential decay function $y(t) = e^{-t/\tau_{H-bond}}$, we can obtain the H-bond lifetime τ_{H-bond} . The exponential decay function $y(t) = e^{-t/\tau_{orientation}}$ is used to fit the autocorrelation function of molecular orientation, then we can obtain the average orientational autocorrelation time $\tau_{orientation}$.

The fitting method of the H-bond autocorrelation functions.

There are multiple fitting method to fit the autocorrelation function of H-bond. We used a single exponential decay function $y(t) = e^{-t/\tau_{H-bond}}$ to obtain the H-bond lifetimes. The temperature from 280 K to 360 K was used to fit the H-bond lifetimes. We have also tried the double exponential fittings in Fig. S4, the detailed lifetime values vary somewhat, but the trend does not change.



Fig. S4 The outermost water H-bond lifetime obtained by double exponential fittings of the autocorrelation function of H-bond with different water thicknesses under different temperatures. The black squares, dark cyan circles and orange triangles

represent the H-bonds lifetimes for the outermost water molecules of water film with thickness 0.41 nm, 0.64 nm and 2.12 nm; the black, dark cyan, orange dash lines are the Arrhenius form fits.