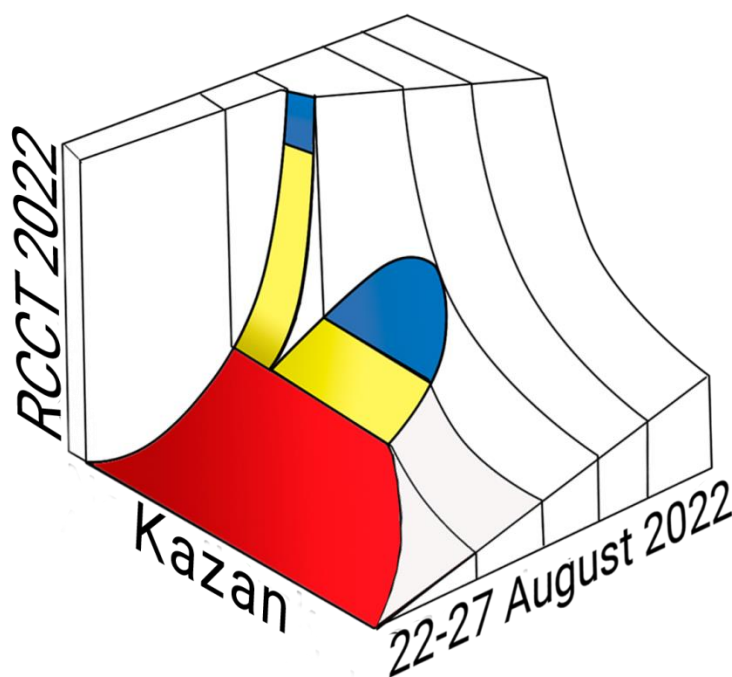


# **XXIII International Conference on Chemical Thermodynamics in Russia**

**August 22-27, 2022  
Kazan, Russia**



**RCCT – 2022**

## **BOOK OF ABSTRACTS**

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# MD SIMULATION OF A POLYCATION CHAIN WITH VARYING COUNTERIONS IN SOLUTION AND PREDICTIONS FROM THE STATISTICAL FIELD THEORY

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Simulations and modeling of polyelectrolyte solutions is a field with long history and numerous practical applications. Nevertheless, the development of an analytical model of a polyelectrolyte that takes into account the location of charge within the ionic species remains as yet a challenging task. In the recent years, the field theory techniques have been advanced considerably, making possible to describe solutions that contain ionic particles of complex electrical structure. An important test of theoretical predictions is the comparison with the results of computer simulations using reasonably realistic model potentials.

In the present work, we perform molecular dynamics (MD) simulations of poly(dimethyl diallyl ammonium) salts in water, with halide or amino acid counterions: PDADMAX where  $X=Cl^-$ ,  $Lys^-$ ,  $Leu^-$ ,  $Gly^-$ . A full-atom model potential (OPLS-AA force field as included in the Gromacs simulation package) is used. We examine the behavior of polycations with different backbone lengths (20, 40, 60, 80, 100, 200, and 400 monomers) in dilute solution at 298 K. For PDADMACl and PDADMALeu systems, we perform simulations in presence of a salt background (0.5M NaCl or 0.5M NaLeu). The simulation results are used for testing a model of polyelectrolyte chains in solution developed with the aid of the variational field theory [1]. The model takes into account the connectivity of the charged monomers along the polyelectrolyte backbone and the hard core interactions between these monomers and the counterions in solution. The charges are located off-center of ions; the many-body Coulomb interactions are treated in the random phase approximation [2].

We compare predictions from the theory with our MD data on the structure and conformation of chains, including the gyration radii and charge-charge correlation functions. Particularly, we discuss effects of the counterion nature and concentration (especially for the amino acid anions as compared with  $Cl^-$ ), and the viability of the model in reflecting these effects.

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[2] V.Y. Borue, I.Y. Erukhimovich, *Macromolecules*, 1988, 21, 3240.