Abstract Submitted
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Molecular Modeling of a Bijel[1] MICKAELA SAMUEL, Rochester Institute of Technology — Bicontinuous Interfacially Jammed Emulsion Gels, bijels, are emulsions of two immiscible liquids "jammed" into a network created by colloids. Bijels could have the capability to improve energy conversion, catalytic reactions, and electrical conductivity and given its potential we aim to understand the thermodynamic conditions for obtaining a Bijel. This involved initially tuning the binary liquid interactions. The competition between vapor-liquid phase separation and liquid-liquid phase separation (LLPS) among the three components complicates the system. To entirely suppress vapor-liquid equilibrium, the well-depth between the liquids is set to 1. Colloids were then incorporated into the system by introducing three parameters: φ_C which represents the colloidal volume, V that sets the strength of the colloidal attractions, and κ which sets the range of attraction. Finally, the interaction between the three components was chosen to be neutral. κ was set at 30 for the entire study while V and φ_C varied. The mean-squared displacement and the radial distribution function were plotted and compared to visual snapshots to classify the behavior of the material. The results of these simulations helped conclude that ε =1 is better at suppressing void formation and the degree of separation between the liquids decreases with increasing colloidal volume fraction. There's also evidence that bijels can form or LLPS can only occur when the colloids form a gel that creates large voids for phase separation. In relation to the overall goal, the thermodynamic parameters that provided the "best" route for a Bijel was ε =1, κ =30, V=5, and φ_C =0.15.

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