Electronic structure of functionalized graphene@group IV/SiC interfaces.

Bachelor or Master project in the group for Computational Condensed Matter Theory – Prof. Wehling

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System

Two-dimensional materials have been the focus of active research since the first successful fabrication of graphene – a flat sheet of carbon atoms arranged in a honeycomb layer – almost 20 years ago. Due to the reduced dimensionality, these materials host many unique properties and fascinating states of matter that can be tailored for applications in technology. A flexible way of tuning the material properties is stacking different two-dimensional materials in heterostructures.

In this thesis project, you will investigate heterostructures of graphene monolayers on top of a SiC bulk substrate with an intercalated buffer layer of group IV atoms (C, Si, Ge, Sn, Pb). The interplay of the buffer layer and the graphene layer give rise to different hybdrization effects in the electronic band structure and the possibility to tune electron correlations.

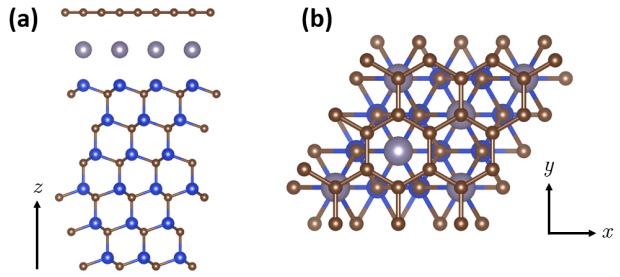

Figure 1: Schematic structure of the graphene@group IV/SiC heterostructure. Carbon atoms are brown, Silicon atoms are blue, and the group IV buffer layer is indicated by gray atoms. (a) Side view. (b) Top view.

Methodology

The aim of this project is to characterize the electronic structures of different graphene@group IV interfaces. You will use density functional theory (DFT) to investigate the influence of the atomic density of the buffer layer and positioning of the graphene layer on the band structure.

In addition, you will employ the tight-binding method to derive low-energy models that can be used to understand the origin of physical effects better. Based on these models, electronic correlation effects can be studied. The results are analyzed to explain experimental measurements and give guidance for further experiments.

Learning outcome and requirements

During the project you will learn about **density functional theory** and **tight-binding modeling** for electronic structure calculations. Additionally, the project will train you in the **usage of high-performance computing** as well as **programming in the context of data processing and visualization**. You will join an international work environment and active collaboration with experimental groups.

A good understanding of **quantum mechanics** and basic knowledge of **condensed matter physics** are helpful for successfully working on the topic.

If you are interested, please contact Niklas Witt and Prof. Tim Wehling:
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