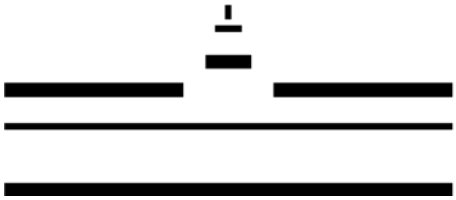

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Physikalisches Institut  Institut für Festkörpertheorie

# Integriertes Seminar

## Aktuelle Probleme dimensionsreduzierter Festkörper

Ort: Seminarraum 718 (Wilhelm-Klemm-Straße 10)

Zeit: **Mittwoch, 26.10.2016, 10:15 Uhr**

# Functionalized 2D multilayer nanosystems: structure, vibrations, optical response, bonding, and electron band engineering

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In my talk I will first briefly outline my research interests. Then I will discuss our theoretical first principles results on structure and bonding in 2D heterosystems made of monolayer, bilayers or trilayers of graphene and graphene-like materials (GLMs), specifically hexagonal boron nitride (hBN). For such atom-thick systems, stacked on top of each other and functionalized through controlled hydrogenation, the effects of electron band gap opening and tuning, as well as formation of covalently bonded multilayers have been predicted. The simulated atomic and electronic structures together with their optical response indicate that submonolayer hydrogenation of the outer surfaces of the multilayer systems of interest not only induces covalent interlayer bonds, but also offers the possibility of electron gap engineering in otherwise gapless graphene or insulating hBN. Linear and nonlinear optical and vibrational spectra were modelled for alternating graphene monolayers with insulating BN films, modified by different hydrogen coverage. Calculated structural, vibrational, electronic and optical properties of the systems of interest aim to enable in-situ noninvasive characterization of graphene based multilayers. Hydrogenated hetero-layers of graphene – incommensurate SiC film were also simulated, and their thermal stability proved. Finally, partially hydrogenated on one side graphene, with nonzero gap and covalently bonded to 3D boron nitride substrates, was considered from the same footing. The discussed results offer new opportunities in 2D microelectronics device applications, while several of our theoretical predictions have been confirmed experimentally.

Einladender: Rohlfing