Network Formation and Ion Conduction in Ionomer Membranes

Many important processes in the physical world can be described as a gradient (overdamped) flow of a variational energy. We present a broad formalism for the generation of new classes of higher-order variational energies with a physically motivated structure. In particular we reformulate the Cahn-Hilliard energy, which is well know to describe the surface area of mixtures, into a higher-order model of interfacial energy for mixtures of charged polymers (ionomers) with solvent. These materials are important as selectively conductive membrane separators in a wide variety of energy conversion devices, including polymer electrolyte membrane fuel cells, Lithium ion batteries, and dye sensitized solar cells.

Our reformulated energy, called the Functionalized Cahn-Hilliard (FCH) energy, captures elastrostatic interactions between the charged groups and the complex entropic effects generated by solvent-ion interactions, and allows us to unfold the bilayer and pore networks formed by the solvent phase imbibed into the polymer matrix. We discuss sharp interface reductions of the FCH energy, its gradient flows, and sharp interface reductions of the gradient flows that give rise to higher-order curvature driven flows. We also describe extensions to models that couple to ionic transport and as well as to multiphase models suitable to describe a wide range of membrane casting processes.

References

Hosted by Prof. Martin Z. Bazant
Department of Chemical Engineering