Molecular modeling and simulations for polymer/nanomaterials

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Significant advances in the field of computer simulations (both methodological and algorithmic) and the rapid increase in computing power have led to the development of powerful multiscale simulation tools. These developments have the potential to address fundamental issues in materials science and technology by revealing the molecular origin of unique phenomena exhibited at the macroscopic level and by elucidating the structure-property-processing relationships in systems with a complex internal microstructure. In this talk, I will describe recent developments of methods of a hierarchy of simulation tools [nonequilibrium molecular dynamics (NEMD) and nonequilibrium Monte Carlo (NEMC) methods based on the principles of nonequilibrium thermodynamics/statistical mechanics] and their applications to the study of the physical properties of complex macromolecular fluids, especially under the application of an external field; e.g., an imposed flow can perturb a polymeric system over several length and time scales, causing it to exhibit a variety of thermodynamical and rheological properties. Further extensions to more complex polymer/nanomaterials will be briefly mentioned.