Dual scale modeling of mobility of additives in a polymer matrix

Authors: Nico F.A. van der Vegt, Kurt Kremer

Max Planck Institute, Mainz, Germany

Abstract:

In my talk I will discuss the development and use of (high-resolution) classical atomistic and (low-resolution) coarse grained models in computer simulations of polymer materials. I will illustrate how coarse grained models can be used to study materials in which all length scales are equilibrated [1] and how by virtue of "inverse mapping of chemical details" [2,3] permeation of small solute molecules can be addressed. I will moreover show an example in which diffusion of small solutes inside a polymeric matrix is predictively modelled with a coarse grained model.

Key references:
[1] S. Leon, N. van der Vegt, L. Delle Site, K. Kremer, Macromolecules 38, 8078 (2005)
[2] B. Hess, S. Leon, N. van der Vegt, K. Kremer, Soft Matter 2, 409 (2006).
[3] V.A. Harmandaris, N.P. Adhikari, N.F.A. van der Vegt, K. Kremer, Macromolecules 39, 6708 (2006)