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Large Scale Molecular Dynamics Simulation of Polymeric Materials MONOJOY GOSWAMI, JAN-MICHAEL CARRILLO, RAJEEV KUMAR, BOBBY SUMPTER, Oak Ridge National Lab — In this talk, I will present a series of large-scale molecular simulations of polymer nanocomposites and block copolymers (BCP). We will discuss three different problems in this talk that requires large-scale computation: 1) hydrated RNA dynamics on a nanodiamond (ND) surface for drug-delivery applications, 2) poly(3-hexylthiophene) (P3HT) and PCBM nanocomposites for the application in organic photovoltaics (OPV) and (3) amphiphilic BCP self assembly in surfactant solution for membrane separation technology applications. We simulate problem (1) using fully atomistic NAMD simulation and discuss the puzzling discovery of faster RNA dynamics on ND surface. LAMMPS MD code is used to simulate problems (2) and (3). Here we explain the importance of nanodomains in P3HT:PCBM nanocomposites in designing OPV and the criterion for surfactant mediated self-assembly of amphiphilic BCP in solution.

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