EXAM assignment

Lecture: Atomistic Computer Modeling of Materials (ÚFV/APMM/19)

Student: Tibor Hošík

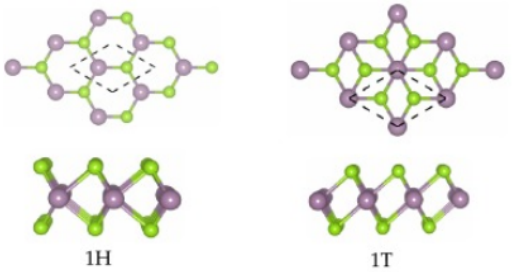
Date: May 18, 2022

Submission Deadline: June 26, 2022 via email: *martin.gmitra@upjs.sk*

Assignment:

Using density functional theory as implemented in Quantum Espresso code suite calculate ground state properties of $CrTe_2$ monolayer. To model quasi two-dimensionality of the monolayers consider separation by a vacuum at least of 12 Å in perpendicular direction. For pseudopotentials use the following provides with the assignment.

1. Find equilibrium lattice constants for both the 1T and 1H polymorphic phases. And decide which polytype is more stable.



2. Calculate ground state energy in open-shell approach, i.e., spin-polarized calculations and find differences for non-magnetic and ferromagnetic phases.

3. For the ground state phase calculate density of states and band structures along the high symmetry lines in first Brillouin zone for both the phases at equilibrium.

4. Calculate enthalpy for both the phases and discuss stability of the magnetic phase with respect to the applied pressure.

Evaluation:
- 30% construction of the input files, self-consistent field and relaxation calculations
- 20% self-consistent field calculations
- 10% calculation of density of states and electronic band structures
- 40% enthalpy calculations
- +20% bonus, online oral exam covering theory topics given on lectures, please submit the requested files 2 days before oral exam.

Submit:
- input files, output files of self-consistent field calculations
- a short text report (pdf/odt/doc) with results figures/tables demonstrating obtained results, please include as a first page this assignment.

Exam evaluation scale:
A: 100% - 90% B: 89% - 75% C: 74% - 60% D: 59% - 40% E: 39% - 20% FX: 19% - 0