

Abstract Submitted
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The superspreading mechanism unveiled via molecular dynamics simulations¹ PANAGIOTIS THEODORAKIS, ERICH MULLER, RICHARD CRASTER, OMAR MATAR, Imperial College London — Superspreading, by which aqueous droplets laden with specific surfactants wet hydrophobic substrates, is an unusual and dramatic phenomenon. This is attributed to various factors, e.g., a particular surfactant geometry, Marangoni flow, unique solid-fluid interactions, however, direct evidence for a plausible mechanism for superspreading has not yet been provided. Here, we use molecular dynamics simulations of a coarse-grained model with force fields obtained from the SAFT- γ equation of state to capture the superspreading mechanism of water drops with surfactants on model surfaces. Our simulations highlight and monitor the main features of the molecular behavior that lead to the superspreading mechanism, and reproduce and explain the experimentally-observed characteristic maxima of the spreading rate of the droplet vs. surfactant concentration and wettability. We also present a comparison between superspreading and non-superspreading surfactants underlining the main morphological and energetic characteristics of superspreaders. We believe that this is the first time a plausible superspreading mechanism based on a microscopic description is proposed; this will enable the design of surfactants with enhanced spreading ability specifically tailored for applications.

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