

Computational Studies of Network Morphologies in Soft Materials

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A material's properties are strongly influenced by their structure at small length scales. The arrangement of molecules into different shapes (or morphologies) will ultimately dictate the properties of the material and its potential applications. One class of morphology that frequently exists in materials is the "network," where the molecules making up a material form a connected domain spanning the entire material. Network morphologies are desirable for wide-spread applications. A connected network of molecules can give a material improved mechanical strength, while a network of water channels through a material can allow ions to transport through the material and enable electric conductivity.

For example, collagen is a protein that forms networks that give strength to bodily tissues, including skin, bones, muscles, and cartilage. Methylcellulose is a synthetic polymer that forms a network in water at elevated temperatures, providing a thickener for food processing applications. In fuel cells, a membrane must permit the flow of ions while being chemically resistant and mechanically durable; a polymer membrane that contains networks of water channels is beneficial for this application.

In these examples, the structural details of the network provide key beneficial properties that allow for use in each application. The connectivity and strand diameters of collagen and methylcellulose networks impact their mechanical strength, while mesh sizes influence how other molecules can move through the network. In ion exchange membranes, the size and connectivity of water channels determine how quickly ions can travel through the membrane, and thus strongly influence their conductivity and performance.

Often, changing the precise molecular makeup of the material will change the network structure and the material properties, leading to the question: "How can molecules be designed to yield the network structure that will give us the desired properties for any given application?" The chemical composition and sequence can significantly affect the network structure in each of the aforementioned examples, but experimentally exploring this design space is often time-consuming and costly. Computational methods can provide a speedup, where designs can be explored in-silico (computationally), and the findings translated to experiments to enable more rapid material discovery.

In this dissertation, I use computational methods to gain insight into the network structure of several materials, how each material's molecular design impacts its network structure, and how

those changes to network structure impact material properties. The materials studied include collagen-like peptides, synthetic peptides aimed to mimic naturally-occurring collagen; perfluorinated ionomers, ionic polymers that compose membranes in fuel cells; methylcellulose, polymer-grafted nanoparticles, particles with polymers attached to them; and, lastly, a study aimed at developing networks that counterintuitively shrink as bonds are broken within them, making the network less connected.