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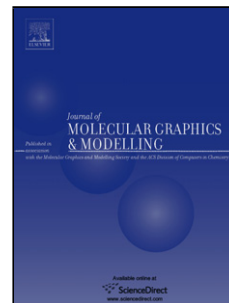
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Adsorption of Poly(ethylene succinate) Chain onto Graphene Nanosheets: A Molecular Simulation

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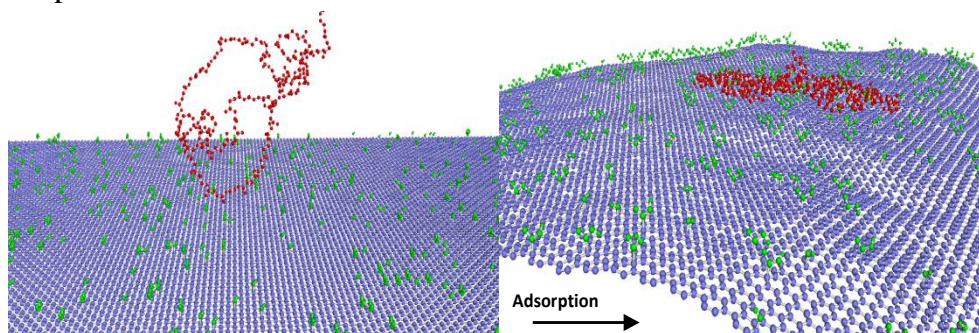
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Graphical abstract



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

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