TECHNISCHE UNIVERSITÄT WIEN
Vienna University of Technology

INSTITUT FÜR ANGEWANDTE PHYSIK
Institute of Applied Physics
vormals/formerly
Institut für Allgemeine Physik

Wiedner Hauptstraße 8-10/E134, 1040 Wien/Vienna, Austria – Tel: +43 1 58801 13401 / Fax: +43 1 58801 13499 – E-mail: office@iap.tuwien.ac.at / http://www.iap.tuwien.ac.at

IAP-SEMINAR

EINLADUNG

Termin: **Dienstag, 25.6.2013 um 16:00 Uhr**
Ort: **Technische Universität Wien,**
Institut für Angewandte Physik,
Seminarraum 134A, Turm B (gelbe Leitfarbe), 5. OG
1040 Wien, Wiedner Hauptstraße 8-10

Vortragender: **Dipl.-Ing. Andreas Garhofer**
TU Wien, IAP, CMS

Thema: **Ab initio studies of Graphene-Metal Interfaces**

Kurzfassung

Graphene (Gr) is a 2D allotrope of carbon with unique electronic and mechanical properties. The isolation of graphene in 2004 has led to a remarkable surge of interest in the scientific community. High quality graphene sheets can be produced via epitaxial growth on metal substrates. The Gr-metal interaction has either been classified as “weak” interaction, e.g. on Au, Ag, Cu, and Pt with merely shifted Gr pibands, or as “strong”, e.g. on Ni, Ti, and Co, with strongly perturbed graphene bands. However, the interaction of graphene with a metallic surface is still not well understood on a fundamental level. In this talk, I will present density function (DFT) theory calculations of different Grmetal interfaces. Gr/Ni(111) usually grows in 1x1 structures, because of a negligible lattice mismatch. Semi-local functionals don’t account for van der Waals forces and are not able to describe the interaction correctly, while vdW-DF functionals reproduce the benchmark calculations. Common concepts of adsorption cannot be applied to this system, as we observe strong signs of chemisorption but with adsorption energies typical for physisorption. While in free-standing graphene the formation energies for single vacancies and Stone-Wales defects are large, these defects are stabilized when a nickel substrate is present. Furthermore, the energy barriers to heal the defects are decreased significantly. Besides 1x1 structures also moiré patterns are observed for Gr/Ni(111). A new growth model of graphene on Ni(111) is presented, where surface nickel carbide plays an important part. An artificially Gr/Ni(111) system, obtained by the intercalation of 1ML Ni leads to a pronounced buckling of graphene due to locally strongly enhanced Gr-Ni interactions for specific adsorption configurations. Theweakly coupled Gr/Ir(111) configuration shows contrast inversion in STM/AFM measurements which could be assigned via DFT calculations.

Alle interessierten Kolleginnen und Kollegen sind zu diesem Seminar
(45 min mit anschließender gemeinsamer Diskussion) herzlich eingeladen.

J. Redinger e.h.
(Seminar-Chairperson)

H. Störi e.h.
(LVA-Leiter)