Abstract Submitted
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Molecular Dynamics Simulations of Ultracentrifuged Polyelectrolyte Complexes[1] DIDDO DIDDENS, ALBERT JOHNER, JÖRG BASCHNAGEL, Institut Charles Sadron, Université de Strasbourg, 23 Rue du Loess, 67034 Strasbourg Cedex 2, France, THÉORIE ET SIMULATION DES POLYMÈRES TEAM — Polyelectrolyte complexes (PECs) are formed by the aggregation of positively and negatively charged polymer species, which precipitate rapidly from solution in case of equimolar mixing. As the fast complexation kinetics prevents the formation of an optimized pairing between positive and negative charges, the microstructure of these aggregates is ill-defined, resulting in a material that is difficult to process further. Recently, Schlenoff *et al.* [1] have demonstrated that the precipitates can be reshaped via ultracentrifugation in concentrated sodium chloride solutions, yielding a compacted, gel-like material, whose rheological properties make them interesting candidates for bioimplants. However, despite the success of this novel route to post-process PECs, the underlying molecular mechanisms are not yet fully resolved. We study the complex structure before, during and after centrifugation in a non-equilibrium Molecular Dynamics simulation of a fully atomistic simulation model. In a second step, we investigate the effect of these structural changes on the dynamics inside the PECs, and discuss these findings in context with the experimental observations.

[1] Porcel and Schlenoff, *Biomacromolecules*, **2009**, 10, 2968

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