Project 6.3. Application of ab initio calculations to determination of the electric properties of 2-D GaN-graphene systems for THz application.

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Background:

Polar GaN-graphene systems constructed from GaN polar surfaces and single- and multi-layer graphene will be investigated using ab initio modelling. GaN has two polar surfaces: gallium and nitrogen of significantly different electrical properties due to their polarity. Current technologies allow to obtain flat segments which allows to obtain an atomic flat contact surface of GaN and graphene. As a result it is possible to construct 2-D contact areas of GaN and graphene. Semiconductor surfaces are subject to a number of different changes, such as reconstruction and relaxation, and also they adsorb foreign atoms. This drastically changes their electrical properties.

Modelling of these systems will be based on knowledge of both GaN surfaces and single- and multilayer graphene layers in different stackings, including AA, ABAB, ABCABC and AA'. Ab initio calculations will be used to determine the crystallographic properties of the pure GaN-graphene contact surface for various reconstructions and also the influence of the presence of other atoms, including alien atoms. The application of methods developed in our research group will allow to obtain both crystallographic and electrical properties. In particular, potential profiles, overlap integrals, surface defect charged states and pinning of the Fermi level will be obtained. The influence of other atoms will allow to propose their use in technology of 2-DEG gas, optimal for THz systems.

Aim:

The objective is to determine basic electrical properties of the GaN-graphene system, using ab initio calculations. Electric potential profiles will be determined in the vicinity of the GaN-graphene contact surface in case of electrical contact and electrical insulation of graphene layer and GaN surface. Adsorption of hydrogen, oxygen, carbon, cesium and other atoms can dramatically change the coupling of these systems and their properties: work function, ionization energy and electron affinity.

Requirements:

- DFT simulations, data analysis experience
- Bachelor or Master degree, or relevant working experience
- written and oral communication skills in English
- experience in programming with C/C++ in a Linux environment
- knowledge of a scripting language, one of Python, Perl, bash, cs