Canadian Association of Physicists
Association canadienne des physiciens et physiciennes

Contribution ID: **3411** Type: **Invited Speaker / Conférencier(ère) invité(e)**

(I) Linking placement of associating groups along polymer chains to phase behavior of polymer blends using PRISM theory and molecular simulations

Tuesday 7 June 2022 11:15 (30 minutes)

Phase behavior of polymer blends (i.e., the miscibility or phase separation of the two or more polymer chemistries in the blend) can be tuned by incorporation of functional groups that allow for favorable association between the polymers in the blend. In this talk, we will present our current work involving Polymer Reference Interaction Site Model (PRISM) theory and coarse-grained molecular dynamics simulations to predict the blend morphology (i.e., macrophase separated, disordered with concentration fluctuations, microphase separated) as a function of placement and fraction of associating groups along polymer chains at varying strengths of association. The features in structure factors [S(k) vs. k] calculated using PRISM theory for varying polymer design and association strengths are used to identify the morphologies within the phase diagram. For the disordered morphologies that exhibit concentration fluctuations, we calculate how the length scales of concentration fluctuations change with the associating group placement for similar fraction of association groups. Then, we use molecular simulations to visualize and quantify the molecular packing that explain these results obtained from PRISM theory. Using this combination of PRISM theory and molecular simulations we are able to explore a large polymer design space with reduced computational intensity and more reliable structure factors than would be possible with an approach involving only molecular simulations.

This work was funded by U.S. Department of Energy, Office of Science (DE-SC0017753)

Authors: KULSHRESHTHA, Arjita (University of Delaware); Prof. JAYARAMAN, Arthi (University of Delaware)

Presenter: Prof. JAYARAMAN, Arthi (University of Delaware)

Session Classification: T2-7 Fluctuations and Disorder in Condensed Matter (DCMMP) | Fluctuations et désordre en matière condensée (DPMCM)

Track Classification: Symposia Day (Tues. June 7) / Journée de symposiums (mardi, le 7 juin): Symposia Day (DCMMP) - Fluctuations and Disorder in Condensed Matter