Study of Volume Phase Transitions in Polymeric Nanogels by Theoretically Informed Coarse-Grained Simulations

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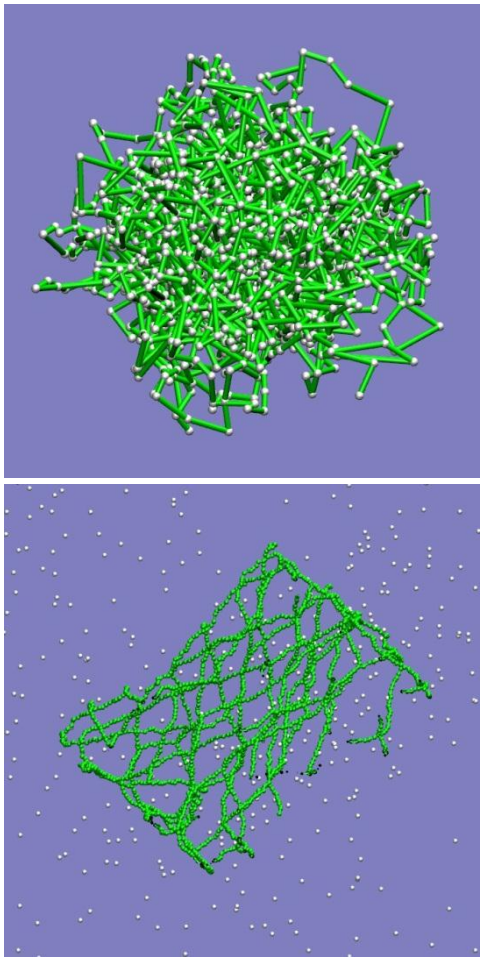
Polymeric nanogels undergo large reversible volume changes with moderate changes in environmental conditions. We report the results of a theoretically informed coarse-grained Monte Carlo simulation of a polymeric nanogel placed in a solvent bath. The nanogel is modelled as a regular network of Gaussian strands, each discretized with coarse-grained polymer beads (‘‘particles’’). The non-bonded interactions are evaluated from the local densities (‘‘fields’’), and include the Flory-like contribution for polymer-solvent interactions, the translational entropy of mobile ions, and the Coulomb energy obtained by solution of Poisson’s equation. While an artificial grid is employed for convenience of implementation, the results are independent of contour and grid discretization within a resolution specified by the level of coarse-graining. We analyze the effects of degree of crosslinking, solvent quality, and charge fraction of polymer backbone, on the volume phase transition behavior of nanogels.



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