Theoretical understanding of the dynamics in polymer systems: from simple polymers to complex electrolytes

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In this presentation I summarize our simulations on macromolecular systems, ranging from simple homopolymers over polymer blends to polymer electrolytes as well as their mixtures with ionic liquids.
The simulations are guided by the aim to obtain a deeper understanding of the mechanisms, governing the dynamics of these different systems. For a closer interpretation of the results two conceptual developments are of importance. First, we have introduced a numerical approach to determine local friction coefficients from simulations. In this way it is possible to characterize the dynamic heterogeneities in polymer blends or the chain-end effects in homopolymers.
Second, we have developed an analytical model to express the ionic dynamics in polymer electrolytes in terms of the different motional mechanisms in these systems. Application of this model to the actual numerical data allows us to characterize the ionic dynamics and the additional impact of ionic liquids on this dynamics.