From crude oil to ice cream: Complexity of nanoparticles at interfaces

Multiscale analysis of the dynnamic interactions of nanoparticles and oil-soluble surfactants at liquid interfaces

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In Short

- Particle-stabilized emulsion systems, despite their daily uses, have very complex behaviors.
- Due to their importance, unprecedented insight into these systems' behavior is needed.
- By conducting experiments and simulations, we aim to shine a light on some aspects of the mechanism of these behaviors at the atomic level.
- As an example of such systems, we will study silica nanoparticles in oil-water interfaces in the presence of surfactants.
- Our goal is to tailor the formation of different types of particle/surfactant emulsion systems.

Particle-stabilized emulsion systems see widespread industrial use in diverse areas, such as floatation in oil recovery or water remediation, in nutritional products, cosmetics and pharmaceutical formulations as well as in materials processing of composites and ceramics. In many of these applications the emulsion systems can be quite complex with various types of particles and surface-active molecules acting in synergy or competition to stabilize the droplet interface. Because of this complexity, the formulation of stable multi-component emulsion systems is usually still a resource-intensive trial and error process. Particularly, the packing density and percolation of mixed interfacial films can currently neither be controlled by adjusting established system parameters like concentrations, pH or surfactant types, nor are there adequate computational models that could support such a task. The aim of this project is to link the molecular details of heterogeneous and multi-component oil/water interfaces containing a mixture of both surfactant molecules and nanoparticles to the macroscopic behavior of these films. This requires a multiscale approach in which an adequate degree of complexity has to be carefully selected at every scale to reach a meaningful and efficient rational description and understanding of the system.

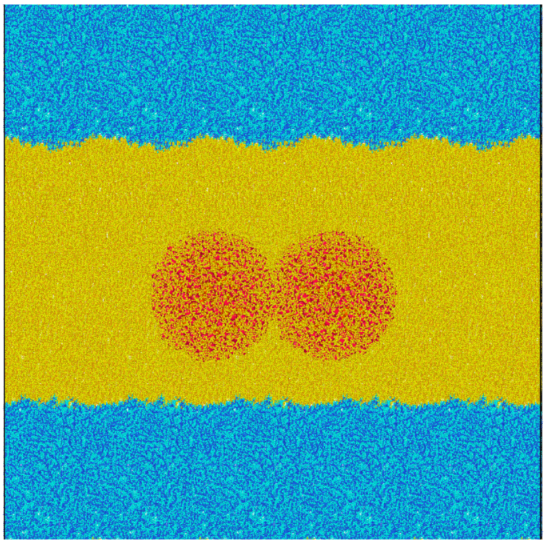

Figure 1: *Example of a model structure includes water (blue), oil (yellow), and nanoparticles (red).*

From this understanding, we aim to generate design rules that allow us to tailor the formation of different types of particle/surfactant emulsion systems by acting on a few selected and easily accessible quantities and parameters, such as the oil/water surface tension and the macroscopic contact angle of an equivalent flat surface (see figure 1 for an example of the system). To achieve this aim, we plan to access the same set of characteristic observables (in particular: contact angles, interfacial energies, adsorption energies, electron density profiles, interfacial microstructure and interfacial rheology) both from experiments and from atomistic and mesoscopic simulations. If the same values of observables are obtained from these complementary approaches, we can safely assume that the simulated models are a faithful representation of the experimental reality. In this way, we will have achieved a satisfying description of particle adsorption at the surfactant-laden interface and of structure formation in the particle film which determines the type of emulsion system.This combination of experimental and simulation methods will allow unprecedented insight into the formation of mixed interfacial films. With this approach we aim both to expand our knowledge on multicomponent interfacial systems on a fundamental level, as well as to enable the formation of complex emulsion systems based on predictable formulation rules. Such design rules will greatly facilitate the resource-intensive formulation processes which are necessary for a wide range of industrial processes from making ice cream to processing hierarchically structured porous ceramics.

The general design of the project is based on water-dispersable, hydrophilic nanoparticles and oil-soluble surfactants. This system prevents volume-phase interactions between particles and surfactants and limits such interactions to the interfacial region. In order to retain a realistic scope of the project, the investigated system is limited to a well-defined set of constituents that allows comparability with other systems. Silica nanoparticles are chosen for their hydrophilicity, monodispersity, sphericity, purity, and availability in small sizes. The surface chemistry of silica can be efficiently tailored via reaction with various silanes. Decane is selected as an organic solvent mainly because it can be purified to the high degree essential for interfacial measurements, which are sensitive to parts-per-billion amounts of surface-active impurities. Lastly, oil-soluble surfactants with a hydrophobic tail with different functional head groups are chosen [1-3].

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https://www.hmi.uni-bremen.de/

More Information

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