Contribution ID: **1062** Type: **Invited Speaker / Conférencier invité**

Complex ordered phases of multiblock copolymers

Thursday, 16 June 2016 13:15 (30 minutes)

Self-assembly of multiblock copolymers presents a great opportunity to generate tailored polymeric materials with hierarchically ordered nano-scale domains. At the same time, the phase complexity of multiblock copolymers presents a great challenge to experimental and theoretical study of their phase behavior. Theoretically the self-consistent field theory (SCFT) provides a powerful framework for the study of inhomogeneous polymeric systems. In particular, many researchers have demonstrated that SCFT can be used to describe the phase behavior of block copolymers. Our recent research focuses on the development of theoretical and simulation methods for the prediction of block copolymer phases, resulting in a generic strategy to discover complex ordered phases of block copolymers within the SCFT framework. Specifically, the strategy utilizes a combination of real-space and reciprocal-space techniques to explore possible ordered phases that could be formed by multiblock copolymer melts, resulting in an array of candidate structures. A comparison of the free energy of the candidate phases can then be used to construct phase diagrams. Our extensive calculations have demonstrated that this strategy could be used to predict the formation of complex and hierarchically ordered phases from multiblock copolymers. In particular, application of this strategy to multiblock copolymers, including linear and star ABC triblock copolymers and BACBA pentablock copolymers, has led to the discovery and understanding of a rich array of ordered phases.

Primary author: SHI, An-Chang (McMaster University)

Presenter: SHI, An-Chang (McMaster University)

Session Classification: R2-1 Computational Condensed Matter (DCMMP) / Matière condensée numérique (DPMCM)

Track Classification: Condensed Matter and Materials Physics / Physique de la matière condensée et matériaux (DCMMP-DPMCM)