

Abstract of the thesis entitled “First-Principles Computational Studies of Semiconductor Crystals with Wurtzite and Zinc Blende Structures for Optoelectronic Applications”

The purpose of this doctoral dissertation was to investigate various polytypes of group IV and III-V semiconductors using numerical theoretical modeling. To achieve this, a wide range of computational techniques based on density functional theory (DFT) were employed. The results were analyzed and compared with the current state of knowledge. The broad spectrum of studied materials and properties allowed for the discussion of the most important chemical trends.

The first chapter provides a description of the research methodology. The DFT method was derived from the fundamental many-body Hamiltonian, and the Hohenberg-Kohn theorem and Kohn-Sham equations were presented. The key approximations used in DFT were then discussed. Finally, the kp model used in this work and the group of materials studied were briefly described.

In the second chapter, the properties of III-V semiconductors in the zinc blende and wurtzite crystal structures were investigated. Initially, physical properties such as geometric parameters, formation energy, elastic constants, and piezoelectric constants were determined. A comprehensive discussion of electronic properties, including band structures, band gaps, band splittings, and relative band positions, was conducted. Finally the influence of strain on the band structure was described.

The third chapter presents a comprehensive study of four crystallographic phases of group IV semiconductors and their binary compounds. Equilibrium geometries and bulk modulus coefficients were determined, and a previously proposed model was used to describe the stability of different polytypes. Also in this chapter significant emphasis was placed on the analysis of electronic properties, including band gaps. A review of materials was conducted with respect to their potential application in optoelectronics, considering the current state of knowledge in this field.

In the final chapter, the impact on the electronic band structure of mixing gallium nitride with various group III and V atoms was examined. For this purpose, the supercell method combined with special quasirandom structures and band structure unfolding was used. The analysis showed that substituting nitrogen with other group V atoms introduces new states in the band gap, which for the case of mixing with arsenic was experimentally confirmed. On the other hand, substituting gallium with aluminum and indium does not introduce any new states but only changes the band gap. The effect was explained by the distortion of the GaN geometry by group V atoms, attributed to differences in atomic sizes and electronegativities.