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Computational Field Theory for Advanced Polymer Design

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Abstract

Field-theoretic representations of many-body problems in classical and quantum statistical mechanics have been known for more than 70 years, but have largely enabled approximate analytical calculations. Over the past 15 years, our group has shown that the complex-valued statistical field theory models of classical fluids can be directly tackled by numerical simulation. Such “field-theoretic simulations” (FTS) are advantaged over conventional particle-based computer simulations in a variety of situations, especially dense mesostructured phases of high molecular weight polymers and systems with long-ranged interactions, such as polyelectrolytes. They are also well-suited for multi-scale simulations spanning nanometers to microns.

This talk will introduce the construction of field theory models of polymeric fluids and the FTS framework. Three application examples will be provided: the design of uniquely hard-tough-elastic thermoplastics [1-2], the complexation behavior of oppositely charged polyelectrolytes in solution [3-4], and unpublished work on the microphase assembly of oppositely charged polymeric ionic liquids in the melt.

[1] W. Shi, A. L. Hamilton, K. T. Delaney, G. H. Fredrickson, E. J. Kramer, C. Ntaras, A. Avgeropoulos, N. A. Lynd, Q. Demassieux, and C. Creton, *Macromolecules* **48**, 5378 (2015)
[2] Yi-Xin Liu, Kris T. Delaney, and Glenn H. Fredrickson, *Macromolecules* **50**, 6263 (2017).
[3] K. T. Delaney and G. H. Fredrickson, *J. Chem. Phys.* **146**, 224902 (2017).
[4] S. P. O. Danielsen, J. McCarty, J.-E. Shea, K. T. Delaney, and G. H. Fredrickson, *Proc. Natl. Acad. Sci. USA* **116** (17), 8224-8232 (2019).