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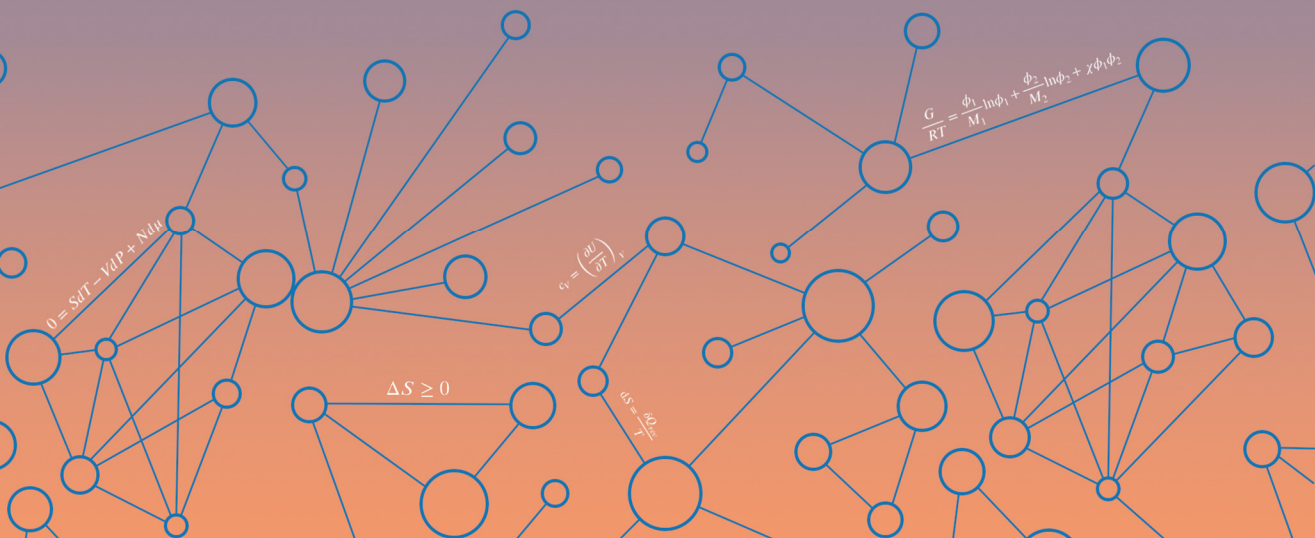

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European Symposium on Applied Thermodynamics

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Linear polyelectrolyte chains with differing counterions in solution: a field theoretic modeling vs MD

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Modeling of polyelectrolyte solutions is a field with long history and numerous practical applications. Nevertheless, the development of a polyelectrolyte model that takes into account any details of the location of charge within the ionic species remains as yet a challenging task. Within the recent years, the field theoretic techniques have been advanced considerably, making possible to describe solutions that contain ionic particles of complex electrical structure [1].

In this work we develop a model of polyelectrolyte chains in solution from 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]. For testing the new model, we perform a series of full-atom Molecular Dynamic (MD) simulations of polyelectrolyte chains PDADMAX poly(dimethyl diallyl ammonium) with different counterions (X=Cl^-, Lys^-, Leu^-, Gly^-), i.e., a halide or an aminoacid polymeric ionic liquid of a varying length of the backbone (20, 40, 60, 80, 100 and 200 monomers) in dilute solution at 298 K. Simulations in presence of a salt background (0.5M NaCl) are performed for PDADMACl systems. 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. The discussion of our results is focused on effects of the nature of counterion and the viability of the model in reflecting these effects.

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References

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[2] V.Y. Borue, I.Y. Erukhimovich, Macromolecules 21 (1988) 3240–3249