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A molecular dynamics approach to modeling effects of detaching force on the compound droplet residue on spherical surfaces[1]
ALI MOGHADAM, NEDA OJAGHLOU, DUSAN BRATKO, HOOMAN V. TAFRESHI, Virginia Commonwealth University — Droplet detachment from a surface is involved in many industrial applications. While single-phase droplet detachments have been broadly explored, the detachments of multi-phase (compound) droplets attracted less attention. Compound droplets, consisting of magnetic and non-magnetic components, have recently shown promise to detach the non-magnetic component by applying a force on the magnetic one. We study the compound droplet detachment from a sphere via Nonequilibrium Molecular Dynamics (NEMD) simulations. The compound droplet is simulated via coarse-grain models for water (polar) and hexane (non-polar), where water is fully cloaked with hexane owing to their interfacial tensions and the positive spread parameter. The compound droplet is subjected to a vertical force, and we gradually increase its magnitude until detachment. In our study, the force acts on hexane molecules and is varied as a function of the hexane bead's position to emulate applications of magnetic forces for the droplet detachment. The outcome strongly depends on the dynamics of the detaching process. At relatively large forces and faster detachments, the hexane (oil) is capable of detaching water. However, weak forces and slow detachments result in oil separation from the aqueous phase, with most of water remaining as a residue on the surface.

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