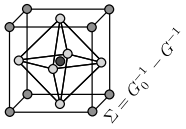
Goethe-Universität Frankfurt
Fachbereich Physik

Institut für Theoretische Physik
Dr. Harald O. Jeschke
Daniel Guterding

Computational Methods in Solid State Theory SS2016



Frankfurt, April 29, 2015

Exercise Set 2

(Due date: Monday, May 16, 2015)

Exercise 2 (**DFT calculation and tight binding fit**) (10 points)

Linarite [$PbCuSO_4(OH)_2$] is a magnetically ordered insulator. It crystallizes in the monoclinic space group $P2_1/m$ (No. 11) with lattice parameters $a = 9.682$ Å, $b = 5.646$ Å, $c = 4.683$ Å, $\alpha = \gamma = 90°$ and $\beta = 102.65°$. The Wyckoff positions are:

Atom	x	y	z
Pb	0.34162	0.25	0.32922
Cu	0	0	0
S	0.66924	0.25	0.11596
O1	0.52562	0.25	0.93314
O2	0.66352	0.25	0.42794
O3	0.25351	0.53644	0.94203
O4	0.96662	0.25	0.71304
O5	0.09532	0.25	0.26983
H1	0.86674	0.25	0.61668
H2	0.05864	0.25	0.45377

	red. coord.	FPLO coord.
D	(0, 1/2, 1/2)	(0.23202, 0.85742, 1.03374)
B	(0, 0, 1/2)	(0.23202, 0, 1.03374)
Z	(0, 1/2, 0)	(0, 0.85742, 0)
Y	(1/2, 0, 0)	(0.51244, 0, 0)

a) Compose the cif file for linarite and visualize it (for example using VESTA).

b) Prepare an FPLO (Full-potential local-orbital minimum basis code) input file and calculate the bandstructure on the path $D - B - \Gamma - Z - D - \Gamma - Y$. Find the main orbital character of the two bands crossing the Fermi level.

Remark: The location of these k-points in reduced and FPLO coordinates is different. Both notations are given in the above table. In some monoclinic space groups the labelling of high-symmetry points can be different from what one would expect.

c) Write a program that fits the two bands crossing the Fermi level with a TB dispersion using an onsite energy and four hopping paramters t_i, $i = 1, 2, 3, 4$. Suitable optimization methods can be found in the `scipy.optimize` module of the Python programming language.

d) Calculate the density of states (DOS) from the DFT code.

e) Calculate the DOS for the tight binding Hamiltonian and compare it to the one calculated from the DFT code.