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Slip Dynamics at the Liquid/Solid Interface in MD Simulations[1]
YALING LIU, SETH LICHTER, WING-KAM LIU, Northwestern University, ALEXANDER ROXIN, CNRS — Determining liquid flows through nanoscale devices requires the proper accounting for slip along the solid boundaries. Using MD simulation, we show how the amount of slip depends on the material properties of the liquid and solid including their energy and size. In agreement with earlier studies, slip length undergoes a drastic increase near a critical value. We analyze the trajectories of individual liquid molecules as they move over the solid surface to reveal the dynamics underlying slip. We observe that below a critical value, localized patches of liquid molecules propagate along the surface: slip is due to the accumulated effect of many such patches. Above a critical value, the entire first layer of liquid slips over the solid. It is found that the liquid structure in the first liquid layer adjacent to the solid plays a crucial role in determining the dynamics. A theory which describes the dynamics of this layer reproduces the main observations. Unlike continuum flows, nanoscale flow properties can be adjusted by modifying the crystal structure of the solid and the relative size of the liquid molecules.

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