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Gas Aggregation and Nanobubbles Stability on Substrates Influenced by Surface Wettability: A Molecular Dynamics Study

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Abstract : The interfacial gas adsorption presents a frequent challenge and opportunity for micro-/nano-fluidic operation. In this study, we investigate the wettability, gas accumulation, and nanobubble formation on various homogeneous surface conditions by using MD simulation, including a series of 3D and quasi-2D argon-water-solid systems simulation. To precisely determine the wettability on various substrates, several indicators were calculated. Among these wettability indicators, the water PMF (potential of mean force) has the most correlation tendency with interfacial water molecular orientation than depletion layer width and droplet contact angle. The results reveal that the aggregation of argon molecules on substrates not only depending on the level of hydrophobicity but also determined by the competition between gas-solid and water-solid interaction as well as water molecular structure near the surface. In addition, the surface nanobubble is always observed coexisted with the gas enrichment layer. The water structure adjacent to water-gas and water-solid interfaces also plays an important factor in gas out-flux and gas aggregation, respectively. The quasi-2D simulation shows that only a slight difference in the curved argon-water interface from the plane interface which suggests no noticeable obstructing effect on gas outflux from the gas-water interfacial water networks.

Keywords : gas aggregation, interfacial nanobubble, molecular dynamics simulation, wettability
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