

Supplementary Information

Spontaneous Propulsion of Water Nanodroplet Induced by Wettability Gradient: A Molecular Dynamics Simulation Study

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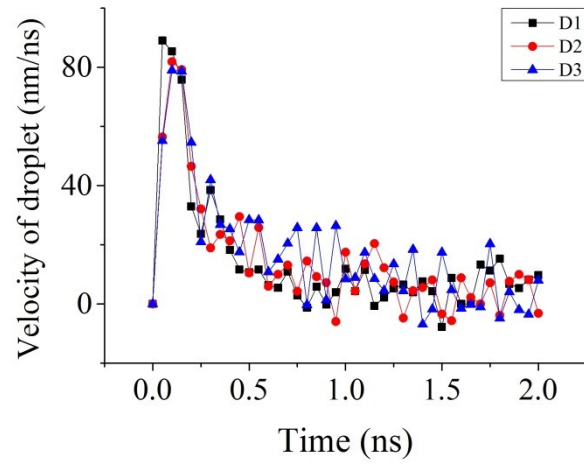


Figure S1: Instantaneous velocity data of different type of MGS during 2.0ns simulation time.

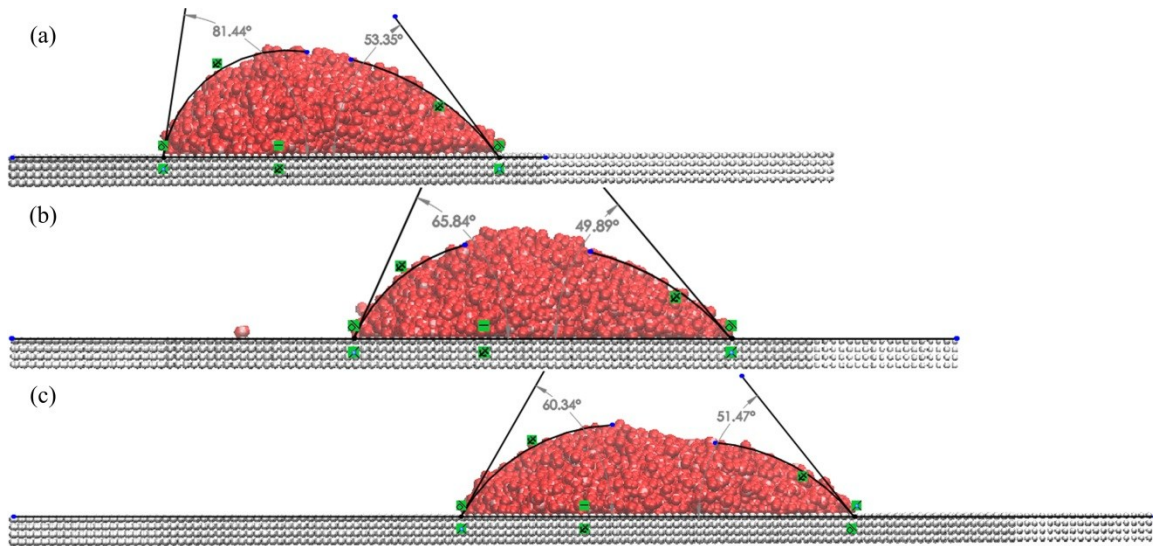


Figure S2: Leading and trailing contact angle of water droplet over (a) D1, (b) D2, and (D3) surface.

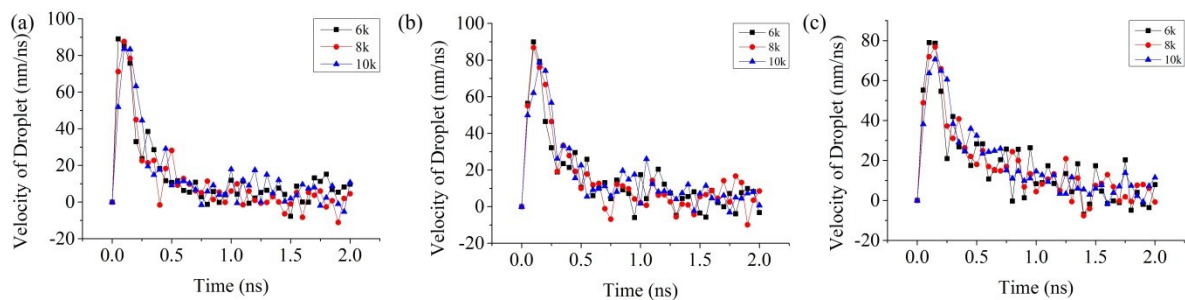


Figure S3: Instantaneous velocity data of different size of water droplet over (a) D1, (b) D2, and (c) D3 MGS.

