

Supporting Information:

An adjustable high-speed and directional diffusion of water nanodroplets confined by graphene sheets

Lijun Deng^{a,*}, Hai Qiu^b, Ben Wang^a, Zaoyang Guo^{a,*}

^aSchool of Science, Harbin Institute of Technology, ShenZhen, 518055, China

^bSchool of Mechanical Engineering, Jiangsu University of Science and Technology, ZhenJiang, 212003, China

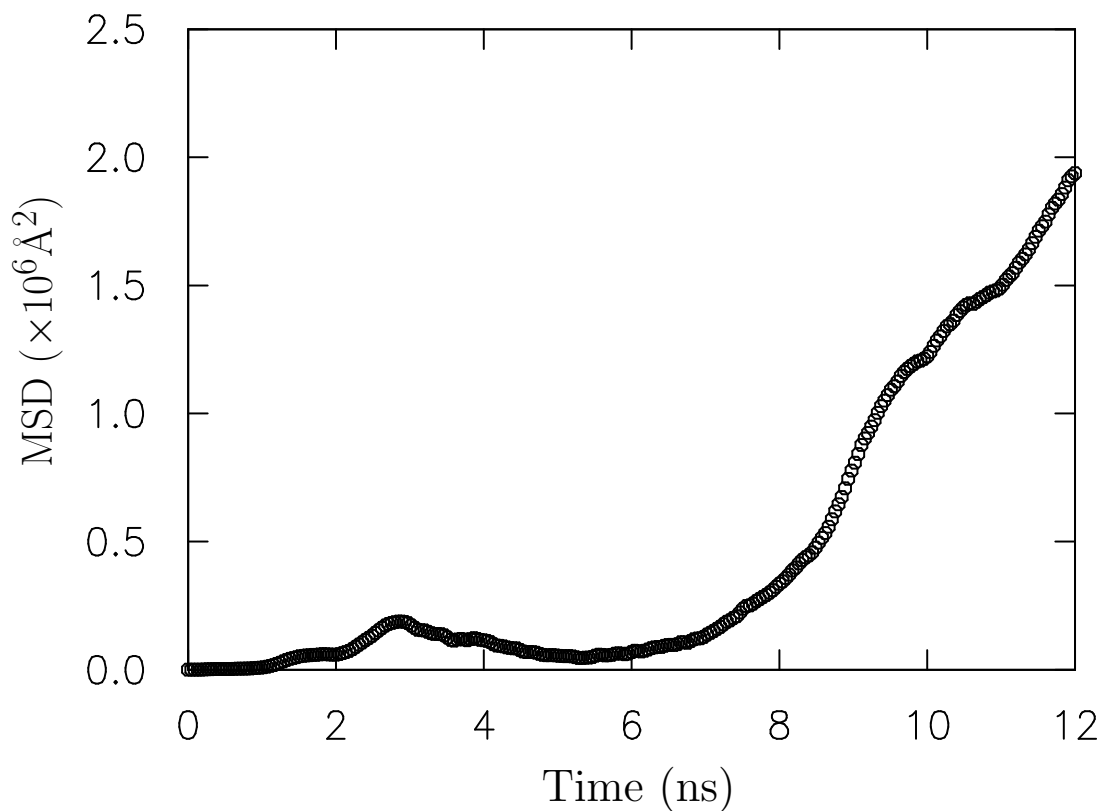


Figure S1: Mean squared displacement (MSD) vs. time for the nanodroplet composed of 252 water molecules at $d = 25 \text{Å}$ over 12 ns.

