Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Development of a Coarse-grained Model of Polypeptoids for Studying Self-assembly in Solution PU DU, Louisiana State Univ - Baton Rouge, STEVEN RICK, University of New Orleans, REVATI KUMAR, Louisiana State Univ - Baton Rouge — Polypeptoid, a class of highly tunable biomimetic analogues of peptides, are used as a prototypical model system to study self-assembly. The focus of this work is to glean insight into the effect of electrostatic and other non-covalent secondary interactions on the self-assembly of sequence-defined polypeptoids, with different charged and uncharged side groups, in solution that will complement experiments. Atomistic (AA) molecular dynamics simulation can provide a complete description of self-assembly of polypeptoid systems. However, the long simulation length and time scales needed for these processes require the development of a computationally cheaper alternative, namely coarse-grained (CG) models. A CG model for studying polypeptoid micellar interactions is being developed, parameterized on atomistic simulations, using a hybridized approach involving the OPLS-UA force filed and the Stillinger-Weber (SW) potential form. The development of the model as well as the results from the simulations on the self-assembly as function of polypeptoid chemical structure and sequences will be presented.

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Date submitted: 11 Nov 2016 Electronic form version 1.4