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Theory and Simulation of Polyelectrolyte Solutions and Gels

Guest Editor:

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Message from the Guest Editor

Polyelectrolyte solutions and gels are of broad scientific and technological interest due to their crucial role in the functionality of many biological processes and they are essential for the development of many modern materials. The main attribute of systems of charged macromolecules is that all molecules are cooperatively correlated both topologically and electrostatically in a medium of highly polarizable solvent/environment and small mobile ions.
The aim of this Special Issue is to highlight the progress on the theoretical and computational modeling of polyelectrolyte solutions and gels in understanding the conformations of isolated macromolecules or nanogels and their charge regularization, polarizability of the medium, specific ion effects, multivalency, mobility of macromolecules of different chemical architectures, intrinsically disordered proteins, crowded solutions, adsorption to charged brushes, dendrimers and membranes, self-assembly of proteins and coacervates, morphology of charged block copolymers, kinetic pathways of complexation among macromolecules, critical phenomena, and flow effects.

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Message from the Editor-in-Chief

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