Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Ion transferring in polyelectrolyte networks in electric fields. HONGHAO LI, AYKUT ERBAS, Northwestern Univ, JOS ZWANIKKEN, University of Massachusetts Lowell, MONICA OLVERA DE LA CRUZ, Northwestern Univ — Ion-conducting polyelectrolyte gels have drawn the attention of many researchers in the last few decades as they have wide applications not only in lithium batteries but also as stretchable, transparent ionic conductor or ionic cables devices. However, ion dynamics in polyelectrolyte gels has been much less studied analytically or computationally due to the complicated interplay of long-range electrostatic and short-range interactions. Here we propose a coarse-grained non-equilibrium molecular dynamics simulation to study the ion dynamics in polyelectrolyte gels under external electric fields. We found a nonlinear response region where the molar conductivity of polyelectrolyte gels increases with external fields. We propose counterion redistribution under electric fields as the driving mechanism. We also found the ionic conductivity to be modulated by changing polylelectrolyte network topology such as the chain length. Our discovery reveals the essential difference of ion dynamics between electrolytes and polyelectrolyte gels. These results will expand our understanding in charged polymeric systems and help in designing ion-conducting devices with higher conductivity.

Honghao Li
Northwestern Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4