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Molecular dynamics simulations of disjoining pressure effects in ultra-thin water films on a metal surface HAN HU, YING SUN, Drexel University — Disjoining pressure, the excess pressure in an ultra-thin liquid film as a result of van der Waals interactions, is important in lubrication, wetting, flow boiling, and thin film evaporation. The classic theory of disjoining pressure is developed for simple monoatomic liquids. However, real world applications often utilize water, a polar liquid, for which fundamental understanding of disjoining pressure is lacking. In the present study, molecular dynamics (MD) simulations are used to gain insights into the effect of disjoining pressure in a water thin film. Our MD models were firstly validated against Derjaguin's experiments on gold-gold interactions across a water film and then verified against disjoining pressure in an argon thin film using the Lennard-Jones potential. Next, a water thin film adsorbed on a gold surface was simulated to examine the change of vapor pressure with film thickness. The results agree well with the classic theory of disjoining pressure, which implies that the polar nature of water molecules does not play an important role. Finally, the effects of disjoining pressure on thin film evaporation in nanoporous membrane and on bubble nucleation are discussed.

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