Ab-initio methods for calculating electronic structure represent an important field of material physics. The aim of this theses — within the project focused on developing the new method for calculating electronic states in non-periodic structures based on density functional theory, pseudopotentials, and finite elements methods — is to convert Kohn-Sham equations into the form suitable for discretisation, to suggest apropriate method for solving generalized eigenproblem resulting from this discretisation and to implement an eigenvalue solver (or to modify existing one).
The thesis describes a procedure for converting the many-particle Schrödinger equation into generalized rank-k-update eigenvalue problem and discusses various methods for its solution. Eigensolver Blzpack, which makes use of the block Lanczos method, has been modified, integrated into the Sfepy framework (a tool for the finite element method calculation) and resulting code has been successfully tested.