

Accepted Manuscript

Research paper

Semi-flexible Polymer Engendered Aggregation/dispersion of Fullerene (C₆₀) Nano-particles: An atomistic investigation

Sunil Kumar, Sudip K. Pattanayek

PII: S0009-2614(18)30320-8

DOI: <https://doi.org/10.1016/j.cplett.2018.04.035>

Reference: CPLETT 35591

To appear in: *Chemical Physics Letters*

Received Date: 9 February 2018

Revised Date: 14 April 2018

Accepted Date: 16 April 2018

Please cite this article as: S. Kumar, S.K. Pattanayek, Semi-flexible Polymer Engendered Aggregation/dispersion of Fullerene (C₆₀) Nano-particles: An atomistic investigation, *Chemical Physics Letters* (2018), doi: <https://doi.org/10.1016/j.cplett.2018.04.035>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



Semi-flexible Polymer Engendered Aggregation/dispersion of Fullerene (C₆₀) Nano-particles: an atomistic investigation

Sunil Kumar^{§*}, Sudip K. Pattanayek[‡]

[§]CSIR-National Metallurgical Laboratory, Jamshedpur, India 831007

[‡]Indian Institute of Technology, New Delhi, India 110016

*Email: sunil@nmlindia.org, suniliitd14@gmail.com

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.

Download English Version:

<https://daneshyari.com/en/article/7837688>

Download Persian Version:

<https://daneshyari.com/article/7837688>

[Daneshyari.com](https://daneshyari.com)