Contribution ID: **17** Type: **poster contributions**

A Computational Model for Interpolyelectrolyte Complexes

Advances in modern polymer science allow to create evermore complex self-assembled structures, which are driven mostly by using electrostatic and hydrophobic forces. An example of such a system are multicompartment interpolyelectrolyte complexes (MIPECs) to be obtained by combining appropriate copolymers of opposite charge and which are stabilized by a hydrophilic corona [1]. These water-soluble colloids of 50-200 nm size combine different solubilisation properties, functionalities, and variable mesoscopic structure that make them interesting for example in the field of drug delivery. The structure of the MIPECs have been already studied e.g. by Small Angle Neutron Scattering (SANS) [2]. However, a detailed description of the architecture and appropriate modeling of the data is still missing. In this poster, we will present a computational model which can describe the existing SANS data and offer further structural insights from the model parameters.

This top-down, coarse-grained model presents micelles of hydrophobic chains as spherical particles confined into a spherical region composed of the IPEC. This simplistic model allowed us to use Molecular Dynamics (MD) simulations to rapidly sample the configurations of the system. The obtained scattering intensities revealed the lack of a fractal behavior [3] and the confinement shape. Moreover, we will show that by considering a third different Scattering Length Density (SLD) we can realistically model the scattering contribution of the confined region and obtain a realistic model of our system. This structural model then was tested on experimental SANS data obtained from complexes of oppositely charged microemulsion droplets and polyelectrolytes.

Primary authors: PREVOST, Sylvain (Institut Laue-Langevin); CZAKKEL, Orsolya; GRADZIELSKI, Michael; CHAMCHOUM, Matteo; SIMON , Miriam

Presenter: CHAMCHOUM, Matteo

Session Classification: Poster session/Wine and Cheese evening