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Interfacial and Dynamical Behavior of Droplet Coalescence: A Molecular Dynamics Study

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ABSTRACT

A lot of consumer products including foods, medications, shampoos, and cosmetics contain emulsions: dispersions of two immiscible fluids. Emulsions are thermodynamically unstable droplet dispersions that undergo coarsening by coalescence, a mechanism of film rupturing between adjacent droplets, which allows the recombination of individual droplets until two liquid phases completely separate out. Our daily activities, industrial output, and frequent oil spill incidents all result in significant amounts of oil/water combination. Therefore, effective oil/water mixture separation and further purification are vitally needed in today's world. Due to their improved separation effectiveness in oil/water mixtures, electrocoalescence and interface theory have gained a lot of interest. In order to comprehend the electrocoalescence process from a micro perspective, molecular dynamics (MD) simulation is a useful tool. It has been extensively utilized to expose the behaviors and microscopic mechanisms of electrical demulsification. According to the findings, the droplets' coulombic attraction is significantly greater than the van der Waals interaction in an electrical field. In our work, we see the surfactant effects and electric field effects during droplet coalescence and subsequently calculate the free energy of droplet coalescence.

Keywords: coalescence, surfactant, electric field, free energy

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