Design of polymeric building blocks: Coarse graining, multiscale and theoretical predictions

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Abstract

Creating novel building blocks, which allow for an easy and large-scale fabrication of complex materials, is a challenge and a central goal in material science. Much effort has been spent in creating tunable units that self-assemble into complex structures with particular features, and this has motivated an extensive analysis of functionalized building blocks of various shapes [1,2,3]. Polimeric systems have proven to be extremely functionaliable self-assembling building blocks with tunable properties [4]. A full atomistic description of such systems with atomistic potentials have proven to be extremely useful when describing the properties of a few particles, but when large scale simulations are required, it becomes essential to coarse-grain some degrees of freedom, while preserving all the underlying properties of the system. This talk focuses on the development and usage of multi-scale methodologies for polymers solutions, in particular on methods that allow to span from properties of single polymers, up to properties of dilute to semi-dilute solution of polymeric systems, with different architectures and chemical details. I will introduce and explain a coarse graining procedures that can, both theoretically and computationally allow to predict, and then represent properties of systems made by many microscopic units. I will show a few example of how such a methodology has been applied to systems of various chemical composition and physical architecture, and become a viable tool to design tunable building blocks whose mesoscopic self-assembly can be controlled by means of a few simple external parameters that can be accessed experimentally, as for example temperature, pressure, density or solvent quality.

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