Molecular Simulations of Complex Formulations

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A mesoscale simulation approach for designing and screening complex chemical formulations is shown. Interaction parameters are derived from first principles via COSMO-RS chemical potentials, converted into Flory-Huggins parameters and mapped onto DPD bead interactions. Benchmark systems demonstrate near quantitative accuracy for interfacial tensions and critical micelle concentrations across anionic, cationic, and non-ionic surfactants. The method is applied to designing a polymer for an emulsion concentrate formulation of a novel fungicide, where the composition space is too large to screen experimentally. Open challenges include strongly differing bead sizes, high coarse-graining levels, charged beads, and directed interactions.