

Seminář odd. 26

Tenkých vrstev a nanostruktur

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TÉMA

In silico studies of electronic current in nano-junctions: Exciting atomic motion

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In the Landauer approach to nanoscale transport the electrons are assumed to bypass a conducting junction ballistically and equilibrate through energy exchange in the electrodes. However, when passing through the junction, the current-carrying electrons has a finite, albeit small, probability to interact with the atomic vibrations (phonons) in the junction leading to local energy and momentum transfer. In the presence of a high current density this will not only lead to Joule heating: Recently a number of other mechanisms have been pointed out in which the current may excite and influence the atomic motion in nano-junctions, and possibly lead to instabilities and contact disruption. I will motivate our research and present computer simulations of the effects in atomic, molecular, and graphene-based junctions using first principles methods.

odborný garant: *Hector Vazquez, PhD.*