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Gegründet im Jahre 1869 von H. Hlasiwetz, J. Loschmidt, J. Petzval und J. Stefan

EINLADUNG

zum Vortrag von

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Metal-graphene / carbon nanotubes hybrids by density functional theory

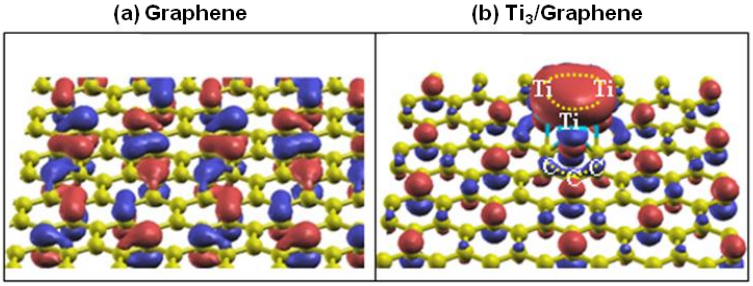
am Dienstag, 13. Juni 2017, um 17:30 Uhr

Ort: Lise-Meitner-Hörsaal, Fakultät für Physik, Universität Wien,
1090 Wien, Strudlhofgasse 4 / Boltzmanngasse 5, 1. Stock

Barrierefreier Zugang: Boltzmanngasse 5, Lift, 1. Stock rechts über den Gang zum Hintereingang des Hörsaals

Abstract:

Metallic nanostructures on graphene and Carbon Nanotubes (CNTs) have attracted considerable attention due to their potential applications in electronic nanodevices, sensors and catalysis. We report on Density Functional Theory results referring to Ti (or Cu) nanoclusters' /nanowires' decoration on graphene or CNT, and to graphene flakes on Cu substrate. For the first systems we aimed at revealing the electronic origin of the grown nanostructures which is – according to experiment - uniform for Ti, and clustering for Cu. For the second ones, we found that the shapes, orientations and edge geometries of CVD-grown graphene flakes are governed by the crystallographic directions of the Cu substrate. In particular, in case of the Cu (101) face, rectangular four-lobed, parallel-sided flakes oriented along [101] directions were formed. These findings are well reflected by DFT calculations; they revealed that due to C2p-Cu3d hybridizations, the zig-zag edge is preferentially aligned along the surface channel [101], thus reducing the lattice mismatch.



Wavefunction representation at the Fermi level demonstrating the alteration of the π C-C bonds (a) to dangling bonds on the C atoms and the charge accumulation on the supported trimmer in the (b) case.

References

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