Computational Chemistry and Materials Modeling
Lab 3, due date is set in Canvas LMS
Topic: computational chemistry of crystals with DFT

***Notes**: Upload solution as a single file "YourName.zip". Provide absolute minimum of supporting info – no copies of work folders. Compare results with published experimental and theoretical data. Solution must be submitted as article-style report supplemented by required technical files: xyz- and cif-geometries, program run log- or out-files, extra figures etc. Be prepared to give a 5 min presentation of everything that you consider nontrivial in your work.*

Take a crystal consisting at least of 2 atoms in primitive unit cell. Using DFT:

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

Sample solution: See Lab3_silicon.zip
Sample solution: See Lab3_TiC.zip