سمینار هفتگی ماده چگال نرم

Molecular Dynamics Simulation of Nanocar Motion on Carbon Structures

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Abstract

Nanomachines are molecules inspired by natural molecular machines and are able to move and transport at the nanoscale. Due to the advancement of nanotechnology, the need to move materials and energy on a small scale is necessary more than ever. Nanocars are artificial molecular machines with chassis, axles, and wheels designed for nanoscale transport at materials' surfaces. Understanding the dependence of surface dynamics of nanocars on the substrate's physico-chemical properties is critical to the design of the transport properties of such man-made nanoscale devices. Among the multitude of potential substrates for the nanotransporters, graphene exhibits intrinsic ripples on its surface, which may affect the surface dynamics of nanocars. In the first step, we report our molecular dynamics study of the motion of C_{60}, a popular nanocar wheel, on the graphitic substrates with systematically-controllable surface ripples. We look for the effect of temperature and surface ripples of Graphene substrate on motion mechanisms. In the next step, 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. It is expected that by using the results of this project and understanding the mobility of this nanocar, beneficial and technical points can be proposed to the design of molecular machines with directional motion.

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