Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Multiscale simulation of complex coacervates KYLE Q. HOFFMANN, Inistitute for Molecular Engineering, University of Chicago, JONATHAN K. WHITMER, Materials Science Division, Argonne National Laboratory, JIAN QIN, DIMITRIS PRIFTIS, SARAH PERRY, LORRAINE LEON, MATTHEW KADE, MATTHEW TIRRELL, JUAN J. DE PABLO, Inistitute for Molecular Engineering, University of Chicago — Aqueous solutions of polymers having opposite charge can separate into a coacervate phase and a supernatant water phase.The conditions leading to such behavior, including chain lenght, ionization fraction, ionic strength, molecular structure, and temperature are poorly understood. Though thermodynamic models of this phase separation exist, they offer little descriptive power for the mechanism of complex coacervation, and the internal structure of the coacervate and precipitate phases. Here we use atomic-level and coarse-grained representations of polypeptides to study features of the phase diagram, scaling relations, and microstructure of complex coacervates, comparing results to experimental data and model calculations.

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Date submitted: 15 Nov 2013 Electronic form version 1.4