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Making coarse grained polymer simulations quantitatively predictive for statics and dynamics

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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 fully entangled but also of systems with low molecular weight additives. Comparisons to rather different experiments such as diffusion constant measurements or NMR relaxation experiments show a remarkable quantitative agreement without any adjustable parameter. 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. References: V. Harmandaris, K. Kremer, Macromolecules, in press (2009) V. Harmandaris et al, Macromolecules, 40, 7026 (2007) B. Hess, S. Leon, N. van der Vegt, K. Kremer, Soft Matter 2, 409 (2006) D. Fritz et al, Soft Matter 5, 4556 (2009)