Abstract

Semiconducting nitride materials are crucial elements of many devices useful in both everyday life and having also some special applications. Thanks to their specific electronic structure, they are used to fabrication of Light Emitting Diodes (LED), which provide visible light from green, through blue, up to violet. They may also be employed as sources of ultraviolet (UV) and infrared (IR) radiation. Solid state solutions of InGaN materials are particularly popular. They are commonly used in energy saving light bulbs and electronic Blue-ray data storage devices.

The investigations of possible novel applications of semiconducting nitride materials are still in progress. The main goal of this project is a study of structural and electronic properties of solid solutions of semiconducting group III (AlN, GaN, InN) and rare-earth elements (ScN, YN, LaN, and LuN), as well as some mixed rare-earth nitrides by *ab initio* calculations.

Modern computational methods based on the Density Functional Theory (DFT) will be employed which allow not only to reproduce available experimental data, e.g., band gaps, but may also be the successful tool for prediction of electronic structures of materials that have not been obtained experimentally up to now.

The investigations planned here will provide novel information on the structural and electronic properties of the semiconducting materials. The acquired knowledge may suggest some possible directions for further experimental studies, of not only the entirely new systems, but also an explanation of the phenomena that have already been reported for known materials in equilibrium and under stress/strain, which is naturally present in thin films and heterostructures.