EXAM assignment

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

Student: Dobromila Danková

Date: May 18, 2022

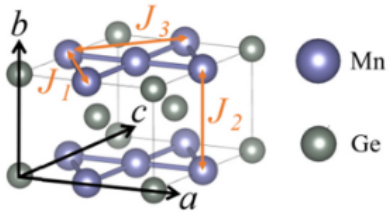
Submission Deadline: June 26, 2022 via email: *martin.gmitra@upjs.sk*

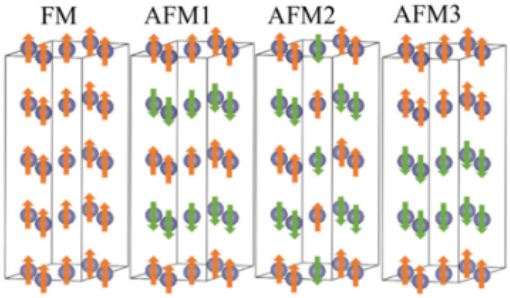
Assignment:

Using density functional theory as implemented in Quantum Espresso code suite calculate ground state properties of Kagome magnet MnGe. For pseudopotentials use the following provides with the assignment. For further structural details see reference DOI: 10.1016/j.jallcom.2022.164389.

1. Find equilibrium crystal structure.

2. Calculate ground state energies for non-magnetic, ferromagnetic and antiferromagnetic phases as show figures below and determine exchange coupling parameters J_1, J_2, and J_3.





3. Calculate density of states and electronic band structures for the lowest in energy magnetic structure.

Evaluation:

- 20% construction of the input files for self-consistent field and relaxation calculations
- 60% self-consistent field calculations and determination of exchange parameters
- 20% calculation of the density of states and electronic band structure
- +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