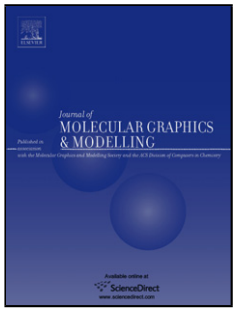


Title: Adsorption of poly(ethylene succinate) chain onto graphene nanosheets: A molecular simulation

Author: Payam Kelich Ahmad Asadinezhad

PII: S1093-3263(16)30134-6
DOI: http://dx.doi.org/doi:10.1016/j.jmgm.2016.08.003
Reference: JMG 6735

To appear in: *Journal of Molecular Graphics and Modelling*

Received date: 16-4-2016
Revised date: 30-7-2016
Accepted date: 8-8-2016

Please cite this article as: Payam Kelich, Ahmad Asadinezhad, Adsorption of poly(ethylene succinate) chain onto graphene nanosheets: A molecular simulation, Journal of Molecular Graphics and Modelling http://dx.doi.org/10.1016/j.jmgm.2016.08.003

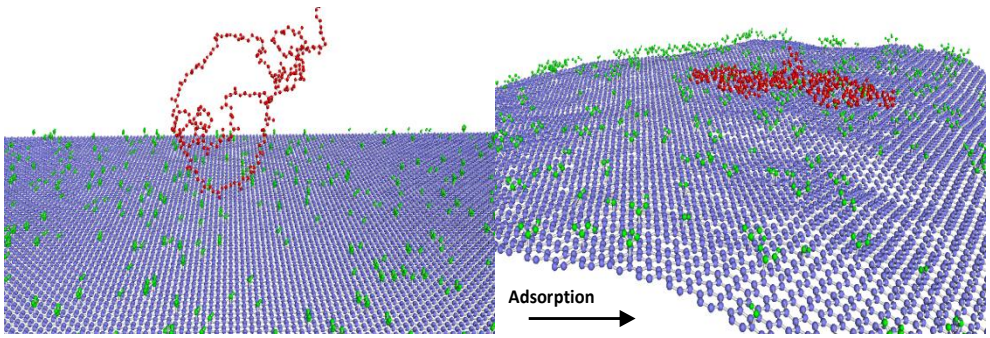
Adsorption of Poly(ethylene succinate) Chain onto Graphene Nanosheets: A Molecular Simulation

Payam Kelich and Ahmad Asadinezhad*

Department of Chemical Engineering, Isfahan University of Technology, 84156-83111, Esfahan, Iran

*Corresponding author: Email address: asadinezhad@cc.iut.ac.ir
Tel: +98-31-33915605
Fax: +98-31-33912677

Graphical abstract



Highlights

- Poly (ethylene succinate) (PES) conformation adopts a folded shape near graphene
- Graphene functionalization induces strong confinement on PES chain conformation
- PES chain motion alters in dynamic mode as it becomes adsorbed onto graphene
- Temperature aids PES chain conformational order and dynamics during adsorption

ABSTRACT

Understanding the interaction between single polymer chain and graphene nanosheets at local and global length scales is essential for it underlies the mesoscopic properties of polymer nanocomposites. A computational attempt was then performed using atomistic molecular dynamics simulation to gain physical insights into behavior of a model aliphatic polyester, poly(ethylene succinate), single chain near graphene nanosheets, where the effects of the polymer chain length, graphene functionalization, and temperature on conformational properties of the polymer were studied comparatively. Graphene