EXAM assignment

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

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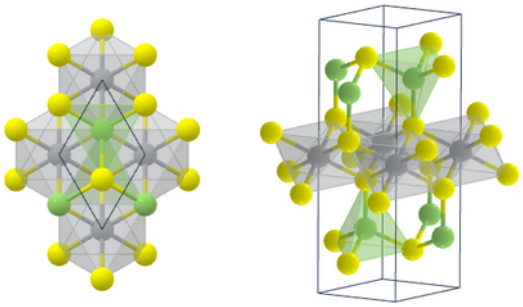
Date: May 19, 2025

Submission Deadline: June 25, 2025 via email: *martin.gmitra@upjs.sk*

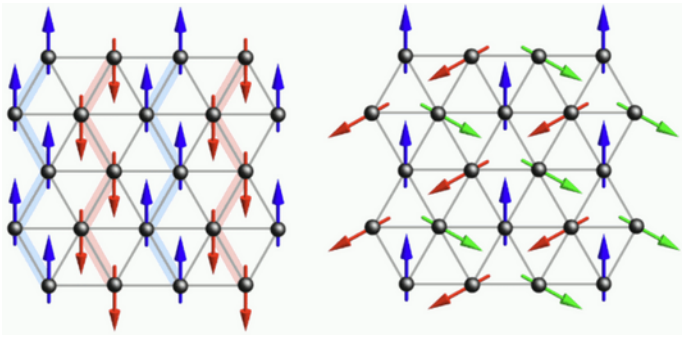
Assignment:
Using density functional theory as implemented in Quantum Espresso code calculate ground state electronic and magnetic properties of $NiGa_2S_4$ monolayer extracted from the bulk crystal structure with space group $P\bar{3}m1$. For vacuum in perpendicular direction to the monolayer use about 12 Å. For crystal structure details see:



https://next-gen.materialsproject.org/materials/mp-6959?formula=NiGa2S4

For pseudopotentials use ONCV norm-conserving pseudopotentials.

1. Find equilibrium atomic configurations for the given structure and non-magnetic phase, and calculate band structure for along the $\Gamma - K - M - \Gamma$ points in 1st Brullouin zone.
2. Perform self-consistent calculations for collinear ferromagnetic phase, calculate band structure and compare it with the nonmagnetic case.
3. Calculate total energy of the collinear antiferromagnetic order and Neel 120° order for Ni atoms



4. Determine the exchange coupling parameters between nearest and next-nearest Ni atoms on the triangular lattice from the total energy approach considering the collinear ferromagnetic and antiferromagnetic, and 120° Neel phase.

Evaluation:
- 20% construction of the input files and structure relaxation
- 20% calculations of electronic band structures
- 30% determination of the magnetic ground state energy
- 30% calculation of the exchange parameters
- +20% bonus, oral exam covering theory topics given on lectures

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 at the beginning this assignment.

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

Further reading:

S. Nakatsuji, et al., Science 309, 1697 (2005), DOI: 10.1126/science.1114727
E. M. Stoudenmire et al., Phys. Rev. B 79, 214436 (2009), DOI: 0.1103/PhysRevB.79.214436
J. Victorin et al., Sci. Rep. 14, 28040 (2024), DOI: 10.1038/s41598-024-77804-w