Seminář odd. 26
Tenkých vrstev a nanostruktur

Fyzikální ústav AVČR, Cukrovarnická 10, Praha 6

datum: 30. 9. 2018 úterý

čas: 10:00

místnost: knihovna, budova A, 1.p.

TÉMA

Tuning the graphene band gap by thermodynamic control of molecular self-assembly on graphene

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Recent interest in functionalised graphene has been motivated by the prospect of creating a two-dimensional semiconductor with a tunable band gap. Various approaches to band gap engineering have been made over the last decade, one of which is chemical functionalisation. In this work, a predictive physical model of the self-assembly of halogenated carbene layers on graphene is suggested. Self-assembly of the adsorbed layer is found to be governed by a combination of the curvature of the graphene sheet, local distortions, as introduced by molecular adsorption, and short-range intermolecular repulsion. The thermodynamics of bidental covalent molecular adsorption and the resultant electronic structure are computed using density functional theory. It is predicted that a direct band gap is opened that is tunable by varying coverages and is dependent on the ripple amplitude. This provides a mechanism for the controlled engineering of graphene's electronic structure and thus its use in semiconductor technologies.

odborný garant: *Hector Vazquez, Ph.D.*