Colloquium of the International Graduate Research Training Group 1524 – SSNI –

Self-Assembled Soft-Matter Nanostructures at Interfaces

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Self-assembly of charged polymers- from Polyelectrolyte Multilayers to DNA bundles

In this talk we will discuss two different ways of self-assembly of charged polymers. The first half of the talk will about polyelectrolyte multilayers (PEMs) that are composed of alternating layers of oppositely charged polyelectrolytes (PEs), which are generally built up based on the Layer-by-Layer technique introduced by G. Decher. Our goal is to understand the interphase and interface structures and interactions via simulation methods. We try to combine coarse-grained (CG) and all-atom (AA) molecular dynamics (MD) simulations to construct a viable model for PEMs. The CG-MD method is very efficient in dealing with the systems in larger time and length scale, and AA-MD approach is necessary to understand the details, e.g., the conformation of adsorbed PE chains, the influence of the aqueous solvent at a higher resolution. We find that the first layers, in particular the second layer, is very important in PEM buildup.

In the second part of the talk we show that even like charged polyelectrolytes can self-assemble, if a sufficient amount of multivalent salt is present. We will start with DNA- like charged stiff rods which serve as model systems for theory and simulations, mimicking charged PPPs. We will present some results obtained on the all-atom level and on the coarse-grained level for the bundle sizes of these systems.