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Theory For The Miscibility Windows In Blends Of Polypropylene And Ethylene-α-Olefin Copolymers DAVID WU, HUIMIN LI, Colorado School of Mines, JOHN CURRO, University of New Mexico, COLORADO SCHOOL OF MINES COLLABORATION, UNIVERSITY OF NEW MEXICO COLLABORATION — The miscibility of isotactic polypropylene (iPP) and ethylene-α-olefin (C2Cx) copolymers has been intensively studied both for its industrial importance and as a model system for complex polymer miscibility behavior. Experiments generally show a window of miscibility for particular regions in the parameter space defined by copolymer composition, volume fraction, and branch chain length. Since the cost of systematic molecular dynamics studies of such systems is still prohibitive, a statistical mechanical approach with the molecular interaction potentials and chain structure as the only input is highly desirable. We present self-consistent Polymer Reference Interaction Site Model (SC-PRISM) calculations of blends of iPP and C2Cx copolymer, where Cx is propylene, butene, and hexene. The calculated enthalpy of mixing is shown to correlate well with experimental trends for the miscibility window. Furthermore, since the theory allows access to molecular-level correlations, insight is provided into the mechanisms for the specific miscibility behavior, including contributions due to chain conformations.

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