

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Field theoretic simulations of the interfacial properties of complex coacervates ROBERT RIGGLEMAN, University of Pennsylvania, GLENN FREDRICKSON, University of California, Santa Barbara — Many biological processes and emerging technologies, such as wet adhesives and biosensors, rely on the association between oppositely charged polyelectrolytes. Such association is driven not only by the electrostatic interactions between the polyelectrolytes, but there is also a substantial entropy gain associated with counterion release upon complexation. In some cases, the association between oppositely charged polymers can lead to a solid precipitate while others can result in a fluid phase rich in polyelectrolytes (coacervate phase) coexisting with a polyelectrolyte-dilute solvent phase. For many of the applications seeking to exploit coacervation, characterization of the interface between the solvent phase and the coacervate is of paramount importance. In this talk, we will present the results of field-theoretic simulations for a coarse-grained polyelectrolyte model that exhibits complex coacervation. Our simulations sample the fully-fluctuating fields in three-dimensions and provide a detailed characterization of the interface between the solvent and the coacervate phase for symmetric polyelectrolytes (where both the polycations and the polyanions carry identical charge densities) as a function of salt concentration and strength of the electrostatic fields. Finally, we characterize the interfacial properties for a select set of asymmetric conditions.

Robert Riggelman
University of Pennsylvania

Date submitted: 20 Nov 2010

Electronic form version 1.4