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Effects of charge inhomogeneities on the phase behavior of Polyelectrolyte gels PRATEEK JHA, Chemical and Biological Engineering, Northwestern University, JOS ZWANIKKEN, Materials Science and Engineering, Northwestern University, JUAN DE PABLO, Chemical and Biological Engineering, University of Wisconsin Madison, MONICA OLVERA DE LA CRUZ, Materials Science and Engineering, Northwestern University — Networks of Polyelectrolyte chains (PE gels) express a wide range of functionality and are intelligent models to study biological responsive materials such as chromosomes. Electrostatic interactions originating from the charge inhomogeneities compete with the short range interactions that result in a rich phase behavior not well explained by the existing models. We study the electrostatic effects in PE gels within two different schemes - a Poisson-Boltzmann and a Green's function formalism. While a numerical free energy minimization is used in the former scheme, a novel Monte Carlo approach is utilized in the latter. We discuss the influence of density and dielectric inhomogeneities together with dynamic fluctuations on the swelling, the collapse, and the phase segregation behavior of PE gels.

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