Molecular Dynamics: Applications In Molecular Biology

NANO: Brief Reports and Reviews
Vol. 6, No. 1 (2011) 19–29

DOI: 10.1142/S1793292011002317

MOLECULAR DYNAMICS SIMULATION OF POPC AND POPE LIPID MEMBRANE BILAYERS ENFORCED BY AN INTERCALATED SINGLE-WALL CARBON NANOTUBE

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Received 1 April 2010
Accepted 4 July 2010

Using classical all-atom molecular dynamics simulation, we investigated the molecular dynamics of palmitoyloleoylphosphatidylcholine and palmitoyloleoylphosphatidylethanolamine membrane bilayers enforced by a single-wall carbon nanotube. We postulated that an insertion of a single-wall carbon nanotube in the center of lipid membrane "strengthens" ambient lipids and prevents the whole system from further destabilization by high temperatures. We implemented root mean square deviation and root mean square fluctuation analyses of simulated structures from their initial states in order to emphasize the molecular dynamics behavior of these structures during 1000 ps simulation time at different temperatures. The data suggest that an intercalated carbon nanotube restrains the conformational freedom of adjacent lipids and hence has an impact on the membrane stabilization dynamics. On the other hand, different lipid membranes may have dissimilarities due to the differing abilities to create a bridge formation between the adherent lipid molecules. The results derived from this work may be of importance in developing stable nanosystems for construction of novel biomaterials and delivery of various biomolecules in the fields of biosensors, biomaterials, and biophysics.

Keywords: Molecular dynamics; lipid membrane bilayer; carbon nanotube; root mean square deviation; root mean square fluctuation.

1. Introduction

The importance of nanotechnology for biotechnological applications is frequently discussed in the scientific community as a powerful tool for the development of nanostructured materials,[1] ranging from novel nanoelectrics to molecular assemblies, to nanocomposites, tissue engineering and biomedicine. The physico-chemical properties of some of these nanomaterials determine their biocompatibility via supporting and stabilizing different biological systems such as lipid membrane bilayers by means of their integration into functional hybrids.[1]

The most basic property of lipid bilayers in biology is to act as a barrier between the inside and outside of a cell, and this depends on the

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Molecular dynamics of macromolecules of biological interest began in with the publication of a paper on the simulation of a small protein.The study of the macromolecular structure is a key point in the understanding of biology. Biological function is based on molecular interactions, Molecular dynamics - Application: understanding - Application: molecular.In this Perspective, we illustrate the application of molecular dynamics simulations to biology by describing several selected examples.Molecular dynamics simulations are used to describe the patterns, strength, and properties of protein behavior, drugreceptor interactions, the solvation of molecules, the conformational changes that a protein or molecule may undergo under various conditions, and other events that require the systematic evaluation of.From: Modeling of Microscale Transport in Biological Processes, Current State-of-the-Art Molecular Dynamics Methods and Applications. Dimitrios.Trove: Find and get Australian resources. Books, images, historic newspapers, maps, archives and more.Molecular Dynamics Simulations of Biological Reactions .. Application of molecular dynamics simulation in food carbohydrate researcha review. Tao Feng.and applicability to other, more challenging areas such as biological systems and . matter systems, namely Monte Carlo (MC) and Molecular Dynamics (MD).PDF Molecular dynamics simulations have evolved into a mature technique that can be used effectively to Advances and Applications in Bioinformatics and Chemistry 3747 and Molecular Biology, University of.Excerpt. Molecular dynamics of macromolecules of biological interest began in with the publication of a paper on the simulation of a small protein, the.Studies of Synthetic and Biological Macromolecules. Lichang Introduction to Molecular Dynamics Simulations: Applications in Hard and Soft.adorationperpetuelle34.com developments-and-applications-in-nanotechnology-and-energy/application-of- molecular-.If you are searched for a book Molecular Dynamics: Applications in Molecular Biology (Topics in. Molecular & Structural Biology) in pdf form, in that case you.Doctoral Thesis in Theoretical Chemistry and Biology. School of The applications in this thesis of molecular dynamics simulations in solution chemistry .Here, we describe the foundations of molecular dynamics and the Center, 4 Department of Biochemistry and Molecular Biology, University of.In recent years, the electric field in the application of biological research has become a hot spot, However, the mechanism still lags behind the experimen.Molecular Dynamics Simulations for Biological Systems: of molecular dynamics for biological studies and application of molecular dynamics simulations.

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