Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

**Theoretical analysis on ion transport through polymer networks in electrochemical capacitors** JOS W. ZWANIKKEN, YUFEI JING, VIKRAM JADHAO, CHARLES E. SING, NIELS BOON, MONICA OLVERA DE LA CRUZ, Northwestern University — The development of predictive methods for deformable electronics calls for an equally composite theoretical foundation that unites traditionally separated fields. We are pioneering theoretical methods that unite polymer physics with liquid state theory, and develop a dynamical algorithm for inhomogeneous polarizable media between capacitor plates. By a quantitative study of the local molecular correlations we can explain the macroscopic behavior and the induced (non-equilibrium) potentials of mean force between the ions, the supporting medium, and the electrodes. Several timescales are found that correspond to different relaxation processes, related to ion diffusion, double layer formation, and the elastic response of the network. The application of an alternating current reveals a complex frequency-dependent response, by which the relative importance of the different underlying processes can be tuned. Typical non-equilibrium forces, generated by the applied field, are found to arise between regions with sharp gradients in the molecular structure or supporting background. The results may inform experimental efforts on noise reduction in soft capacitors, and suggest new functionality based on frequency-dependent non-equilibrium forces.

Jos W. Zwanikken
Northwestern University

Date submitted: 15 Nov 2013 Electronic form version 1.4