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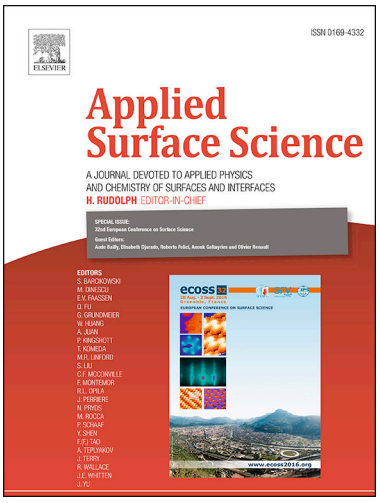

Full Length Article

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

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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_2-NH_2 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_2 amine results in more strength polymer/nanotube interactions than CH_2-NH_2 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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