

İTÜ FEN-EDEBİYAT FAKÜLTESİ

FİZİK BÖLÜMÜ SEMİNERİ

“Molecular dynamics simulations to probe dynamics and transport in mesoscopic systems: Application to nanotubes and polymer droplets”

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Molecular dynamics is a powerful tool allowing us to have a direct in-sight into the microscopic motion of atoms. Thanks to statistical mechanics and non-equilibrium transport relations, properties such as diffusivity, viscosity or friction can be computed. We show that macroscopic irreversible phenomena such as friction and viscous dissipation are already present at mesoscopic scales, hence bridging the gap between microscale and macroscopic scales. Two case studies are presented: (1) Nanotube systems: multi-walled nanotubes are promising candidates for mechanical parts of nanomachines. Experiments show that systems such as oscillators or rotational axis at the nanoscale are feasible. However, an important practical aspect is the energy dissipation which can cause rapid increase of temperature and thus hinder the efficiency of the device. A study of the dynamics and friction in double-walled nanotube is presented. (2) Microfluidics: lab-on-a-chip technologies permit to process fluids at the picoliter scale. As a consequence the flow control is highly increased and important practical and economic benefits arise from the fact that small volumes are involved in the experiments. However, for hydrodynamic flows at the microscale the standard no-slip boundary condition fails to describe the flow of polymers, finite slip can occur at the substrate/fluid boundary. This slippage while introducing a new source of dissipation at the surface decreases dissipation in the volume and hence permits to have more efficient flows. In this scope, a study of driven polymer droplet on a substrate is discussed.

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SAAT 15:30'DA ÇAY SERVİSİMİZ VARDIR