Project 6.2. Application and development of ab initio methods for determination of the properties of surfaces and quantum structures of group III nitrides.

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Background:

1. Ab initio methods will be used to determine the physical properties of polar and non-polar surfaces of AlN, GaN and InN semiconductors. The principal physical properties of non-polar and semi-polar nitride surfaces will be determined: structure (including reconstructions), electronic properties, including Fermi level pinning and their influence on fundamental adsorption processes on these surfaces.

2. The basic properties of multiquantum wells in the size, such as used in the construction of LED, LD and HEMT devices, will be determined. The modelling will cover polar and non-polar nitride structures of pure nitrides and those based on solid solutions. Results will include: electric properties, such as field distribution, screening, and optical such as oscillator strength, probability of optical transitions, critical for applications. The results will be used mainly to simulate structures operating in the near and far UV range.

3) Programing and development of phase-amplitude functional theory, which is based on quantum mechanics equations that will solve problem of multiple electron systems with smaller computational effort than DFT theory. Reduced computational complexity will allow for the simulation of larger systems, i.e. atomic steps on crystal surfaces or large area electronic devices. The research work includes the implementation of a new method for atomic, molecular and crystal systems.

Implementation - the student chooses one or more issues.

Aim:

The aim of the project is to determine the principal physical properties of polar, non-polar and semi-polar nitride surfaces also the basic properties of multiquantum wells in the size, such as used in the construction of LED, LD and HEMT devices, will be determined. The scientific goal of the project "Phase-Amplitude Functional Theory – implementation and development" PAFT will be to construct method equations, implement them in a computer program and check the properties obtained for simple molecular systems, as well as predict the properties of optoelectronic devices such as electroluminescence LED diodes, LD laser diodes and electromagnetic radiation detectors.

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