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Coarse grained polystyrene simulations: Static and dynamic properties[1] KURT KREMER, Max Planck Institute for Polymer Research, Mainz, Germany — By combining input from short simulation runs of rather small systems with all atomistic details together with properly adapted coarse grained models we are able quantitatively predict static and especially dynamical properties of both pure polymer melts of long entangled chains but also of systems with low molecular weight additives. Comparisons to rather different experiments such as diffusion constant measurements, NMR relaxation experiments and dielectric spectroscopy show a remarkable quantitative agreement without any adjustable parameter. The model is also able to distinguish different tacticities and to study the consequences for static and dynamic properties. Reintroduction of chemical details into the coarse grained trajectories allows the study of long time trajectories in all atomistic detail providing the opportunity for rather different means of data analysis.

[1]Work done in collaboration with D. Fritz, V. Harmandaris and N. van der Vegt.

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