Electronic Supplementary Material (ESI) for Nanoscale.

Supporting Information

Initial-position-driven Opposite Directional Transport of Water Droplet on Wedge-shaped Groove

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Section 1. Configuration of the system

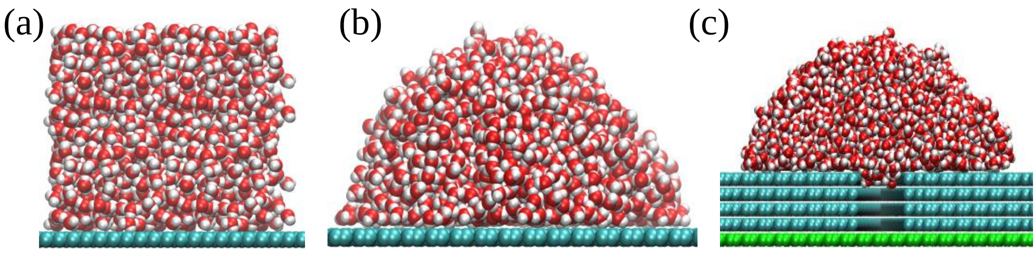

Figure S1. Snapshots of equilibrating process. (a) The initial configuration of the water cube (4×4×4 nm^3) on a graphene layer, (b) snapshot of the water droplet on the graphene layer after simulation of 2 ns, and (c) snapshot of the water droplet on the wedge-shaped groove surface after equilibration.

Section 2. Effect of cutoff radius

In order to check the influence of the cutoff radius on the movement behavior of water droplets, we performed molecular dynamics simulations with increasing it to 2 nm and decreasing it to 1nm. The results demonstrate that water droplets, placed near the narrower end, move towards the groove tip and transport in the opposite direction when put near the wide end whether the cutoff radius increases or decreases (Figure

S1). As is shown in Figure S2, the interaction energy of water-upper layers E_{w-u} play a dominant role when droplets move left, and the interaction energy of water-substrate E_{w-s} increase with droplets moving to the side with a wider opening. This also prove that the opposite movement direction is caused by the opposite interactions from the groove substrate and the upper layers with water droplets.

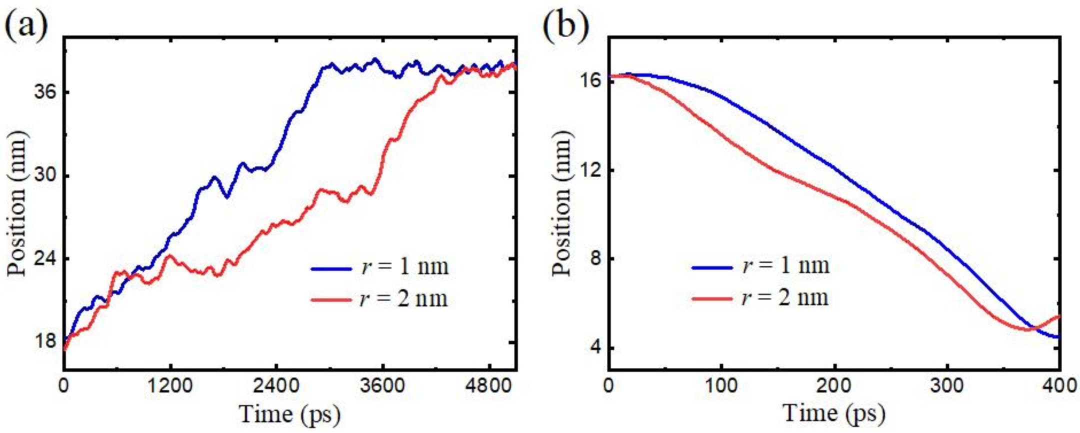

Figure S2. Evolutions of center of mass position and velocity of the water droplet with time along *x* direction. The water droplet is initially placed near the (a) wider and (b) narrower end. The blue and red lines are for the cutoff radius equals to 1 nm and 2 nm, respectively.

