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# Mechanisms of self-assembling of non-conventional surfactants by multiscale modelling and data-driven approaches

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The dynamics regulating self-organisation of surface-active compounds is
at the basis of the living matter; for example, it is involved into the definition of cellular boundaries, cell compartmentalisation and molecular trafficking. Surfactants are also broadly used in soft matter technology, from responsive materials, to nanodelivery. The problem associated with their characterisation at molecular level lies in the non-reducible size of the systems of interest, spanning several orders of magnitude from the nm to the $\mu$m, and in their relatively long relaxation times, which can often pass the millisecond. Here, I will give an overview of recent advances in modelling of the self-assembling dynamics of surfactants, using a hierarchy of approaches at different resolution. I will discuss how external factors like ionic-strength, or photoactivation can have a major role in controlling aggregation [1].
I will also show how combining soft density-functional based models [2] to enhanced sampling metainference approaches [3] can be used to describe the aggregation of non-conventional surfactants that do not respect the common core-shell packing [4], and propose data-driven approaches for systematic calibration of such models [5].

**References**

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