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Designing the Morphology of Separated Phases in Multicomponent Liquid Mixtures[1]

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Phase separation of multicomponent liquid mixtures plays an integral part in many processes ranging from industry to cellular biology. While the physics of binary and ternary liquid mixtures is well-understood, the thermodynamic properties of N-component mixtures with $N > 3$ have remained relatively unexplored. This makes it challenging to understand how cells control concentrations of molecules and their interactions to navigate phase diagrams to achieve target structures. To address this issue, we developed novel algorithms for constructing phase diagrams and for predicting the morphology of separated phases. To determine the number of coexisting phases and their compositions, we developed a new algorithm for constructing complete phase diagrams, based on numerical convexification of the discretized free energy landscape. Furthermore, we developed a graph theory approach to predict the topology of coexisting phases from a given set of surface energies (forward problem), enumerate all topologically distinct morphologies, and reverse engineer conditions for surface energies that produce the target morphology (inverse problem).

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