*Corresponding authors, Email: lijun_deng@foxmail.com; z-guo@foxmail.com

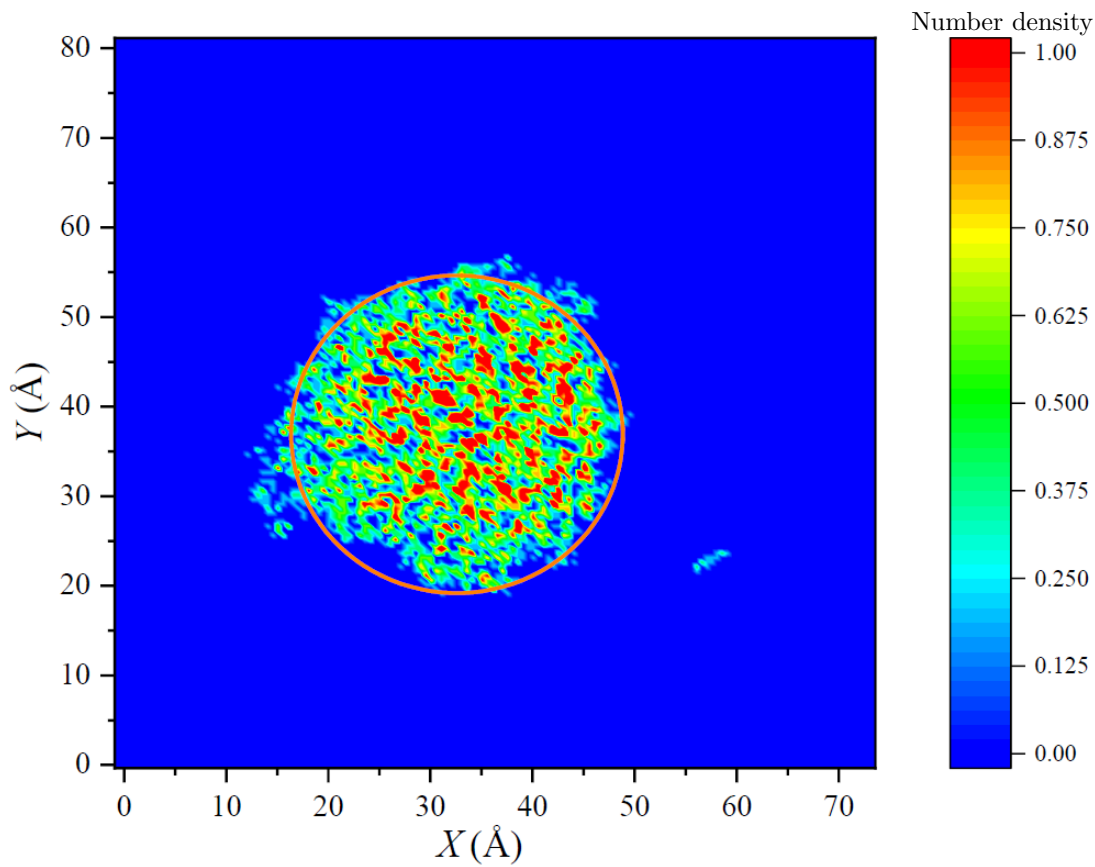


Figure S2: A density profiles of confined water nanodroplets in the $x - y$ plane. R is obtained from the schematic circle (the yellow circle).

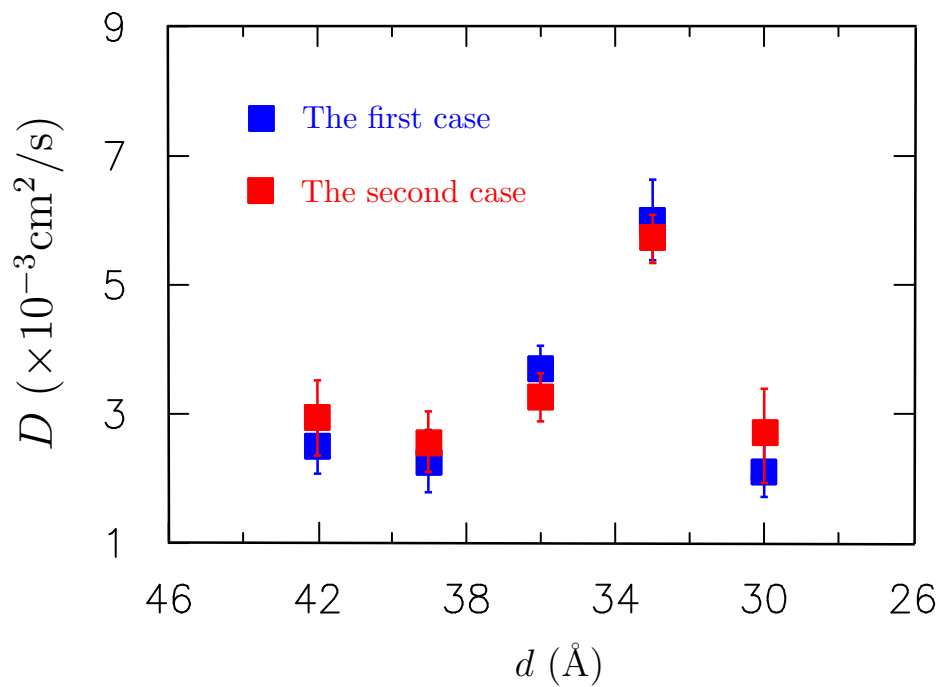


Figure S3: The diffusion coefficient D as a function of d for 512 molecules nanodroplet. The blue and red represent the first case and the second case, respectively.

