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A molecular picture: How composition influences the dynamic and static properties in a polyolefin blend, as observed with molecular simulation ANDREW MAY, JANNA MARANAS, Pennsylvania State University, PENN STATE TEAM — We use molecular dynamics simulation to investigate dynamic and static properties in a blend of poly(ethylene-propylene) [PEP] and poly(ethylene-butene) [PEB]: this is a simple model for blend dynamics because the mixture behaves athermally and each component has similar pure packing characteristics and glass transition temperatures. The use of simulation allows us to examine a full spectrum of compositions, ranging from the dilute (single chain) to concentrated limits (all but one chain). As composition is varied, mobility is observed through the self-intermediate scattering function, while the pair distribution function and local concentrations are used to examine static features. Attention is given to both average values and the distribution within the average. Despite the simplicity of this system, the influence of composition varies between the two components, most noticeable in the dilute region. Molecular packing and concentrations on a local length scale are investigated as a possible source for this variation.

Prefer Oral Session
 Prefer Poster Session

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