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Counterion correlations in charged macromolecular systems ARBEN JUSUFI, YU MEI, MATTHIAS BALLAUFF, Physical Chemistry I, University of Bayreuth, 95440 Bayreuth, Germany — We perfomed Molecular Dynamics simulations of a charged macroion surrounded by counterions. Various scattering contributions result from correlations between counterions, macroion, and between both of them. Experimentally, these scattering contributions can be measured by anomalous small-angle X-ray scattering (ASAXS) experiments. As a result the cross-correlation between the rigid macroion and counterions yields always a meanfield expression for the counterion density distribution even if the counterions exhibit correlated fluctuations. In contrast, in star-like polyelectrolytes, representing a fluctuating macroion, meanfield approximations are valid only if the functionality is sufficiently high. A systematic investigation of the strength of correlated fluctuations and their effect in scattering intensities is demonstrated for these systems. Furthermore, we demonstrate a collapse transition for spherical polyelectroylte brushes (SPB) by adding trivalent counterions. The collapse of the SPB is observed by simulations and experiments.

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