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Substrates sort solute from solvent molecules¹ METEHAN CAM, Northwestern University, Mechanical Engineering Department, CHRISTOPHER G. GOEDDE, DePaul University, Physics Department, SETH LICHTER, Northwestern University, Mechanical Engineering Department — The dynamics of a monolayer of Lennard-Jones atoms driven by an external force over an atomically-spaced solid substrate is presented. As the magnitude of the external force is increased, two bifurcations are observed, from no-slip to defect slip and then to global slip. In the defect slip regime, while the majority of atoms remain stationary in their equilibrium positions, a small percentage of atoms propagate as nonlinear waves over the substrate. In defect slip regime, atoms do not follow the direction of the external driving force. In a solution, solvent and solute atoms follow different directions from one another, resulting in the solute atoms partitioning from the solvent. Using the monolayer dynamics, we aim to understand the physics of the liquid-solid interface and apply this knowledge for molecular-level separation mechanisms mediated by solid substrates.

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