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Influence of Charge and Network Inhomogeneities on the Swollen-Collapsed Transition in Polyelectrolyte Nanogels PRATEEK JHA, JOS ZWANIKKEN, Northwestern University, FRANÇOIS DETCHEVERRY, LPMCN, Universite de Lyon, JUAN DE PABLO, University of Wisconsin-Madison, MONICA OLVERA DE LA CRUZ, Northwestern University — Polyelectrolyte nanogels are sub-microscopic networks of solvent-permeated polyelectrolyte chains that undergo large reversible volume changes for a range of environmental stimuli. This volume phase transition behavior finds use in targeted drug delivery, optical switching in photonic crystals, and many other applications that require controlled tunability. Although the strength of electrostatic interactions have a strong influence on the nanogel response, these interactions are not well captured by the classical mean-field theories of macroscopic gels. We develop a simplified Poisson-Boltzmann model of spherical gels, that highlights the importance of charge inhomogeneities and the associated Coulomb interactions in determining the response of gels. Our analysis reveals that nanometer-sized gels, collapsed gels, and gels in media with low salinity or high dielectric constant, have large regions of excess charge, and show clear deviations from the classical Donnan picture of polyelectrolyte gels. The detailed swelling-collapse behavior is obtained using the theoretically-informed coarse-grained simulations, which includes the effects of network imperfections and thermal fluctuations. The simulations capture the universal features of volume phase transition in nanogels.

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