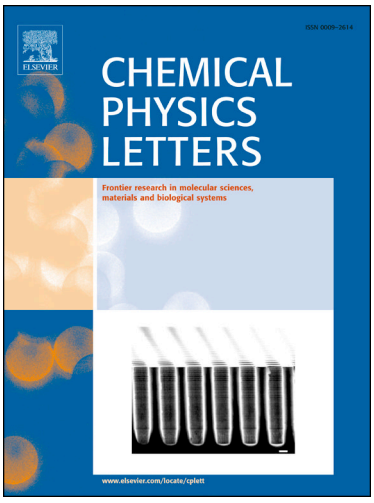

Research paper

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Semi-flexible Polymer Engendered Aggregation/dispersion of Fullerene (C_{60}) Nano-particles: an atomistic investigation

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Abstract

Semi flexible polymer chain has been modeled by choosing various values of persistent length (stiffness). As the polymer chain stiffness increases, the shape of polymer chain changes from globule to extended cigar to toroid like structure during cooling from a high temperature. The aggregation of fullerene nano-particles is found to depend on the morphology of polymer chain. To maximize, the number of polymer bead-nanoparticle contacts, all nano-particle have positioned inside the polymer globule. To minimize, the energy penalty, due to bending of the polymer chain, all nano-particle have positioned on the surface of the polymer's cigar and toroid morphology.

Key-words: Semi-flexible polymer, Fullerene, Molecular Dynamics simulations, LAMMPS.