

Title: Dynamic model of monovalent-divalent cation exchange in polyelectrolyte gels

Authors: Matan Mussel¹, Owen Lewis², Peter Bassler³, Ferenc Horkay³

¹ University of Haifa, Israel; ² University of New Mexico, NM, USA; ³ National Institutes of Health, MD, USA;

Abstract: Incremental changes in ionic composition can lead to reversible and abrupt structural changes in many synthetic and bio-polymer systems. In the biological milieu, for example, this nonlinear response is believed to play an important functional role in DNA condensation, cell secretion, and water flow in the xylem of vascular plants. While these systems are markedly different from one another, their similar response to ionic composition suggests that universal principles may play an important role in governing the transient behavior of these systems. In this talk we describe an investigation of a multicomponent model that imposes conservation laws and constitutive relations to describe a negatively charged gel exposed to a solution containing both mono- and divalent cations. Association of ion exchange with gel volume is achieved by imposing a linear relation between the polymer-solvent interaction parameter and the concentration of divalent cations adsorbed onto the polymer chains. Semi-quantitative compatibility with measurements made on sodium polyacrylate gels is demonstrated in three aspects: (1) dynamics of gel swelling and deswelling, (2) ion partitioning coefficient, and (3) effect of crosslink density. These results imply that the multicomponent approach can be useful for quantitative predictions over macroscopic length and time scales in both man-made applications and biological functions that rely on steep response to the environment.