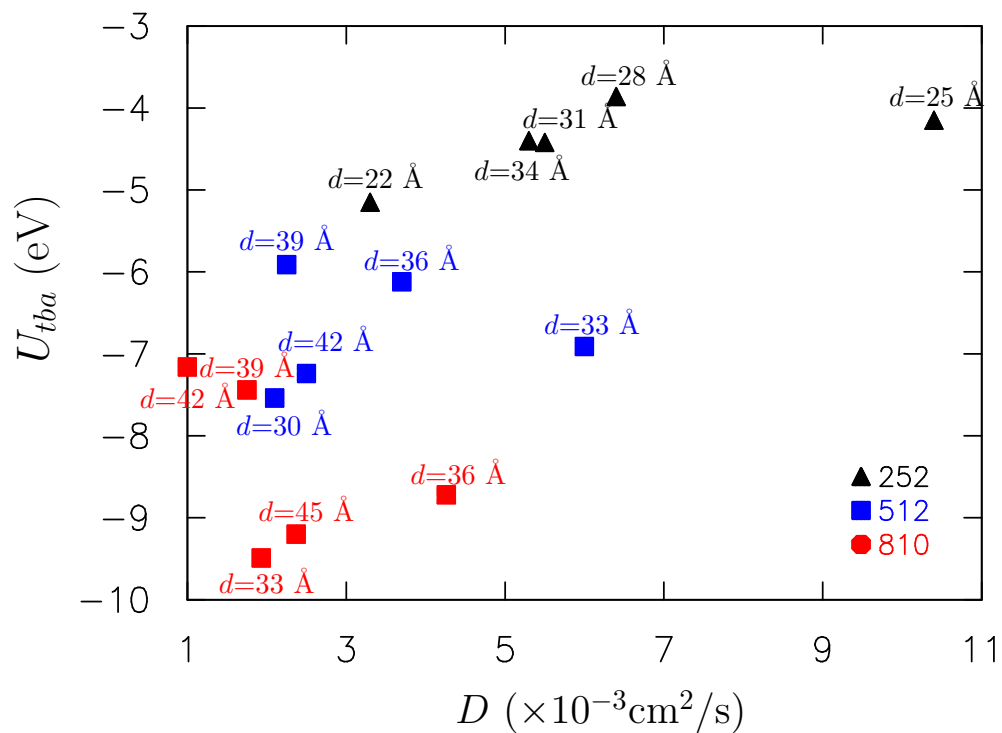


Figure S4: U_{tba} vs. D at different values of d for the three water nanodroplets.

