



سمینار هفتگی ماده چگال نرم

Mobility of Surface-Moving Nanocars

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Abstract

Tremendous functioning of natural molecular machines in life with high efficiency and accuracy have trigger research on fabricating molecular structures able to perform special duties in nanoscales. The idea of conducting a work at the expense of chemical energy at the molecular level has led to the emergence of the new area of query, namely, “molecular machines”. These tiniest possible machines were the issue of interest so that Nobel Prize in chemistry 2016 was awarded to three scientists for “design and synthesis of molecular machines”. Several synthetic molecular machines have been developed for transporting nanoscale materials called Nanocars. Since the high-cost experimental imaging data can not disclose all details of Nanocars motion, it is necessary to study and simulate Nanocars. Molecular Dynamics simulation can be a promising tool for understanding the Nanocars motion, in addition to providing a way to perceive the directional motion on surfaces. Nanocars with C60 wheels were the first generation of synthesized Nanocars. To understand these Nanocars, first the motion of C60 should be investigated. We focused on the motion on carbon structures like graphene and graphite examining the effect of temperature and surface ripples on the dynamics of the molecule. As a second instance, we focus on the motion on Ethylene molecule on Si (100) to see the effect of applying a charge on the motion of the molecule. To consider the quantum effects of applied charge on the system we focused Density Functional based Tight Binding theory by utilizing DFTB+ package.

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