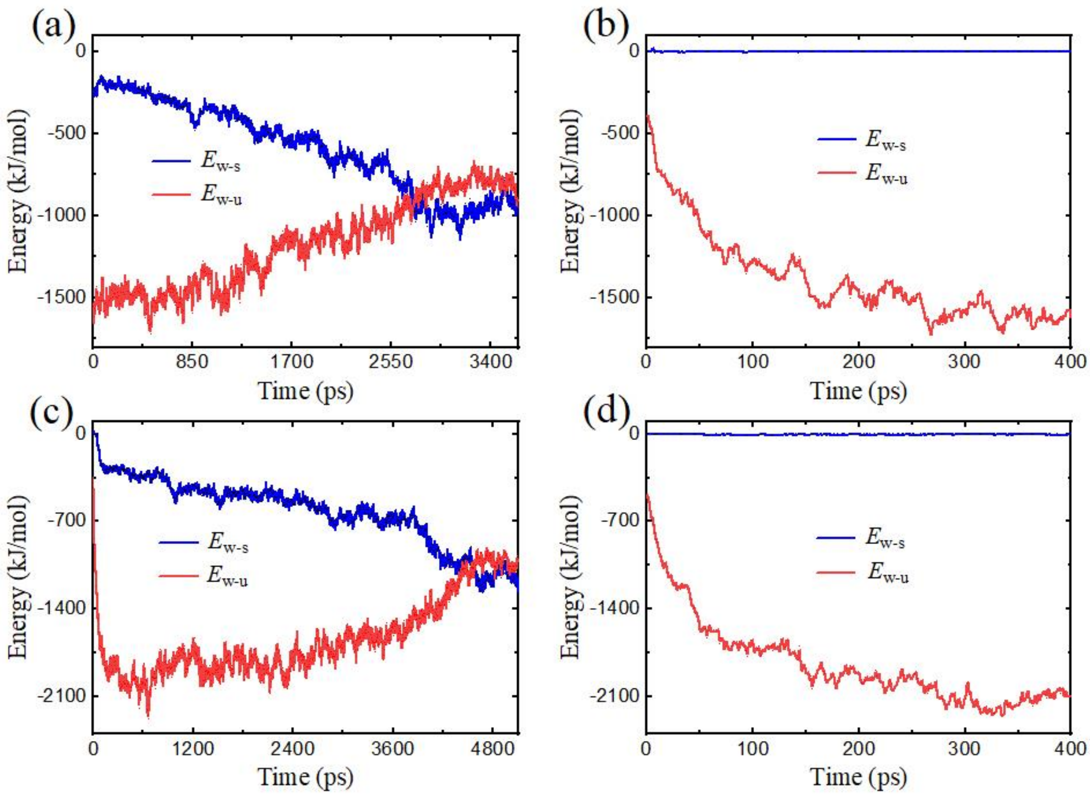

Figure S3. The interaction energy between the water droplet and the grooved surface: (a) (b) for the cutoff radius equal to 1 nm and water droplet initially placed near the wider and narrower end, respectively; (c) (d) for the cutoff radius equal to 2 nm and the water droplet initially placed near the wider and narrower end, respectively. Interaction energies from the upper layers ($E_{w\text{-}u}$) and the substrate ($E_{w\text{-}s}$) are colored by red and blue.

Section 3. Effect of surface wettability

The surface wettability in this research is adjusted to study its effect on the droplet transportation. We tuned the wettability of the surface by multiplying the energy parameter of carbon atoms, ε by a parameter (i.e. 0.8, 0.9, 1.1 and 1.2). As is shown in Figure S3, the same conclusions can be drawn.

