EXAM assignment

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

Student: Dominik Husz

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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 structural properties of Lithium Chloride. For further reference see DOI: 10.1002/zaac.200900357. For pseudopotentials use the one provided with the assignment.

1. Find equilibrium atomic configurations and lattice parameters for $\alpha-$LiCl (rock-salt structure) and $\beta-$LiCl (wurtzite structure).

2. Calculate density of states and band structures along the high symmetry lines in first Brillouin zone for the equilibrium structures.

3. Calculate cohesive energies for $\alpha-$LiCl and $\beta-$LiCl, and enthalpy. Find pressure induced transition between the two structural phases.

Evaluation:
- 20% construction of the input files for self-consistent field calculations
- 40% finding equilibrium structures
- 20% calculations of density of states and electronic band structures
- 20% calculations of cohesive and ethalpy
- +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