سمینار هفتگی ماده چگال نرم

عنوان سمینار

Molecular Dynamics Simulation of Nanocar Motion on Carbon Structures

ارائه دهنده

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چکیده

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, 'the 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 synthesized molecular machines have been developed for transporting nano-scaled materials which are called Nanocars. Since the high cost experimental imaging data can not disclose all details of Nanocars motion, the study and simulating of Nanocars seems necessary. Nanocars with C_{60} wheels were the first generation of synthesized Nanocars. To understand these Nanocars, first the motion of C_{60} should be investigated. We focused on the motion on carbon structures like graphene and graphite. As a second instance we focus on the motion on Ethylene molecule on Si (100) to see the effect of applying charge on the motion of molecule. Molecular Dynamics simulation can be considered a promising tool to understand the Nanocars motion, in addition to provide a way to perceive the directional motion on surfaces

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