



Contribution ID: 58

Type: Poster

Macroion Conformation in Electrolyte Solution – Modelling, Experiment and Slender Body Hydrodynamics

Tuesday, 28 September 2021 18:03 (3 minutes)

Macroions are an important class of compounds with properties characteristic both of polymers and charged molecules. Most commonly, macroions are studied using only experimental techniques such as dynamic light scattering (DLS), laser Doppler velocimetry (LDV) and viscosity measurements. This allows one to evaluate their molar mass distribution, the radius of gyration, the contour length, intrinsic viscosity and sedimentation coefficient.

However, despite of extensive experimental research, no comprehensive characteristics of most studied macroions were acquired using simultaneously theoretical modelling and different experimental techniques. This results in only semiquantitative information about macroion conformation and may led to wrong conclusions about their properties.

Therefore, we have performed thorough characteristics of carrageenan, chitosan and poly(L-lysine) solutions using a combination of the all-atom molecular dynamics (MD) modelling, DLS, LDV and viscosity measurements. Our investigations yielded quantitative information about the macroion molecule properties such as its ionization degree, chain length and cross-section area under a broad range of conditions. We have shown that all studied macroions exhibit a flexible-rod shape with no sharp bending.

The obtained data allows the prediction of macroion adsorption kinetics and facilitate a proper interpretation of experimental techniques that require calibration, especially quartz crystal microbalance or the streaming potential measurements.

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Session Classification: Poster Session