EXAM assignment

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

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Date: May 21, 2024

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

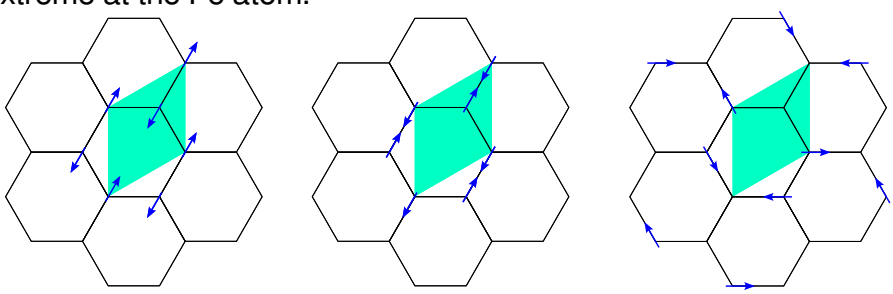
Assignment:
Using density functional theory as implemented in Quantum Espresso code suite calculate ground state electronic and structural properties of a monolayer FeI_2 extracted from the bulk crystal structure with space group $P\bar{3}m1$ and Wyckoff positions 1a for Fe, and 2d for I atom. Crystal structure details here: https://next-gen.materialsproject.org/materials/mp-571122
For pseudopotentials use ONCV norm-conserving pseudopotentials.

1. Find equilibrium atomic configurations and lattice parameters for the monolayer. Determine the magnetic ground-state.

2. Calculate density of states and band structures along the high symmetry lines in first Brillouin zone for the magnetic ground state. Discuss role of the Hubbard U parameter.

3. Perform wannierization and calculate exchange parameters using tb2j package for the ferromagnetic ground state. Consider spin-orbit coupling and find Dzyaloshinkii-Moriya parameters.

4. Consider three structural deformations of iodine atoms shown below. Assume shifts of about 0.2 Å depicted by the blue arrows. Investigate possible stabilization of the deformations by an applied perpendicular electric field to the monolayer plane with a ramp extreme at the Fe atom.



Evaluation:
- 20% construction of the input files for self-consistent field calculations
- 40% calculations of density of states and electronic band structures, Hubbard U
- 40% wannierization and calculations of exchange interactions
- +20% bonus, electric field stabilization, 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