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Effect of Composition and Chain Length on χ Parameter of Polyolefin Blends: A Molecular Dynamics Study RAJESH KHARE, ASHWIN RAVICHANDRAN, CHAU-CHYUN CHEN, Texas Tech Univ — Polymer blends exhibit complex phase behavior which is governed by several factors including temperature, composition and molecular weight of components. The thermodynamics of polymer blends is commonly described using the χ parameter. While variety of experimental studies exist on identifying the factors affecting the χ parameter, a detailed molecular scale understanding of these is a topic of current research. We have studied the effect of blend composition and chain length on χ parameter values for two model polyolefin blends. The blends studied are: polyisobutylene (PIB)/polybutadiene (PBD) and polyethylene (PE)/atactic polypropylene (aPP). Molecular dynamics simulations in combination with the integral equation theory formalism proposed by Schweizer and Curro [Journal of Chemical Physics, 91, 5059 (1989)] are used to determine the χ parameter for these systems and thereby study the effect of blend composition and chain length. The resulting χ parameter values are explained in terms of the molecular structure of these polymeric systems.

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