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Exercises for Computational Methods in Solid State Theory
SS 2014

Exercise Set 2

(Due date: Monday, May 11, 2014)

Exercise 2 (**Density functional theory calculation and tight binding fit**) (10 points)

$Sr_2CuO_2Cl_2$ is an antiferromagnetic Mott insulator. It crystallizes in the tetragonal space group $\mathrm{I}4/\mathtt{mmm}$ (No. 139) with lattice parameters $\mathtt{a} = 3.9716$ Å and $\mathtt{c} = 15.6126$ Å. The Wyckoff positions are:

Atom	x	y	z
Sr	0	0	0.39259
Cu	0	0	0
O	0	1/2	0
Cl	0	0	0.18309

a) Compose the cif file of $Sr_2CuO_2Cl_2$ and visualize it (for example using VESTA).

b) Prepare an FPLO (Full-potential local-orbital minimum basis code) input file and calculate bandstructure and density of states (DOS). Find the main orbital character of the single band crossing the Fermi level.

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

d) Calculate the density of states (DOS) for the tight binding Hamiltonian and compare it to the one calculated by the DFT code.