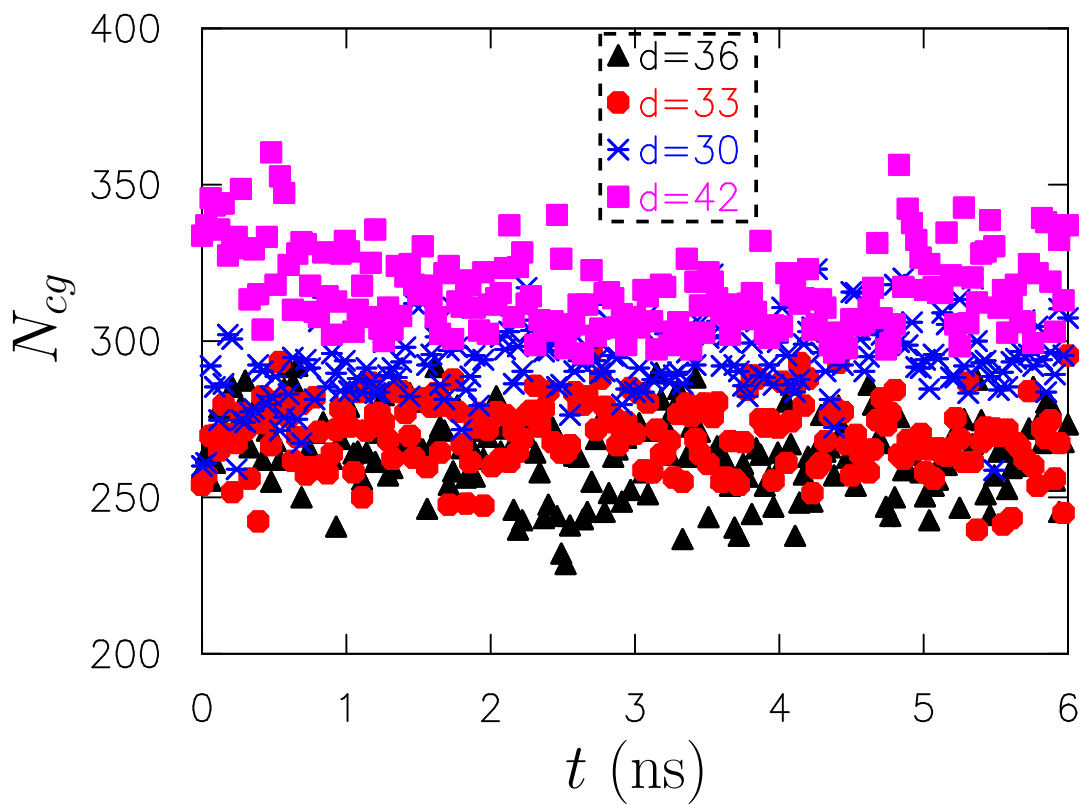


Figure S5: Number of water molecules N_{cg} close to the two graphene sheets as a function of time for 525 molecules droplet at different values of d . The cut-off distance (1.0 nm) described in section 2 in the manuscript is used to determine the statistical range.