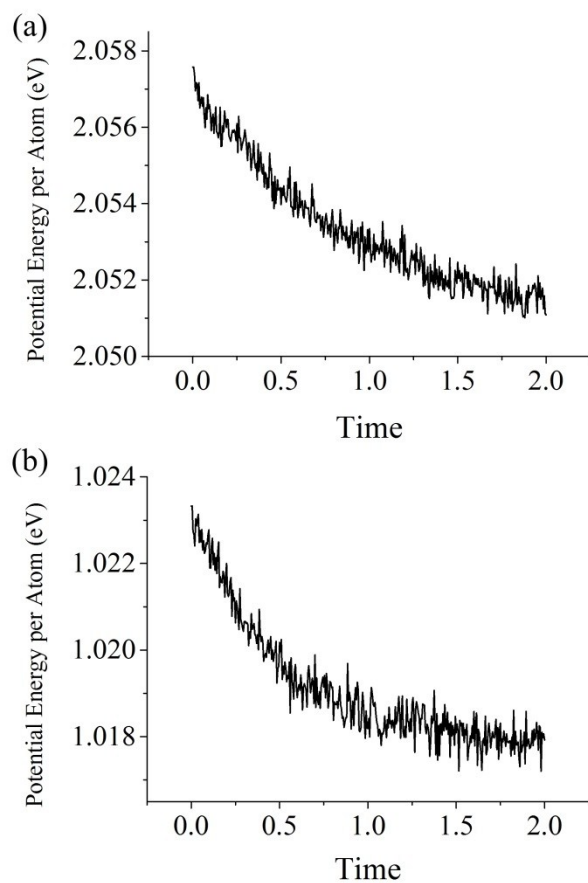


Figure S4: Potential energy per atom water droplet during 2.0ns simulation time over (a) Parallel strip (PS) surface (b) Wedge strip (WS) surface.

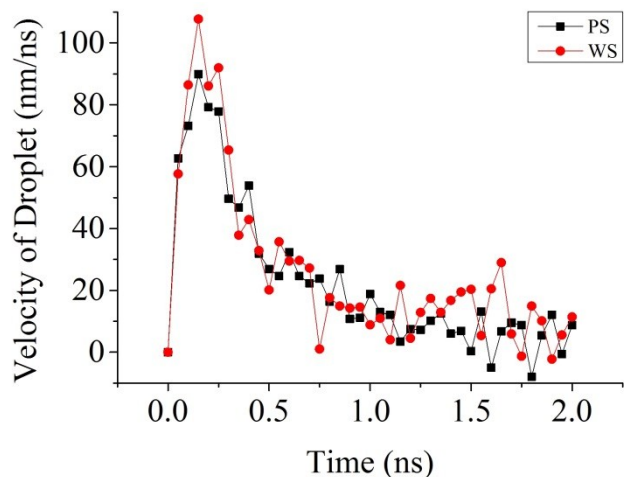


Figure S5: Instantaneous velocity data of 6000 molecules water droplet over PS and WS surface during 2.0ns simulation time.

