

Accepted Manuscript

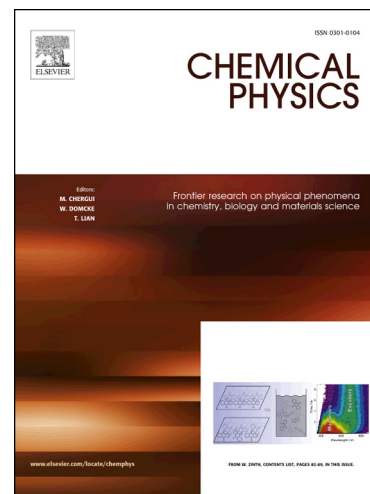
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PII: S0301-0104(18)30017-X
DOI: <https://doi.org/10.1016/j.chemphys.2018.08.037>
Reference: CHEMPH 10153

To appear in: *Chemical Physics*

Received Date: 5 January 2018
Revised Date: 10 June 2018
Accepted Date: 15 August 2018



Please cite this article as: S. Kumar, S.K. Pattanayek, Force Induced Removal of an Encapsulated Semi-flexible Polymer from Single Walled Carbon Nanotube, *Chemical Physics* (2018), doi: <https://doi.org/10.1016/j.chemphys.2018.08.037>

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Force Induced Removal of an Encapsulated Semi-flexible Polymer from Single Walled Carbon Nanotube

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Abstract

Encapsulation of a variety of atoms, molecules, polymers, bio-polymers into a Single Wall Carbon Nanotube (SWCNT) depict unexpected properties such as unique morphology, physical properties, high thermal stability etc. The encapsulation and pull-out processes are very important parts of synthesis and characterization of new materials at atomic length scale, which controls the overall desirable properties. Here, we investigate the encapsulation and the pullout process of a long-polymer chain into/from a SWCNT by molecular dynamics (MD). However, during externally applied force induced pull-out process of polymer chain from SWCNT depict a significant transition in an organization with the creation of additional surface area. We have observed that the amount of applied force highly influences the organization and creation of additional surface area of polymer chain during pull-out process.

Key words: SWCNT, Polymer, Encapsulation, Pull-out, Molecular Dynamics Simulations.

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