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Stability, deformation and rupture of Janus oligomer enabled self-emulsifying water-in-oil microemulsion droplets

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Microemulsions exist widely in nature, daily life and industrial manufacturing processes, including petroleum production, food processing, drug delivery, new material fabrication, sewage treatment, etc. The mechanical properties of microemulsion droplets and a correlation to their molecular structures are of vital importance to those applications. Despite studies on their physicochemical determinants, there are lots of challenges of exploring the mechanical properties of microemulsions by experimental studies. Herein, atomistic modelling was utilized to study the stability, deformation, and rupture of Janus oligomer enabled water-in-oil microemulsion droplets, aiming at revealing their intrinsic relationship with Janus oligomer based surfactants and oil structures. The self-emulsifying process from a water, oil and surfactant mixture to a single microemulsion droplet was modulated by the amphiphilicity and structure of the surfactants. Four microemulsion systems with an interfacial thickness in the range of 7.4-17.3 Å were self-assembled to explore the effect of the surfactant on the droplet morphology. By applying counter forces on the water core and the surfactant shell, the mechanical stability of the microemulsion droplets was probed at different ambient temperatures. A strengthening response and a softening regime before and after a temperature-dependent peak force were identified followed by the final rupture. This work demonstrates a practical strategy to precisely tune the mechanical properties of a single microemulsion droplet, which can be applied in the formation, de-emulsification, and design of microemulsions in oil recovery and production, drug delivery and many other applications.

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