Computational Chemistry and Materials Modeling
Homework 4, due date is set in Canvas LMS
Topic: computational chemistry of crystals with DFT

1. Lab. Take a crystal consisting of 2-30 atoms in unit cell. Using DFT:

- Optimize geometry.
- Plot pDOS.
- Plot bands and calculate effective mass at CB minimum or VB maximum.
- Visualize charge density distribution.
- Calculate vibrational frequencies at Gamma point.
- Calculate elastic tensor and its eigenvalues.
- Estimate EoS.
- Calculate dielectric function and UV-Vis absorption spectrum.

The solution should be prepared in the form of a written report supplemented by the required technical files: cif-geometries, program run log-files, figures not inserted into the report etc. Be prepared to give a 5 min presentation of everything that you consider nontrivial in your work.

Comments to all the exercises: 1) "method" means determination of both electronic structure level and basis set; 2) Briefly explain your answers.

2. Exercise. Which method(s) you would likely use to study energy gaps in bulk semiconductors?