



DFT SIMULATIONS OF AMORPHOUS SELENIUM FILMS



MOTIVATION:

The structural trends of group-16 elements (valence configuration ns^2np^4) have been discussed for many years. The stable forms show a systematic change from diatomic molecules (O) through rings, chains, and helices (S, Se, Te) to the only simple cubic lattice found in an element (Po). Single bonds become stronger with respect to double bonds from O to Te, and there is a parallel change in the electrical properties from insulator to semiconductor to metal, even in the liquid state, where Se is a semiconductor and Te is a metal. We have applied Density Functional Theory (DFT) approaches for chalcogenide materials (including Te) in the past, and we shall investigate amorphous Se films next. Experimentally, it has been observed that melt-quenched and vapour deposited amorphous samples exhibit different physical properties, and we wish to elucidate the origin of this behaviour by preparing similar atomic structures *in silico*. Presumably, chain formation of two-fold coordinated atoms is the key property to monitor, and it may be sensitive to the applied DFT exchange-correlation functional.

WHAT THE STUDENT WILL DO IN THE PROJECT:

The student will study profoundly the DFT methodology. He/She will perform benchmark DFT simulations for liquid and amorphous Se with different DFT exchange-correlation functionals. Also crystalline structures will be optimized for reference. The DFT simulations will be performed on local supercomputers using an existing code (VASP), and we shall test several popular and/or new exchange-correlation functionals. The results will complement the DFT simulation activities on larger samples in the Tampere University of Technology (Finland) and Forschungszentrum Jülich (Germany) by theory collaborators (CPMD code, IBM Blue Gene).

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:

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 DFT training, the student may visit theory collaborators in the Tampere University of Technology and/or Forschungszentrum Jülich.

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