Modelling polyion complex aggregation

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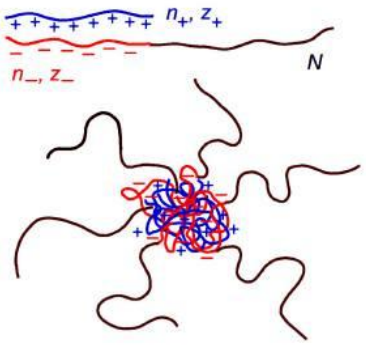
Abstract

IPEC solver is a windows program designed to analyze the stability of core-shell inter-polyelectrolyte complexes formed by complexation of oppositely charged block co-polymers. The two-dimensional size distribution (number of anions and cations) of the complexes is calculated based on the scaling model of block co-polymer aggregation and Poisson-Boltzmann theory for electrostatic interactions[1]. Salt effects, charge distribution and distributions of small ions around the complexes are calculated numerically as a function of chains composition and solvent properties.



[1] VA Baulin, E. Trizac, Soft Matter, 8(25), 6755-6766 (2012)