Towards developing Mesoscale Models for Organic and Bioorganic Polymers. A Case Study on PMMA and Carbohydrate Polymers

Karl N. Kirschner, Kathrin Heikamp, Dirk Reith, and Astrid Maaß
Fraunhofer Institute SCAI, Schloss Birlinghoven, 53754 Sankt Augustin, Germany

Poly(methyl methacrylate), also known as plexiglas or PMMA, is a common organic polymer with a vast range of uses and applications. PMMA can occur with isotactic, syndiotactic, and atactic configurations, which affects its physical properties; these properties include its glass melting temperature, chain stiffness, miscibility, surface activity, and absorption behavior. Similarly, carbohydrate polymers posses a vast range of function - from energy storage to biochemical mechanical reinforcements and cellular identity markers – that depend upon it compositional makeup. In both polymer systems there is a need for accurate modeling at both the atomic and mesoscale levels.

Atomistic molecular dynamics (MD) simulations were performed on isotactic and atactic PMMA polymer systems composed of various residue lengths (n=3, 8, and 16) using our new force field for saturated and unsaturated alcohols and esters. The simulation performed on the shortest polymer length was performed to determine the allowed conformational families of a PMMA triad. The longer chain polymer simulations were performed for developing coarse grain potentials and to reproduce experimental observalbles.

In our desire to develop a coarse graining scheme for carbohydrates we conducted atomistic MD studies of disaccharides. Using the Glycam06 force field, simulations were performed on isolated disaccharides and on a concentrated solution of disaccharides. The two sets of simulations will provide information on intra- and intermolecular contacts, which are needed for developing a course-grained model. Based on the resulting data and statistics we present the most promising coarse graining scheme for disaccharides, which we will extend to poly- and oligosaccharides in the future.