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Atomistic Insights into the Droplet Size Evolution during Self-Microemulsification

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Microemulsions have been attracting great attention for their importance in various fields, including nanomaterial fabrication, food industry, drug delivery, and enhanced oil recovery. Atomistic insights into the self-microemulsifying process and the underlying mechanisms are crucial for the design and tuning of the size of microemulsion droplets toward applications. In this work, coarse-grained models were used to investigate the role that droplet sizes played in the preliminary self-microemulsifying process. Time evolution of liquid mixtures consisting of several hundreds of water/surfactant/oil droplets was resolved in largescale simulations. By monitoring the size variation of the microemulsion droplets in the self-microemulsifying process, the dynamics of diameter distribution of water/surfactant/oil droplets were studied. The underlying mass transport mechanisms responsible for droplet size evolution and stability were elucidated. Specifically, temperature effects on the droplet size were clarified. This work provides the knowledge of the self-microemulsification of water-in-oil microemulsions at the nanoscale. The results are expected to serve as guidelines for practical strategies for preparing a microemulsion system with desirable droplet sizes and properties.

Participation

In-Person

References

Fu, Y.; Xiao, S.; Liu, S.; Zhang, Z.; He, J., Atomistic Insights into the Droplet Size Evolution during Self-Microemulsification. Langmuir 2022, 38 (10), 3129-3138.

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