



**Einladung  
zum  
Seminarvortrag  
SONDERTERMIN!**

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**“Graphene Engineering: An *ab initio* Study of the Thermodynamic Stability of Epitaxial Graphene and the Surface Reconstructions of Silicon Carbide”**

SiC is a widely used substrate for the growth of mono- and few-layer graphene. By Si sublimation, large ordered areas of graphene form on the Si side as  $(6\sqrt{3} \times 6\sqrt{3}) - R30^\circ$  commensurate periodic films [1]. In experiment, a first, partially covalently attached zero layer graphene (ZLG) can be grown in a small temperature window, followed by a monolayer of graphene (MLG) at higher temperatures, and finally, few-layer graphene.

What is not *a priori* clear is whether the ZLG and MLG phases are the result of some (narrow) thermodynamic equilibrium condition, and how the substrate affects the atomic and electronic structure. Both are natural questions for theory, but a challenge for two reasons: (1) system size (up to 2800 atoms in this work) and (2) van der Waals interactions, not accounted for by most standard density functionals. We show that the ZLG and MLG phases are in fact equilibrium phases within all-electron density functional theory (DFT) including van der Waals effects. The equilibrium geometry emerges as a direct prediction, including the significant graphene layer corrugation.

By hydrogen intercalation of epitaxial graphene, the zero layer decouples from the substrate forming quasi-free-standing monolayer graphene (QFMLG) [3]. For the QFMLG, we find an adsorption height in excellent agreement with X-ray standing wave experiments, a very low buckling of the graphene layer, and a very homogeneous electron density at the interface. All these features improve the electronic properties of QFMLG compared to epitaxial graphene.

The situation on the C face of SiC is very different. Here, growing monolayer graphene films is difficult. A phase mixture of different surface phases is observed just when surface graphitization first sets in. However, the atomic structure of some of the competing surface phases as well as of the SiC-graphene interface is unknown. We compare the surface energies of the known  $(2 \times 2)$  phase with several structural models of the  $(3 \times 3)$  phase proposed in the literature [4]. We present the results of a *ab initio* random structure search and propose a new model for the  $(3 \times 3)$  reconstruction.

[1] K. V. Emtsev *et al.*, Nature Materials **8**: 203 (2009).

[2] L. Nemec, P. Rinke, V. Blum, M. Scheffler Phys. Rev. Lett. **111**: 065502 (2013).

[3] J. Sforzini, L. Nemec, T. Denig, *et al.* Phys. Rev. Lett. **114**: 106804 (2015).

[4] L. Nemec, F. Lazarevic, P. Rinke, *et al.* Phys. Rev. B: Rapid Comm, **91**: 161408 (2015).