Project 6.1. Electronic band structure calculations of nitride and oxide superlattices

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Background:
In light emitting diodes or laser diodes, it is crucial to tune the energy band gap to obtain the desired emission wavelength in a possible wide spectral range. It is realized by using as components of optoelectronic devices multiple quantum wells or superlattices, i.e., multi-layered quantum structures of the type: quantum well/quantum barrier. The light emission is tuned by adjusting the chemical composition of the quantum structure and/or layer thicknesses and consequently the band gap of the active region material.
Considering the light emission in the **deep UV** range, useful for water purification, disinfection and other medical applications, structures based on AlGaN, like GaN/AlGaN, are presently a choice. However, they suffer frequently from low efficiency due to doping problems, which limits the range of light emission. Other semiconductor systems, interesting for UV region are quantum structures based on ZnMgO in a rocksalt structure. Another, currently considered material for deep UV is less popular nitride – boron nitride, BN.
Very important is **red emission** in the context of monolithic RGB displays. Unfortunately, it is not possible up to now to get sufficient quality InGaN/GaN QWs with high In content, what limits the spectrum of emitted light to blue and green color. Another interesting possibilities are superlattices based on wurtzite CdZnO and on CdMgO in a rocksalt structure.

Aim:
Aim of the Project is to investigate by means of theoretical calculations, new solutions, structures and materials to extend the spectral span of semiconductor devices to long and short wavelengths beyond the existing ranges. The following quantum structures will be studied for this aim:

1. Al(Ga)N/BN and Ga(B)N/BN
2. Zn(Mg)O/MgO and Cd(Mg)O/MgO in a rocksalt structure

The project will bring some indications for improvement the performance of optoelectronic devices.

Requirements:
Master degree in physics or a related field and predispositions to work in theoretical or computer physics.