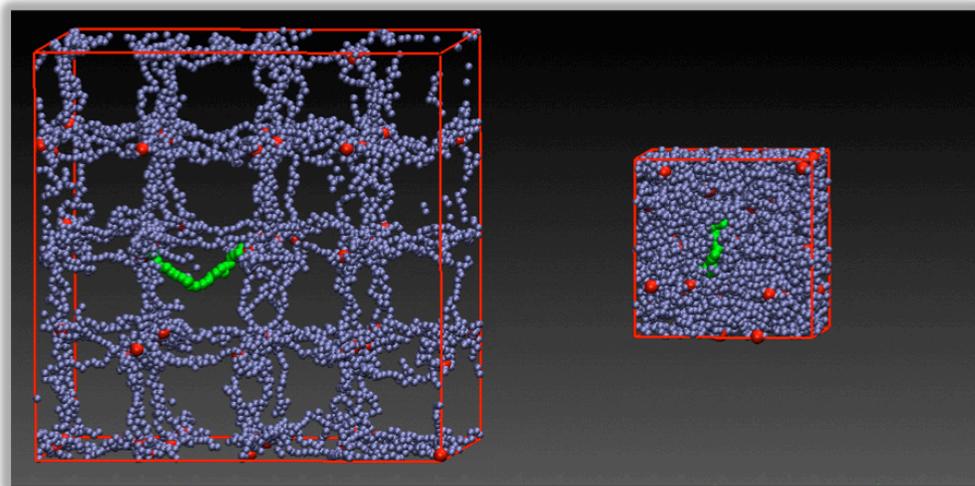


# Molecular Theory of Weak Polyelectrolyte Gels: The Role of pH and Salt Concentration

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Hydrogels of ionizable polymer chains are of great interest for numerous applications in a wide range of fields because they can swell many times their volume in response to a variety of external stimuli, such as changes in solution pH and ionic strength.



**Figure.** Molecular model of the polyelectrolyte gel at two different volume fractions. Cross-links are represented by larger red spheres, and one chain is shown in a different color (for illustration purposes).

We develop a detailed molecular theory that describes the response of weak polyelectrolyte gels to changes in both the pH and the salt concentration of the solution. This approach accounts for conformational degrees of freedom of the cross-linked polymer network, acid-base equilibrium, solution entropy, and electrostatic, van der Waals and excluded-volume interactions. In addition, the theory explicitly incorporates specific molecular details of the polymer gel molecule.

The physical properties of the gel are found to depend on the coupling between charge regulation and the molecular interactions.

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