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

***Notes**: In multiple choice problems explain your answer. Add references if needed. Your solution must be uploaded as a single file "YourName.pdf" or "YourName.zip".*

1. **(Lab)** Take a crystal consisting at least of 2 atoms in primitive 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.

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