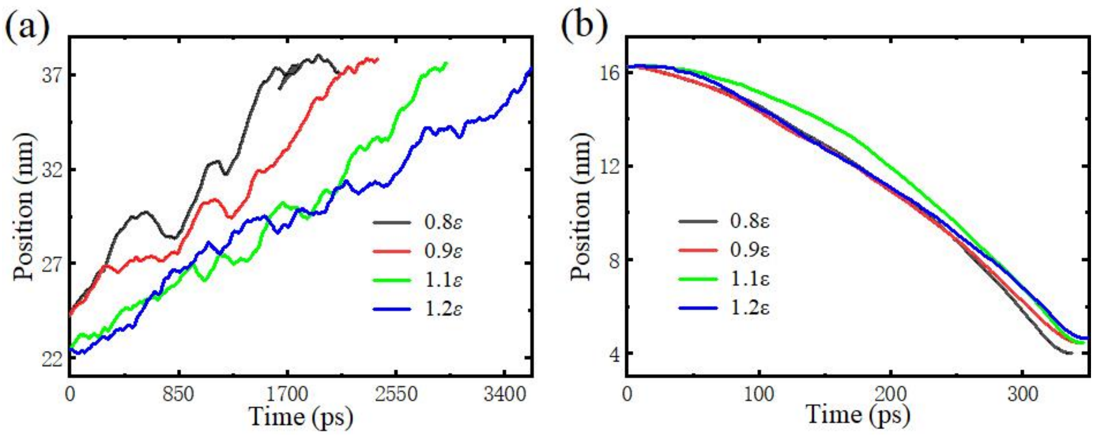

Figure S4. Evolutions of center of mass position of the water droplet with time along x direction: the water droplet initially placed near the (a) wider end and (b) narrower end with the energy parameters of 0.8*ε* (black), 0.9*ε* (red), 1.1*ε* (green) and 1.2*ε* (blue).

Section 4. Effect of droplet size

We further performed simulations of smaller (1181 water molecules) and larger water droplets (2621 water molecules) transporting on the wedge-shaped groove to check the effects of droplet size on the movement. As can be seen from Figure S4, water droplets exhibit the same movement direction, i.e. they move towards the narrow and wide opening of the groove when placed near the narrower and wider opening, respectively.

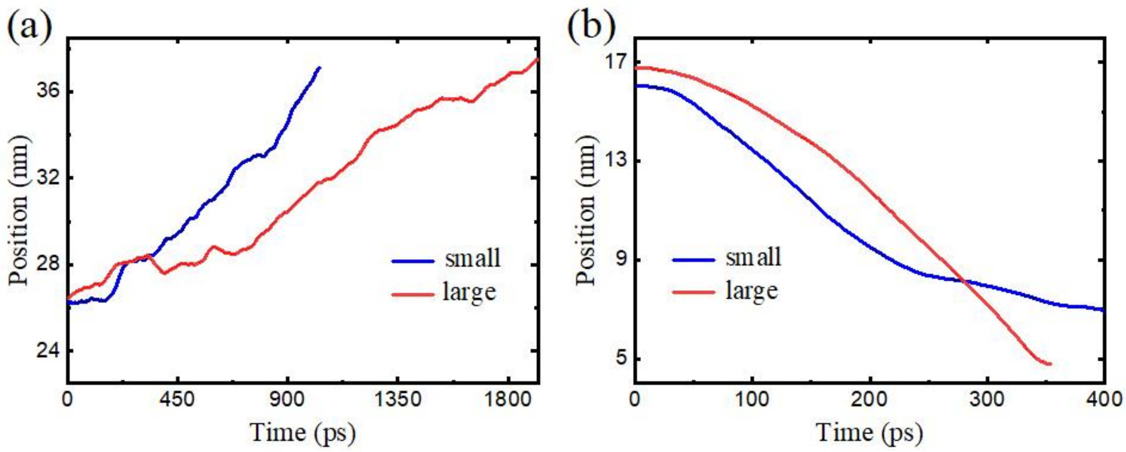

Figure S5. Evolutions of center of mass position of the water droplet with time along *x* direction: the water droplet initially placed near the (a) wider end and (b) narrower end with the smaller droplets (blue) and larger droplets (red).

Section 5. Effect of groove angle

We further constructed a graphene layer model (see Figure S5) with groove angle of 2° . We placed the water droplets near the wider end (Figure S5(a)) and narrower end (Figure S5(b)) to observe their movements. The results prove that the water droplets have the same moving trend with that in Figure 1.

