Physics Colloquium

Professor Gary S. Grest

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"Going up in time and length scales in modeling polymers"

Friday, September 21, 2018

2:30pm—3:30pm

210 Robeson Hall

Polymer properties depend on a wide range of coupled length and time scales, with unique macroscopic viscoelastic behavior stemming from interactions at the atomistic level. The need to probe polymers across time and length scales and particularly computational modeling is inherently challenging. Here new paths to probing long time and length scales including introducing interactions into the traditional bead-spring model that has been widely used for the past thirty years and coarse graining of atomistic simulations will be compared. Using linear polyethylene as a model system, the degree of coarse graining with two to six methylene groups per coarse-grained bead derived from a fully atomistic melt simulation were probed. Using these models we were successful in probing highly entangled melts and were able reach the long-time diffusive regime which is computationally inaccessible using atomistic simulations. We simulated the relaxation modulus and shear viscosity of well-entangled polyethylene melts for scaled times of a microsecond. The long time and length scale is coupled to the macroscopic viscoelasticity where the degree of coarse graining sets the minimum length scale instrumental in defining polymer properties and dynamics. Results will be compared to those obtained from the bead-spring model to demonstrate the additional insight that can be gained from atomistically inspired coarse grained models.