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Linear surfactant-mediated spreading of nanodroplets: molecular dynamics simulation HYE-YOUNG KIM, Department of Chemistry and Physics, Southeastern Louisiana University, Hammond, LA 70402, YONG QIN, Silverstorm Technologies, King of Prussia, PA, KRISTEN FICHTHORN, Department of Chemical Engineering, Penn State University, University Park, PA 16802 —
We utilized molecular dynamics simulations to probe surfactant-mediated spreading of nanodroplets on a solid surface. We find that the spreading speed is strongly influenced by the attraction of the hydrophobic surfactant tail to the solid surface. When this attraction is sufficiently strong, surfactant molecules partition to the liquid-solid interface and can lead to an inhomogeneous distribution of surfactant over the liquid-vapor interface, which could drive the Marangoni convection. The result also shows that the surfactant molecules can assemble into micelles. The repulsion between micelles leads to break-off and migration of the micelles from the liquid-solid to the gas-solid interface and spreading is facilitated in this way. Our model system contains features that have been connected with superspreading in experimental studies and provides insight into the workings of a successful surfactant.
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