

Frankfurt, April 24, 2012

Exercises for Computational Methods in Solid State Theory
SS 2012

Exercise Set 2

(Due date: Monday, May 7, 2012)

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

(1) $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ is an antiferromagnetic Mott insulator. It crystallizes in the tetragonal space group $I4/mmm$ (No. 139) with lattice parameters $a = 3.9716 \text{ \AA}$ and $c = 15.6126 \text{ \AA}$. 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

- Compose the cif file of $\text{Sr}_2\text{CuO}_2\text{Cl}_2$ and visualize it (for example using vesta).
- Prepare an FPLO (Full-potential local-orbital minimum basis code) input file and calculate bandstructure and density of states (DOS). Find the main character of the single band crossing the Fermi level.
- Write a program that fits the band crossing the Fermi level with a TB dispersion using an onsite energy and three hopping parameters t_i , $i = 1, 2, 3$. The fit can for example be done with the help of the conjugate gradient method.
- Calculate the density of states (DOS) for the tight binding Hamiltonian and compare it to the one calculated by the DFT code.