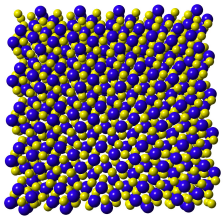
NTNU TAMPERE UNIVERSITY OF TECHNOLOGY

DFT SIMULATIONS OF DYSPROSIUM SULPHIDE FILMS



MOTIVATION:

Interfaces offer a unique playground for exploring novel concepts in physics. For example, electrons spin at the interface between magnetic materials and materials with strong spin-orbit coupling must satisfy the two sets of "rules" enforced by the two classes of materials. It is therefore interesting to create, measure and understand the spintronic/electronic properties of such interfaces. Our experimental actives at NTNU have therefore focussed on the growth and characterisation of highly magnetic Dy compounds (Dy_2S_3 and Dy_2O_3) on the prototypical spin-orbit coupled semiconductor MoS_2.

From the theoretical side, rare-earth elements are known to be pathological cases for the standard Density Functional Theory (DFT) approaches due to the partially occupied 4f or 5f shells (electronic bands) which are not described correctly. Our first goal is to test the most straightforward extensions (corrections) of the DFT methods in the context of crystalline Dy_2S_3 and Dy_2O_3 compounds. Once a satisfactory approach is found, we will perform DFT simulations for Dy_xS_y thin-film model geometries on MoS_2 to provide insight for the experiments. Our primary interest lies in the atomic structure and energetics at this stage, but we shall also focus on the details in electronic band structure.

WHAT THE STUDENT WILL DO IN THE PROJECT:

The student will study profoundly the DFT methodology. He/She will perform benchmark DFT simulations for crystalline Dy sulphides and oxides with different DFT approaches (U-parameter, hybrid functionals). The best method will be applied for Dy_xS_y thin-film model structures on MoS_2 support. The DFT simulations will be performed on local supercomputers using an existing code (VASP). The generation of model thin-film geometries will require using modelling tools and/or scripts. Input to the simulations will come from close experimental collaboration with other researchers and students working at IFY (Condensed Matter section).

REQUIRED FROM THE STUDENT:

Background in materials physics (solid state physics), and interest in materials science will be an advantage. We need a student interested in modelling and programming, and working independently in a larger group of scientists. An interest in using and developing simulation tools is required. Experience with C++ or Python is essential. Previous knowledge with the basics of DFT will provide a good starting point for further learning.

OTHER ASPECTS:

The experimental group by Prof. Justin Wells has been working for some time on the growth of Dy sulphide and oxide thin films on MoS_2. A wealth of chemical characterisation data exists, and additional data on the crystal structure and electronic structure is currently being collected. An opportunity for the student to be involved in some of the experimental activities is also possible.

Within this field there are possibilities for a summer job. This topic is closely related with the other research projects in the Condensed Matter section and TEM Gemini Centre. As part of the initial DFT training, the student will visit theory collaborators in the Tampere University of Technology, Finland (Prof. Akola's previous group).

CONTACT PERSONS:

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