Supplementary information

The following supplementary information contains: Effect of MD time step; the effect of CNT type.

Terahertz electric field induced melting and transport of monolayer water confined in double-walled carbon nanotubes

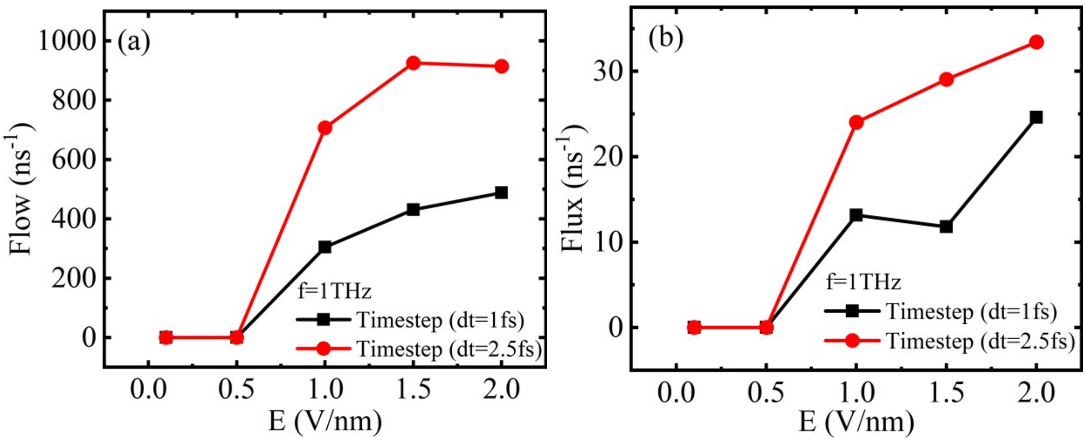
Yue Wu, Zi Wang, Shuang Li, Jiaye Su*

MIIT Key Laboratory of Semiconductor Microstructure and Quantum Sensing, and Department of Applied Physics, Nanjing University of Science and Technology, Nanjing 210094, China

*Corresponding author: jysu@njust.edu.cn

Effect of MD time step

As we can see in Figure S1, although the absolute values of water flow, flux and occupancy number are different at some field strengths, the behaviors for the two time steps are quite similar. Thus, the main conclusion should be same for different time steps. For the time step of 2.5 fs, the water flow and flux are greater, which may be caused by a more intensive vibration of Hbond with the terahertz electric field. Actually, the water flow and flux are sensitive to many parameters and even the employed water models [S1]. In most of previous atomic MD simulations, the time step of 2 fs was used, and in order to save the MD simulation time we used 2.5 fs in the present work and also our previous work.



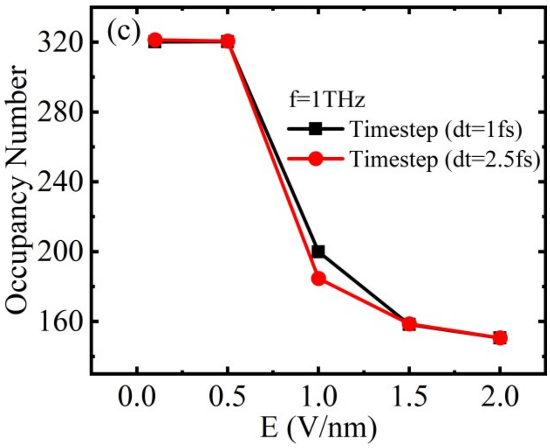


Figure S1. Water (a) flow, (b) flux and (c) occupancy number as a function of the field strength with f = 1 THz for different MD time steps.

Effect of CNT type

In the present work, we used the combination of (7,7) and (17,17) CNTs to create the monolayer water structures. We focus on the effect of terahertz electric field on the structures and dynamics of confined water molecules. To test the effect of CNT types, we have conducted additional MD simulations for CNTs (5,5), (15,15), (16,16), (18,18) and the results are shown in Figure S2. As we can see in Figure S2a, the behaviors of water flow for different CNT types are quite similar and the values at large field strengths exhibit a slight difference because of the slight difference in channel shape and volume. The behaviors of water flux in Figure S2b also are similar to each other, but the combination of CNT (5,5)&(15,15) has obvious greater values at large field strengths because of the stronger confinement. The water occupancy numbers in Figure S2c also are quite similar to each other, where the values of ice structures at E = 0.1 and 0.5 V/nm for CNT (7,7)&(17,17) are greater because of the greater ice diameter. The ice structures in Figure S2d also are similar for different CNTs, but for the smaller inner CNT (5,5) the ice tube should have more defects because of greater curvature. On the whole, for different CNT types, the main results and conclusions should be similar.

