Multiscale Modeling of Polymers and Biopolymers:
Methods and Applications

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Molecular simulations provide a very useful tool for understanding the structure-property relations of various materials. Application of these techniques to polymeric materials, however, is not straightforward due to the broad range of length and time scales characterizing them [1,2]. For example, even a single polymer chain exhibits length scales ranging from the bond length (~1 Å) to the size of the chain (~10 nm) and corresponding time scales ranging from a few femtoseconds for the bond vibrations up to the order of milliseconds or even seconds for the whole chain relaxation. In order to increase the length and time scales accessible by simulations coarse-grained (CG) models have proven to be very efficient [1-3]. Here we present a general overview of the most popular CG methods for the simulation of macromolecular systems, focusing more on hierarchical CG models, which developed directly from the chemistry and provide a clear way for connecting the atomistic-microscopic and the mesoscopic scale. As a test case we discuss in details an application of this hierarchical approach to polystyrene (PS) [3].

Next a short overview of the application of the CG models to the modeling of biopolymers is given. As an example the study of biological membranes through CG mesoscopic simulations is presented. These simulations have the advantage of being able to relate the membrane properties with structure and composition at the molecular level. We discuss two examples: the first is a proposed novel methodology for studying the curvature elasticity of membranes [4], whereas the second considers the interaction between proteins and biological membranes [5].

Finally we discuss the (many) open questions in the field of multi-scale modeling of polymers and/or biopolymers: how do many-body terms are incorporated in the mesoscopic description? Is it possible to estimate in advance the error due to the loss of some degrees of freedom, when we go from the microscopic to the mesoscopic description? Can we obtain a mathematical consistent multiscale simulation tool for the quantitative predictions of both structural and dynamical properties of soft matter [6]?

REFERENCES