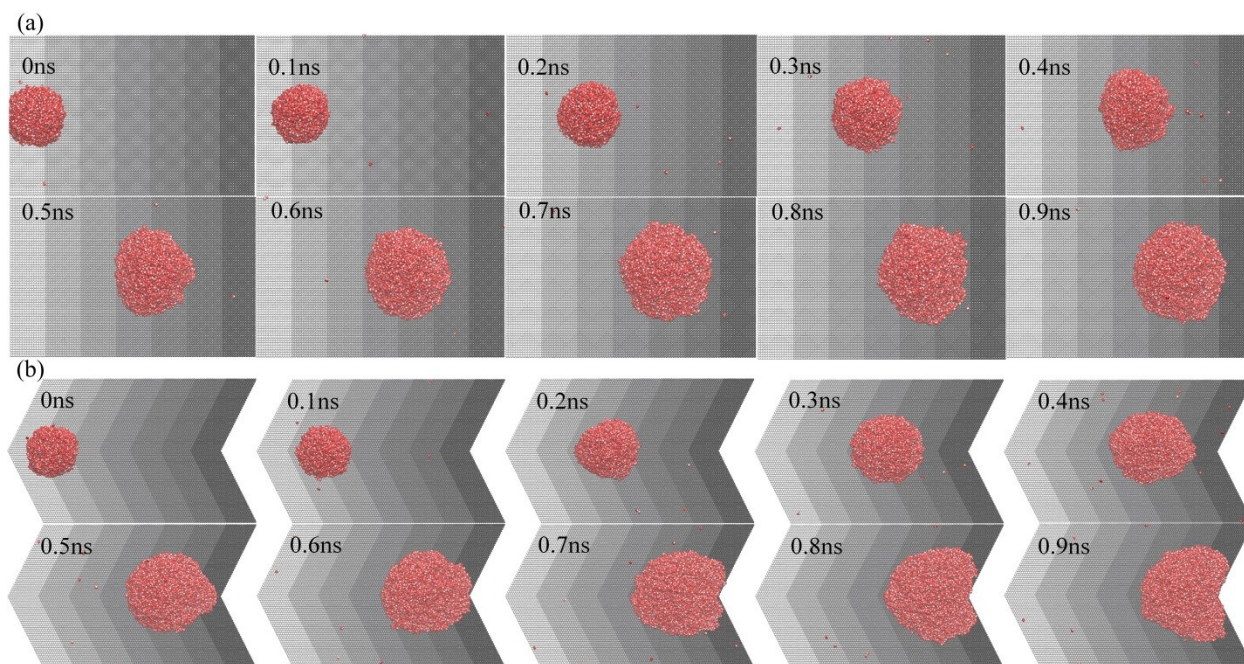


Figure S6: Snapshots of water droplet moving spontaneously over a (a) PS and (b) WS surface.

It can be seen in Figure S6 that the water droplet move comparatively faster on the WS surface as it reaches to the last strip in 0.6 ns while for PS it took around 1.0ns to reach to the last strip.

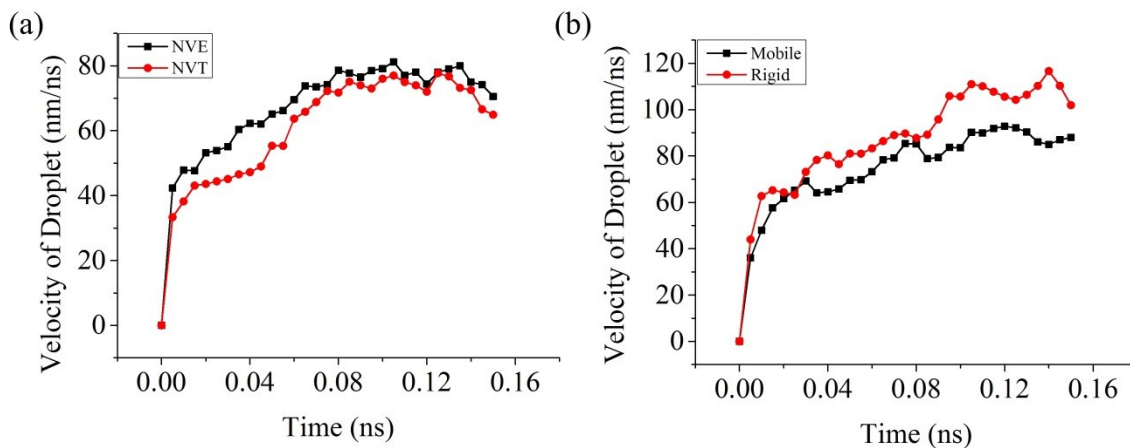


Figure S7: Instantaneous velocity data of 6000 molecule water droplet over (a) D3 surface with NVT ensemble and NVE ensemble (b) on WS surface with rigid substrate and mobile top layer substrate.

It can be seen in Figure S7 that the trend of velocities are same and a slight difference is observed at different conditions. In this study, most of the simulations were done by utilizing NVT ensemble with rigid solid substrate.