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**Molecular Simulation of Olefin Oligomer Blend Phase Behavior**

QILE CHEN, TIMOTHY LODGE, ILJA SIEPMANN, University of Minnesota, MRSEC COLLABORATION — Material properties (e.g. toughness) of polyolefin mixtures are closely tied to their phase behavior that often cannot be accurately predicted by the widely used Flory–Huggins (FH) theory. In this work, configurational-bias Monte Carlo (CBMC) simulations in the Gibbs ensemble were used to compute the phase behavior of oligomeric olefins. The cohesive energy density of pure melts and the free energy of mixing were obtained from these simulations, and the discrepancy between the binary interaction  $\chi$  parameter from simulation and from the FH theory was quantified. Structural analysis and the calculated excess mixing properties provided some rationale into the interpretation of these results.

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