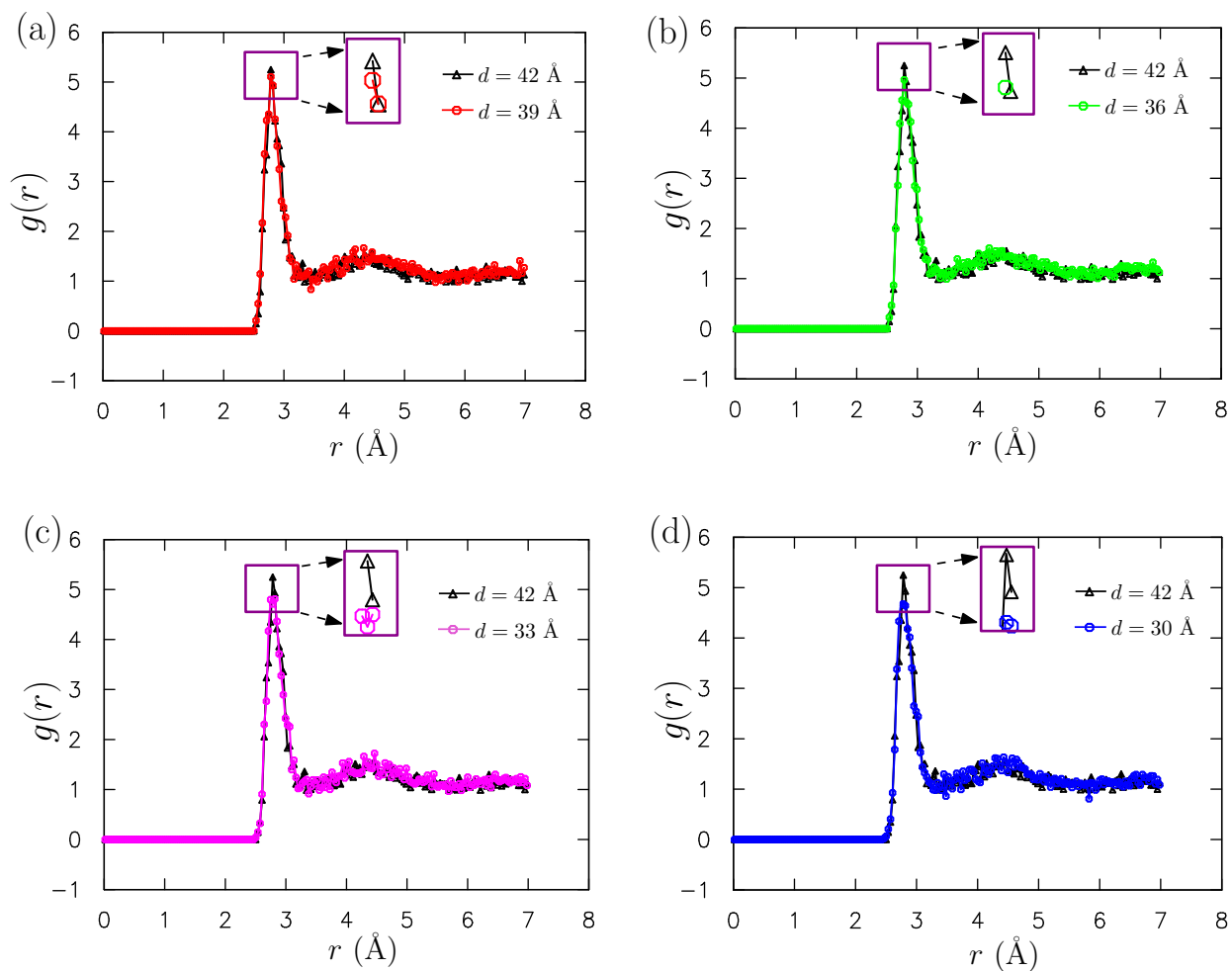


Figure S6: The radial distribution functions of oxygen-oxygen for 512 molecules nanodroplet at different values of d . Note that only the oxygen atoms from the water molecules which have an interaction effect with graphene sheets are counted. The dark purple box represents an amplification of the peak position for easy observation.

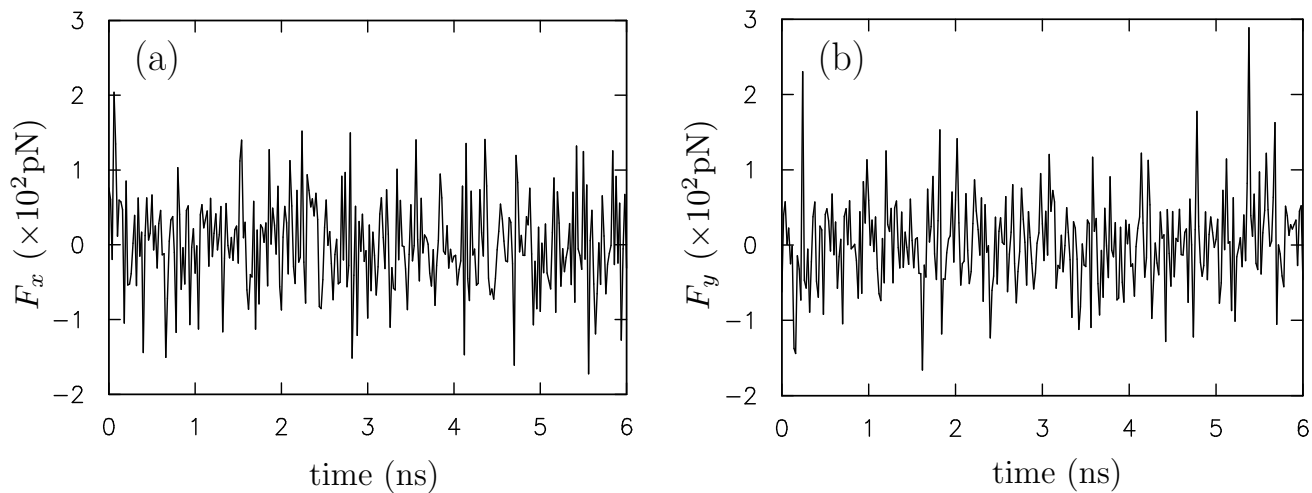


Figure S7: The tangential force along (a) x direction and (b) y direction acting on the water nanodroplet as a function of time t .

Table S1: The values of R for the three nanodroplets at different values of d . N represents the number of water molecules. The units of R and d are both Å.

$R \backslash d$	22	25	28	30	31	33	34	36	39	42	45
N											
252	23.5	21	20.5		24		24				
512				31		28		27.4	25.5	34	
810						33.2		31.6	30.6	30	44

Table S2: The diffusion coefficient D of water nanodroplets on other surfaces, including Boron nitride (BN), Aurum (Au), Molybdenum disulfide (MoS₂), Wrinkled graphene (WG) and self-diffusion of water molecules in liquid water. The unit of D is cm²/s.

Surfaces	D
BN ^[1]	3.7×10^{-5}
Au ^[2]	2.7×10^{-5}
MoS ₂ ^[3]	2.6×10^{-4}
WG ^{Ref.[26]}	7.5×10^{-3}
self-diffusion ^[4]	2.4×10^{-5}
our results	10.4×10^{-3}

References

- [1] H. Li and X. C. Zeng, *ACS nano*, 2012, **6**, 2401-2409.
- [2] M. Foroutan, M. Darvishi and S. M. Fatemi, *Phys. Rev. E*, 2017, **96**, 033312.
- [3] P. Bampoulis, *J. Chem. Phys.*, 2021, **154**, 134705.
- [4] J. Wang, *J. Am. Chem. Soc.*, 1951, **73**, 510-513.