EXAM assignment

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

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Date: May 28, 2023

Submission Deadline: June 23, 2023 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 MnF_2. For further structural reference see DOI: 10.1103/PhysRevB.102.014422. For pseudopotentials use the one provided with the assignment.

1. Perform self-consistent field calculations for non-magnetic, ferromagnetic, and antiferromagnetic Mn spin moment orientation. Determine the magnetic ground state configuration.

2. Calculate band structures along the high symmetry lines in the first Brillouin zone and density of states for all the three magnetic configurations.

3. Estimate the exchange parameter J_1 between the nearest neighbor Mn atoms and Curie critical temperature in mean-field approximation.

4. Calculate J_2 exchange parameter between the next-nearest neighbor Mn atoms.

Evaluation:

- 20% construction of the input files for self-consistent field calculations
- 40% calculations of density of states and electronic band structures
- 20% calculations of J_1-parameter
- 20% calculations of J_2-parameter
- +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