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Methods to calculate the corresponding neutron scattering length density from spin-polarised density functional theory

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Spin polarised density functional theory can predict the magnetic moment and arrangement of spins in a crystal structure from ab initio calculations. We will present DFT calculations on transition metal doped SnTe, predicting the size of the magnetic moment for Fe,Cr, V, Ti dopants.
Once the size and spatial distribution of the magnetic moments is known from DFT, it is straightforward to calculate the neutron scattering length density, which is the measurable in polarised neutron reflectometry experiments. To achieve this, we will present a simple Python-based procedure that converts the output files from Quantum Expresso and VASP into the corresponding neutron scattering length density.

Topics

Neutron Instruments and Techniques

Primary author(s) : Mrs SHABBIR, Syeda Amina; Dr DAVID, Cortie

Presenter(s) : Mrs SHABBIR, Syeda Amina; Dr DAVID, Cortie

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