Goethe-Universität Frankfurt
Fachbereich Physik

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

GOETHE UNIVERSITÄT FRANKFURT AM MAIN

Frankfurt, April 28, 2015

Exercises for Computational Methods in Solid State Theory
SS 2015

Exercise Set 2

(Due date: Monday, May 11, 2015)

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.