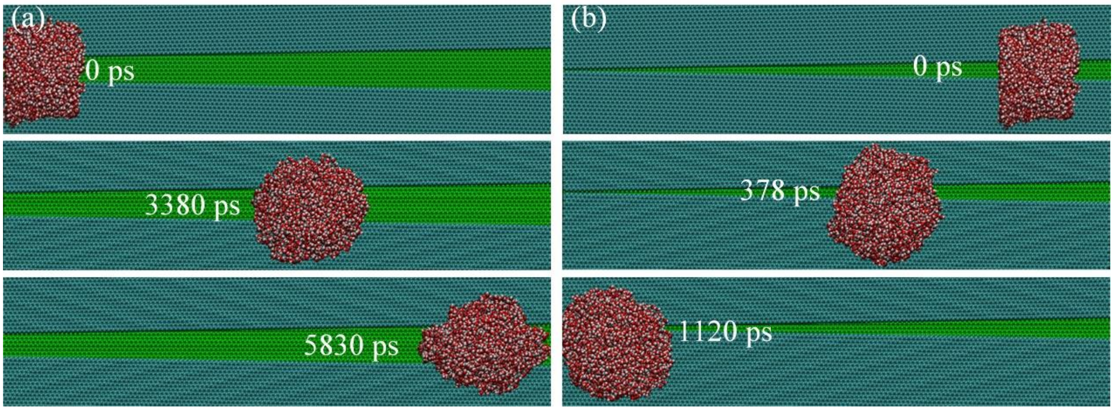

Figure S6. Snapshots of a moving water droplet on the wedge-shaped groove surface. (a) The water droplet initially placed near the wider end will move to the wider end; (b) the water droplet initially placed near the narrower end will move to the narrower end. The planes colored by cyan and green are the upper layers and the substrate layer, respectively. Water molecules are described by spheres with oxygen in red and hydrogen in white.

Section 6. Computational Method of Contact Angle and Viscous Resistance

By fitting the shape of the water droplet on the groove surface with circle equation (Fig S6), the average contact angle θ_{avg} can be calculated through the geometrical relationship between the droplet radius R = 2.5179 nm and contact radius r = 2.5159 nm. Here, the average contact angle θ_{avg} =87.72° .

Moreover, the droplet width $2r$ is 5.0318 nm and the height h' = 2.42 nm. The average groove width δ_{avg} = 2.18 nm. Therefore, the viscous resistance

$$F_{v2} = \frac{h'\eta L v}{2r} = k'\frac{h\eta L v}{\alpha x}$$

Where $k' = \frac{h\prime/h}{2r/\delta_{avg}}$ = 0.78. Thus,

$$\mathrm{F}_v = \mathrm{F}_{v1} + \mathrm{F}_{v2} = (1+k')\frac{h\eta L v}{\alpha x} = k\frac{h\eta L v}{\alpha x} = 1.78\frac{h\eta L v}{\alpha x}$$

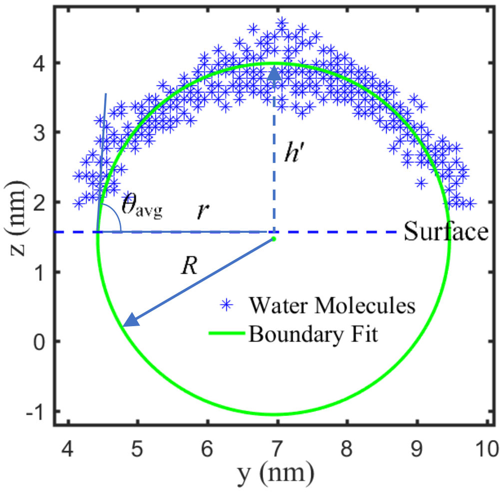

Figure S7. Schematic of water droplet interface on the groove surface. Blue stars are the simulated interface of the water droplet and the green circle is the fitting curve using circle equation. The blue dashed line is the top surface of the groove. The blue arrow is the circle radius R, and the blue solid line is the contact radius r. The blue dashed arrow is the height of the droplet h' and θ_{avg} is the average contact angle.