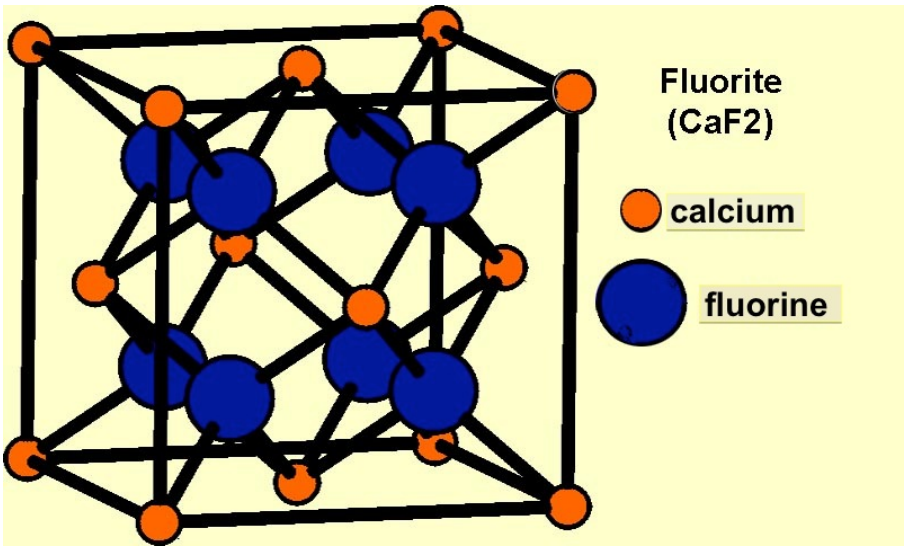
Condensed Matter Physics I
final written test
academic year 2017/2018
January 22, 2018

(*Time: 3 hours*)

NOTE:
Give all the steps necessary to understand in detail the solution procedure. Answers with the final result only or with insufficient details will not be considered valid.

Exercise 1: *Crystalline lattices*



With reference to the figure above, and using a, the side of the unit cube, as the length unit, find:

1. the type of lattice and the primitive lattice vectors
2. the number, type and position of the atoms in the basis
3. the atomic density
4. the structure factor for a generic reciprocal lattice vector
5. the specific combinations/values of reciprocal lattice vectors that reduce the general formula of the structure factor to simpler expressions, and write such expressions (consider always different form factors for Ca and F)

Exercise 2: *Free electron energies*

1. Show that for a 2D simple square lattice the kinetic energy of a free electron at a corner of the first Brillouin zone is higher than that of an electron at the midpoint of a side face of the zone (i.e., center of a Bragg plane) by a factor of 2.

2. What is the corresponding factor for a 3D simple cubic lattice?

3. What would this last result imply concerning the insulating or metallic behaviour of 3D divalent elemental solids?

Exercise 3: *Tight binding in 1D*

1. Give the explicit expression of the tight-binding s-band E(k) for a 1D lattice of spacing a, including only the nearest-neighbor hopping term $\gamma(R_{NN})$ and neglecting all the overlap integrals $\alpha(R)$ terms. Draw it out in the first Brillouin zone ($-\pi$/a, $+\pi$/a), assuming that the original atomic level position is at -6 eV, that the on-site potential integral is $\beta = 1$ eV and $\gamma(R_{NN}) = 1.5$ eV. *(Note: the definition of hopping and overlap integrals used here follows the text book, Ashcroft-Mermin)*

2. Write E(k) upon inclusion of next-nearest-neighbor hopping integral $\gamma(R_{NNN})= 0.5$ eV.

3. Write E(k) upon further inclusion of nearest-neighbor overlap integral $\alpha(R) = 0.2$.

4. Draw the band in the three different approximations in the same plot.