EXAM assignment

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

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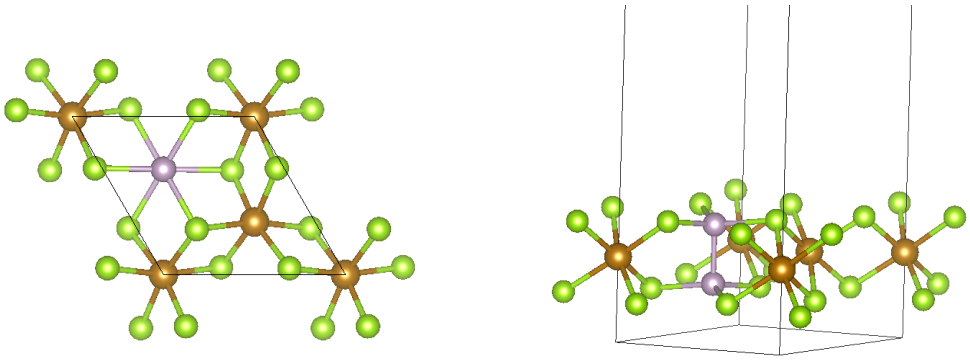
Submission Deadline: June 24, 2024 via email: *martin.gmitra@upjs.sk*

Assignment:
Using density functional theory as implemented in Quantum Espresso code suite calculate ground state electronic and magnetic properties of Ising-type monolayer $FePS_3$ extracted from the bulk crystal structure with space group $R\bar{3}$. For vacuum use about 15 Å. For crystal structure details see: https://next-gen.materialsproject.org/materials/mp-2928. For pseudopotentials use ONCV norm-conserving pseudopotentials.



1. Find equilibrium atomic configurations for the given lattice.

2. Determine the magnetic ground-state, considering collinear magnetic calculations and ferromagnetic and antiferromagnetic orders on Fe atoms.

3. Determine the exchange coupling parameters from total energy approach considering nearest Fe atoms only.

4. Calculate density of states and band structures along the high symmetry lines in the first Brillouin zone for both the the magnetic states.

Evaluation:
- 20% construction of the input files and structure relaxation
- 20% determination of the magnetic ground state
- 30% calculation of the exchange parameters
- 30% calculations of density of states and electronic band structures
- +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 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