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Atomistic water droplet simulation JOHN THOMAS, MADHUR PAHARIA, ERIC LANDRY, GARY LEE, ALAN MCGAUGHEY, Carnegie Mellon University — A water droplet in equilibrium with its own vapor is modeled using molecular dynamics simulations. The density, velocity distribution, orientation, and energetics of liquid and vapor molecules near the droplet surface are examined. Deviations from Maxwellian statistics are predicted in both phases. Hydrogen bonding and molecular orientation also vary with distance from the droplet center. We predict the force landscape near the interface over a range of temperatures and explore the mechanisms responsible for evaporation.

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