Activated Dynamics in Dense Model Nanocomposites SHIJIE XIE,
KENNETH SCHWEIZER, University of Illinois at Urbana-Champaign — The non-
linear Langevin equation approach is applied to investigate the ensemble-averaged
activated dynamics of small molecule liquids (or disconnected segments in a polymer
melt) in dense nanocomposites under model isobaric conditions where the spherical
nanoparticles are dynamically fixed. Fully thermalized and quenched-replica integral
equation theory methods are employed to investigate the influence on matrix dy-
namics of the equilibrium and nonequilibrium nanocomposite structure, respectively.
In equilibrium, the miscibility window can be narrow due to depletion and bridging
attraction induced phase separation which limits the study of activated dynamics to
regimes where the barriers are relatively low. In contrast, by using replica integral
equation theory, macroscopic demixing is suppressed, and the addition of nanopar-
ticles can induce much slower activated matrix dynamics which can be studied over
a wide range of pure liquid alpha relaxation times, interfacial attraction strengths
and ranges, particle sizes and loadings, and mixture microstructures. Numerical
results for the mean activated relaxation time, transient localization length, matrix
elasticity and kinetic vitrification in the nanocomposite will be presented.

Shijie Xie
University of Illinois at Urbana-Champaign