



سمینار هفتگی ماده چگال نرم

Mobility of Surface-Moving Nanocars, How Surface Ripples and Chassis Rigidity Contribute

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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 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. After studying the Dynamics and PES analysis of fullerene motion, we focused on the motion of fullerene-based nano-machines on carbon structures like graphene and graphite examining the effect of surface ripples, Chassis rigidity and temperature on the dynamics of the molecules. 6 different system design were investigated and the diffusion coefficient, anomaly parameter, vertical oscillation, vertical and horizontal rotation of a Nanocar with flexible chassis and a Nanotruck with rigid chassis are presented.

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