Electrostatic Control of Nanoscale Phase Behavior of Polyelectrolyte Gels

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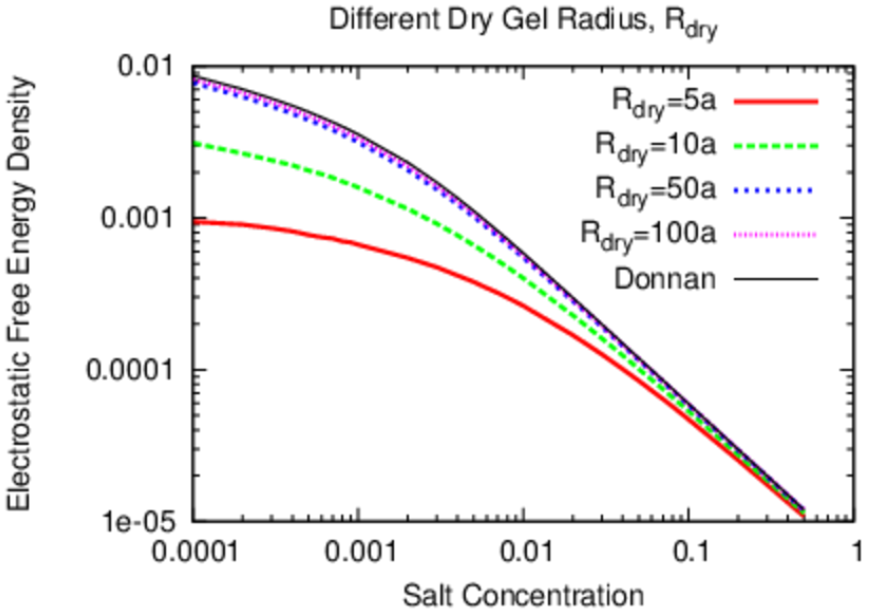

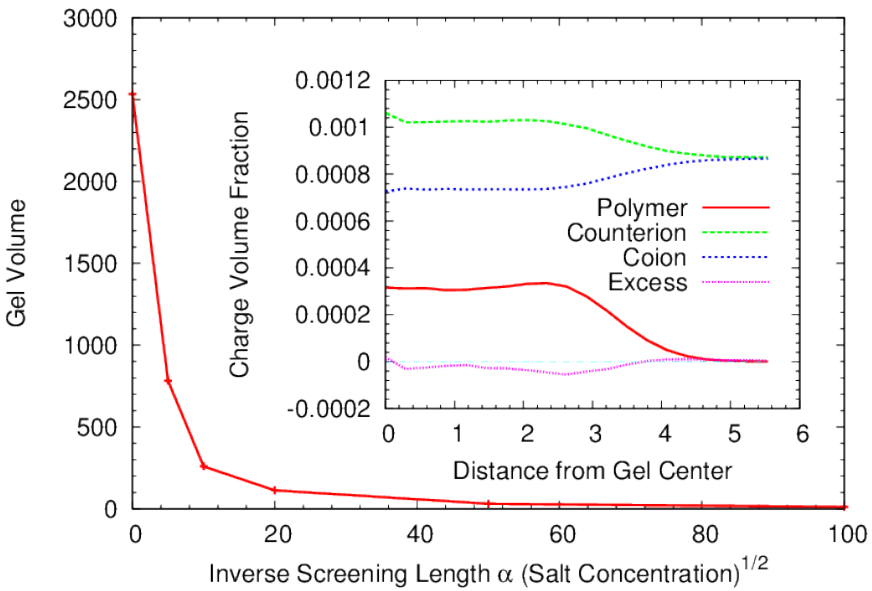

Polyelectrolyte gels are intelligent materials that undergo large reversible volume changes for a range of environmental stimuli. Although the strength of electrostatic interactions have a strong influence on the gel response, these interactions are not properly accounted in the classical mean-field theories that assume a homogeneous charge-neutral gel. Using Poisson–Boltzmann theory and theoretically informed coarse-grained simulations, we emphasize 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. We also observe that the addition of salt can induce collapse in swollen gels by compensating the polymer charge.

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