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Polyolefin blends: Coarse-grained study of melt structures relevant for predicting blend miscibilities SANDEEP JAIN, SHEKHAR GARDE, SANAT KUMAR, Department of Chemical Engineering, Rensselaer Polytechnic Institute, Troy, New York 12180 — Miscibility of polyolefins has been the subject of intense research both due to its fundamental importance and industrial applications. Detailed Molecular Dynamics (MD) simulations of long chain polymers and their phase behavior is limited by the enormous computational effort involved. Naturally, emphasis is being placed on development of coarse-graining strategies that allow more efficient sampling of conformational space while retaining the chemical identity of the polymer of interest. We will present results from a novel coarse-graining approach that combines detailed MD simulations of oligomers with inverse (Monte Carlo based) methods to obtain interaction potentials in coarse-grained system. We show that the coarse-grained potentials, thus generated, reproduce a variety of structural properties of the underlying polymer melt systems. The computational efficiency of our coarse-graining apporach allows simulations of truly polymeric (long chain) melts. Extension of these ideas to studies of polyolefin blends with emphasis on miscibility will be presented briefly.

Sandeep Jain

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