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Multiscale modelling of polymers at soft-bio interface

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The behaviour of polymers at a liquid/liquid interface has become increasingly technologically important in recent years. For example, many of the self-assembly processes involving macromolecules occur at such interfaces and one of the most common chemical processes used to produce polymer nanoparticles –the solvent displacement method– involves the diffusion of the polymer chains from a good solvent, where the polymer initially dissolves, to a non-solvent where the nanoparticles are formed. Finally, polymer-based drug nanocarriers (either nanoparticles or micelles) are becoming increasingly popular in drug delivery and their behaviour at fluid interfaces (such as a lipid/water boundary) should be properly understood in order to predict their biological activity. Here we show how using a multiscale approach it is possible to gain a detailed picture of the thermodynamic stability of homo- and co-polymers at fluid interfaces spanning from universal rules valid to any polymer systems at high dilution to the specific cases of amphiphilic linear and branched polymers.

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