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Optimizing a Mesoscale Model for Polyisoprene-Polystyrene Melts QI SUN, ROLAND FALLER, Dept of Chem Eng & Mat Sci, UC Davis — Coarse-graining, the systematic mapping from the atomistic to meso-scale has made significant progress in pure polymers or polymers in solution. However, it has not yet been attempted in melts of polymer mixtures. Our project is aiming at building a multiscale model of Polyisoprene (PI) and Polystyrene (PS) mixtures. The positions of the meso-scale interaction centers (superatoms) are chosen in order to produce a single peaked bond distribution on the meso-scale as well as a harmonic bond stretching potential. For PI, twelve atoms are joined into one superatom positioned in the middle of the single carbon-carbon bond. The superatom center for PS is at the backbone carbon connected to the side ring and represents sixteen atoms. We apply the newly developed "Inverted Boltzmann Method" to derive numerical potentials from atomistic models where the interaction potential is iteratively optimized against the atomistic structure using potentials of mean force. We optimize the iteration process and analyze the concentration and temperature dependencies of the evolving potential, investigating further what parameters induce the phase separation in longer chains and miscibility in shorter chains. All the work eventually leads to a better understanding of the mechanisms governing material properties.

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