

Abstract

Electronic structure engineering of group IV crystals for optoelectronic applications
– first principles study

by

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This dissertation concerns the theoretical studies of the influence of different types of band structure engineering on electronic properties of group IV semiconducting materials. The aim is to find such systems that allow for optoelectronics applications.

Four methods to manipulate the parameters of the material were presented along with step by step procedure how to achieve and process the results of calculations to acquire necessary properties. For some specifications more detailed explanation was needed, due to difficulties in interpretation or the way of conducting the calculations. In case of each method: strains, alloying, structural changes and spacial confinement, the most important physical effects are shown along with the explanation of the mechanism. Also in the materials where the electronic properties allow to use in optoelectronics systems, the most important parameters for applications, e.g. electrons and holes mobility, are estimated.

In addition to presenting results and their analysis, the dissertation contains expanded theoretical introduction, related to all discussed problems. Also some useful derivations and proofs can be found in the Appendix attached to the thesis.