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Capillary imbibition dynamics under various solid–liquid interactions: A molecular dynamics study

Friday, 4 June 2021 09:40 (1 hour)

Capillary imbibition, i.e. the spontaneous flow of a liquid into fine pores and cracks without the assistance of external forces such as gravity, is universal and critically important in many natural processes and industrial applications. On the nanoscale, the intensity of solid–liquid interactions (ϵ_{S-L}), which controls the wettability of the capillary walls, plays a critical role and directly affects the imbibition rate, the shape of the meniscus, the evolution of the dynamic contact angle, and even the viscosity of the confined fluid. Here we use molecular dynamics simulations to systematically investigate how ϵ_{S-L} influences the capillary imbibition dynamics in a nanochannel. We quantify the relationship between the equilibrium contact angles and ϵ_{S-L} , and find that the cosine of equilibrium contact angle increases linearly with ϵ_{S-L} . Subsequently, we investigate the capillary dynamics under a wide range of solid–liquid interactions. We show that the capillary rate increases with ϵ_{S-L} , while an overlarge ϵ_{S-L} may hinder the further growth of the imbibition rate. We also characterize the evolution of the dynamic contact angle, imbibition rate, imbibition length. The findings in this work could provide new insights into the capillary imbibition dynamics on the nanoscale.

Time Block Preference

Time Block A (09:00-12:00 CET)

References

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