TlXSe2 Report

Nosenko A.

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Contents

Chapter 1

Computational details

All computations have been performed using the Vienna Ab Initio Software Package (VASP) version 5.4.4.pl2. PBE parametrization of GGA functional was used within a projector-augmented-wave scheme taken from the standard VASP PAW library.

There are some problems with the calculation of f-electrons. This is not a VASP problem, this is a DFT problem in general. Therefore, the potential in which the f-electrons are included in the core was chosen for the calculation

The density of states for both materials was performed with cutoff energy set to 700 eV with Gamma-centred k-points mesh 28x28x28. Band calculation using spin-orbit coupling has been performed in the next k-path $\Gamma - T - H_2|H_0 - L - \Gamma - S_0|S_2 - F - \Gamma$ with 20 intersections.

Post-processing produced with pymatgen python library.

Chapter 2

Results

2.1 TlErSe2

Figure 2.1: dos

Figure 2.2: band

Figure 2.3: band + dos

2.2 TlTmSe2

Figure 2.4: dos

Figure 2.5: band

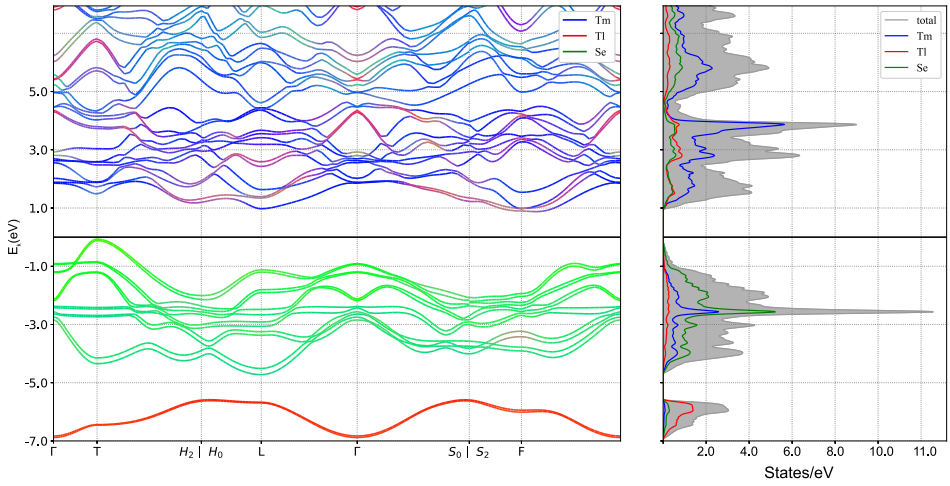

Figure 2.6: band + dos