Title: Self-assembly of polyelectrolytes in aqueous solutions (dissipative particle dynamics)
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Abstract

In the thesis, the coarse-grained dissipative particle dynamics (DPD) is used for the study of self-assembly of equimolar mixtures of oppositely charged symmetric block PEs with one PE block (either strong polycation or strong polyanion) and one readily water-soluble neutral block in aqueous media.

In the first part of the diploma thesis, the principles of DPD simulations are described and the correct implementation of electrostatic interactions in the DPD method is demonstrated on the example of counterion (Manning) condensation.

In the second main part, the effect of the blocks solubility, incompatibility and the interplay of different forces on electrostatic assembly is investigated. The corresponding neutral systems are also simulated for comparison. The study shows that the hydrophobicity of the PE backbone and the incompatibility of blocks significantly affects the electrsotatic co-assembly. The presence of opposite charges on different chains promotes the aggregation process and the aggregation number increases in comparison with the corresponding neutral system. In systems with well soluble charged blocks, only dimers are formed, while in systems with hydrophobic charged blocks, core-shell aggregates are formed for incompatible blocks and nano-gel particles for compatible blocks.

Keywords: polyelectrolytes, block copolymers, computer simulations