

CB-I-1**Managing Complexity in the Design of Multicomponent Polymers****Glenn H. Fredrickson****Departments of Chemical Engineering & Materials
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Multicomponent polymer blends prove challenging to design because they often contain many components and can exhibit self-assembly and phase behavior of daunting complexity. I will describe a suite of new modeling tools that are under development in my group and are well suited to this class of soft material design problems. Rather than applying conventional computer simulation techniques (e.g. MC, MD) to particle-based models of complex fluids, we have developed “field-theoretic computer simulation” schemes for numerically sampling functional integrals comprising field-theory models of complex fluid systems [1]. Such methods can be viewed alternatively as strategies for relaxing the mean-field approximation inherent in self-consistent field theories, or as new computer simulation schemes. I will discuss how these tools can be used to “combinatorially explore” phase diagrams of complex block copolymers and will highlight a specific application to the design of clear-tough-hard plastics for optical media.

[1] G. H. Fredrickson, V. Ganesan, and F. Drolet, *Macromolecules* **35**, 16 (2002).