Computational Chemistry and Materials Modeling
Lab 4, due date is set in Storion web page
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 les: 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 non trivial in your work.*

The Lab work is separated into three parts: *practical part*, which includes all calculations; one-minute *oral presentation* and *written report*.

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

- (5 %) Optimize geometry.

- (10 %) Calculate EoS.

- (5 %) Calculate vibrational frequencies at Γ point.

- (10 %) Calculate elastic tensor and its eigenvalues.

- (10 %) Visualize and analyze charge density distribution.

- (10 %) Plot PDOS

- (10 %) Plot bands and calculate effective mass at CB minimum or VB maximum

- (optional, 10%) Calculate dielectric function and UV-Vis absorption spectrum.

Oral presentation. On the day of Lab report, you have to make a 5-minute one-slide presentation with the main results of your work, which include the optimized structure of your selected crystal, PDOS, elastic properties and any interesting results, according to you.

Lab report. Using the example of Lab report, you need to make your own, which includes all the results, their analysis and names of the input files. The following points are graded:

- (20%) Analysis of the results.

- (5%) Presence of input files names.

- (5%) Appropriate grammar and vocabulary.

Total grading: Practical work (60 %) + Oral presentation (10 %) + Written report (30 %).

Sample solution: See Lab4_silicon.zip.

Sample solution: See Lab4_TiC.zip.