

# Accepted Manuscript

Full Length Article

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R. Ansari, S. Rouhi, S. Ajori

PII: S0169-4332(18)31093-6

DOI: <https://doi.org/10.1016/j.apsusc.2018.04.133>

Reference: APSUSC 39132

To appear in: *Applied Surface Science*

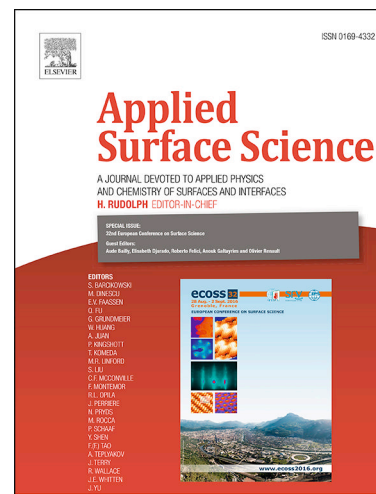
Received Date: 10 November 2017

Revised Date: 6 April 2018

Accepted Date: 12 April 2018

Please cite this article as: R. Ansari, S. Rouhi, S. Ajori, Molecular dynamics simulations of the polymer/amine functionalized single-walled carbon nanotubes interactions, *Applied Surface Science* (2018), doi: <https://doi.org/10.1016/j.apsusc.2018.04.133>

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# Molecular dynamics simulations of the polymer/amine functionalized single-walled carbon nanotubes interactions

R. Ansari<sup>1</sup>, S. Rouhi<sup>2\*</sup>, S. Ajori<sup>1</sup>

<sup>1</sup>Department of Mechanical Engineering, University of Guilan, P.O. Box 3756, Rasht, Iran

<sup>2</sup>Young Researchers and Elite Club, Langroud Branch, Islamic Azad University, Langroud, Guilan, Iran

## Abstract

In this paper, the interactions of polymer chains with single-walled carbon nanotubes (SWCNTs) are studied. To this end, molecular dynamics (MD) simulations are used. The effects of functionalization factor type and weight percent, polymer type, nanotube diameter and randomness of functionalization are studied. Comparing the results for (7,7) and (12,12) single-walled carbon nanotubes, it is observed that increasing the nanotube diameter results in decreasing the difference between interaction energies of different polymers/functionalized single-walled carbon nanotubes systems. Besides, it is observed that mapped distribution of the CH<sub>2</sub>-NH<sub>2</sub> amines on the single-walled carbon nanotube surface has not significant effect on the polymer/functionalized nanotube interaction energies. It is seen that functionalization of nanotubes by NH<sub>2</sub> amine results in more strength polymer/nanotube interactions than CH<sub>2</sub>-NH<sub>2</sub> amine.

*Keywords:* Single-walled carbon nanotubes; Functionalization; Amine; Polymer chains; Adsorption

## 1. Introduction

Since the publication of the first paper on the carbon nanotubes (CNTs) by Iijima [1], their fantastic properties have led to applicability in different fields [2-7]. One of the most significant applications of CNTs is their application in nanocomposites reinforcement [8-10]. But, this application is limited by the poor solubility of CNTs in most organic solvents [11]. This problem

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\*Corresponding author: Tel.: +98 1425244411; fax: +98 1425244422.

E-mail addresses: s\_rouhi@iaul.ac.ir

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