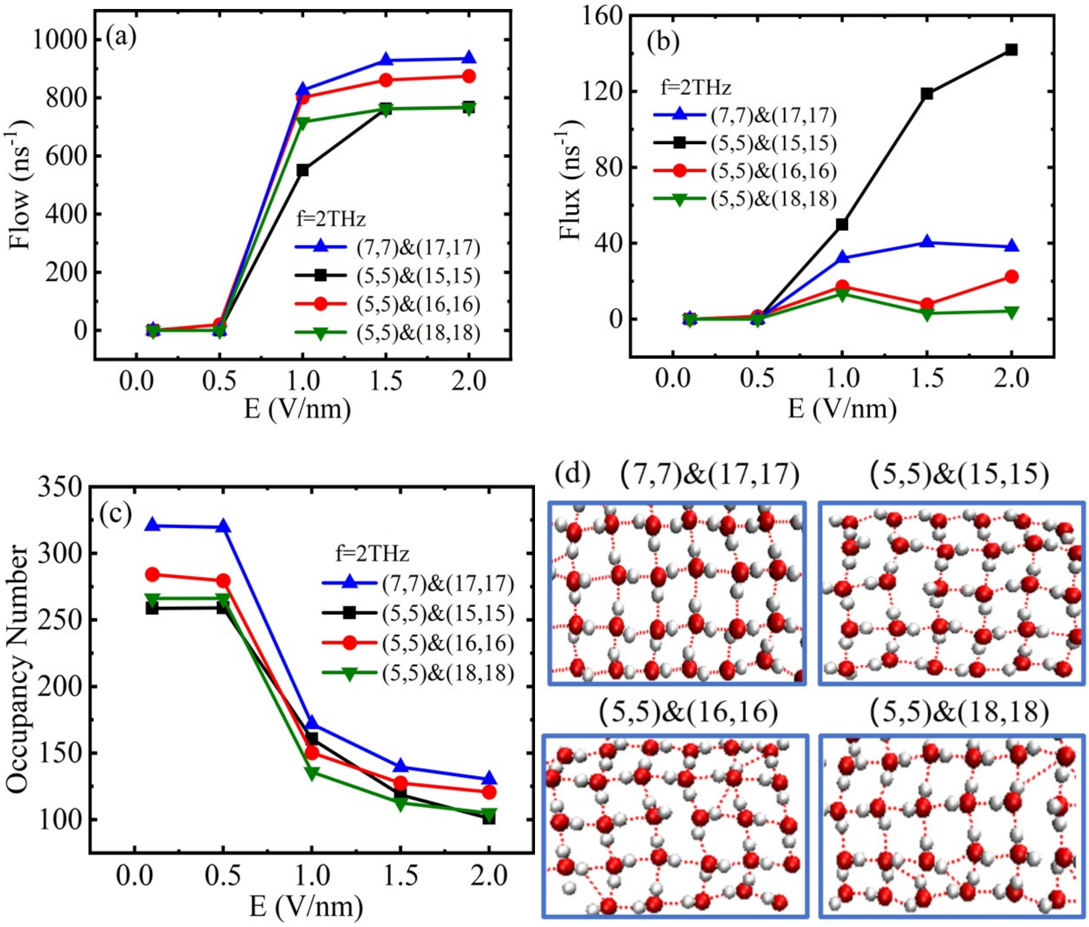


Figure S2. Results for different CNT types. Water (a) flow, (b) flux and (c) occupancy number as a function of the field strength with f = 2 THz. (d) Water structures in different combinations of inner and outer CNTs.

References

[S1] S. Salman, Y. Zhao, X. Zhang, J. Su, Effect of temperature on the coupling transport of water and ions through a carbon nanotube in an electric field, J. Chem. Phys. 2020, 153, 184503.