Multiscale modeling of structure and dynamical processes of oligomeric polyelectrolyte gelators

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Structural characterization of a hydrogel consisting of an oligomeric electrolyte as an ionic gelator in a number of solvents in terms of the solvent and counterion distributions around gelator polymeric chains, macromolecular mobility, and gel network formation ability are carried out theoretically and computationally by combining different models and scales where each level addresses a phenomenon over a specific window of length and time and uses an input of the information from the models of other levels. On the quantum mechanical level, we calculate the geometry and charge distribution of solvent and the structure and charge distribution of anions and polymer chains depending on the solvent, polymer chain length and polymer concentration of practical interest. The information obtained is used on the atomistic level where we solve the reference interaction site model integral equation theory of molecular liquids. Here we determine the 1D and 3D spatial distributions of solvent and solute molecules in the solution and the thermodynamic properties of the solvent. The former allow one to visualize the picture of gel network formation, while the latter are used as an input at the coarse grained level of description where we run dissipative particle dynamics and analyze dynamical properties of the coarse grained system. Based on the dramatic change we observe in the macromolecular mobility in the solution depending on thermodynamic conditions and polymer concentration, we conclude about the gelation ability of the mixture [1-3].

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