Course contents

Elementary introduction into quantum mechanics, methods of the electronic structure calculations, density functional theory, magnetism. Overview of the first-principles methods, finite temperature modeling of thermodynamic properties.
Accuracy and limitations of first-principles modeling of materials.
Overview of existing software.

Intended learning outcomes

After passing the course, the student should be able to:
Apply first-principles methods for investigation of materials and their properties;
Have some knowledge about limitations with regard to the size of the evaluated systems and the time scale;
Identify which type of materials science problem (threshold displacement energy, mechanical, kinetic etc.) that is possible to solve or can be solved by means of ab initio tools, and reach the expected precision and the reliability for ab initio modelling for different properties and materials;
Justify for and use one of the available ab initio programs, setup the structure for the corresponding ab initio modelling and select the main parameters for first principle calculations.