Modelling at the appropriate lengthscale for industrial applications

Massimo Noro

Strategic Science Group, Unilever R&D Port Sunlight (UK)

email: Massimo.Noro@Unilever.com

A large portion of the European manufacturing sector is based on complex liquid formulations, for example, in the area of home care and personal care products. Many of them are underpinned by similar liquid mesostructures. We need to choose the appropriate length-scale tools for the appropriate product mesostructure application [1]. Coarse-grained mesoscale calculations insights to be gained, for example, on the mechanism of structure formation and on the interactions with surfaces of interest.

Dissipative Particle Dynamics is a core mesoscale capability that has been used to calculate the structure of typical products like laundry liquids, containing, often, complex mixtures of surfactants, polymers and a range of other ingredients. The challenge is to develop and employ appropriate force field parameters that accurately reproduce the essential thermodynamic questions of interest [2]. The issue becomes especially important when dealing appropriately with charged and partially dissociated surfactant ingredients [3].

Reproducing and predicting the self-assembly behaviour at the low concentration regime is not trivial. We have studied complex surfactant/polymer mixtures [4] and developed rapid phase-diagram calculation approaches that shed light on transient structures as well. Recent extensions make these approaches more palatable for industrial applications. The shape, symmetry and size of complex aggregates can be detected automatically thanks to modern computational methodologies.

References

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