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From Atoms to Flow: Exploring Evaporation and Condensation in Nano-Channels

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Abstract

In this talk, we present nonequilibrium Molecular Dynamics (MD) simulation results on thin-film evaporation in a nano-pump driven by phase change, using liquid argon confined between parallel platinum plates. Our simulation captures a self-regulating and self-sustaining net flow in a statistically stable steady-state, featuring a thin-film evaporation region near the heater and a one-dimensional condensing interface at the condenser side. We first explore the dynamics of evaporating menisci for different channel heights and provide insights into the underlying flow physics using velocity vectors and temperature contours. Notably, our MD simulations reveal evaporation from the adsorbed layer—a region traditionally considered nonevaporating. This discovery offers a potential explanation for the deviations from theoretical maximum evaporation rates observed in recent experiments. We also compare the MD findings with predictions from continuum-based thin-film evaporation models. Additionally, we examine the temperature profiles and the resulting temperature jumps across the interfacial region under varying heat flux conditions, and investigate their relationship with the energy dynamics of atoms crossing the liquid-vapor interface. Finally, using Lagrangian particle tracking techniques, we assess the validity of the Hertz-Knudsen-Schrage relations and extract mass accommodation coefficients for the steady-state condensing surface. This comprehensive analysis provides new insights into nanoscale phase change dynamics and has implications for enhancing evaporation models.