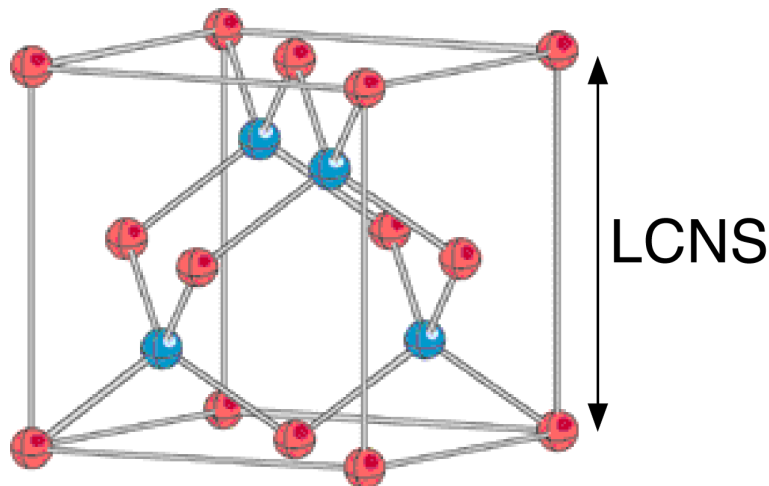


## PHYS516 ASSIGNMENT 5—TIGHT BINDING MODEL OF ELECTRONIC STRUCTURES

**Due: Wednesday, March 23, 2016**

In this assignment, you will calculate the electronic structure of a small crystal of silicon atoms, based on the tight binding model explained in the lecture.

To set up the atomic coordinates in a Si cluster, use the function `InitConf()` in the program `tb_util.c` at the class homepage. This function reads the numbers of crystalline unit cells, `InitUcell[0]`, `InitUcell[1]` and `InitUcell[2]`, to be repeated in the x, y and z directions, respectively. Since the cubic unit cell of Si crystal (which takes the diamond structure, see the figure below) contains 8 atoms, your crystal will consist of  $n_{\text{Atom}} = 8 \times \text{InitUcell}[0] \times \text{InitUcell}[1] \times \text{InitUcell}[2]$  atoms. In the bulk Si crystal, the lattice constant (the edge length of the cubic unit cell) is  $\text{LCNS} = 5.43 \text{ \AA} = 10.2622 \text{ atomic unit}$ .



The following lists relevant data structures.

```
int nAtom;           /* # of atoms */
double r[NMAX][3];   /* r[i][0|1|2] is the x|y|z coordinate of atom i */
```

where `NMAX` is the maximum number of atoms that can be handled with this program.

1. Write a program that sets up a  $4n_{\text{Atom}} \times 4n_{\text{Atom}}$  Hamiltonian matrix (using the s-p basis set explained in the lecture, 4 orbitals/atom  $\times n_{\text{Atom}}$  atoms) and diagonalizes it to obtain  $4n_{\text{Atom}}$  eigenenergies. (Use the periodic boundary condition, as implemented in the molecular dynamics program, `md.c`, to mimic a bulk crystal.)

To use matrix diagonalization functions in *Numerical Recipes* (given in `eigen.c` at the class homepage), you need to define a matrix and vector as follows:

```
double **h;          /* Hamiltonian matrix */
double *d;           /* Eigenvalues */
double *e;           /* Work array for matrix diagonalization */
```

Then the following code section uses the *Numerical Recipes* utility functions, `dmatrix` and `dvector`, to allocate memory to use matrix, `h[i][j]`, in the range  $1 \leq i \leq n4$  and  $1 \leq j \leq$

$n4$ , and vectors,  $d[i]$  and  $e[i]$ , in the range  $1 \leq i \leq n4$ , where  $n4 = 4 \times n_{\text{Atom}}$  is the size of the basis set.

```
n4 = 4*nAtom;
h = dmatrix(1,n4,1,n4);
d = dvector(1,n4);
e = dvector(1,n4);
```

After setting up the  $n4 \times n4$  Hamiltonian matrix, you will diagonalize it with the *Numerical Recipes* functions, `tred2` (which reduces the symmetric Hamiltonian matrix into a tridiagonal form) and `tqli` (which diagonalizes the tridiagonal matrix).

```
tred2(h,n4,d,e);
tqli(d,e,n4,h);
```

2. Choose `InitUcell[0] = InitUcell[1] = InitUcell[2] = 1` and diagonalize the resulting  $32 \times 32$  Hamiltonian matrix for three different values of lattice constant:  $LCNS = 1.8 \times 10.2622$  au,  $1.4 \times 10.2622$  au, and  $1 \times 10.2622$  au. For each lattice constant, plot the density of states defined as follows:

$$D(\varepsilon) = \sum_{v=1}^{n4} \frac{1}{\sqrt{\pi}\sigma} \exp\left(-\frac{(\varepsilon - \varepsilon_v)^2}{\sigma^2}\right)$$

where  $\sigma = 0.1$  eV  $= 0.003675$  au is the energy spread given to each energy eigenvalue,  $\varepsilon_v$ , to obtain a smooth density-of-states curve. Plot  $D(\varepsilon)$  vs.  $\varepsilon$  and discuss the effect of lattice constant on the density of states.

3. Choose `InitUcell[0] = InitUcell[1] = InitUcell[2] = 2` ( $n_{\text{Atom}} = 8 \times 2^3 = 64$ ), diagonalize the resulting  $256 \times 256$  Hamiltonian matrix for  $LCNS = 10.2622$  au, and plot the density-of-states  $D(\varepsilon)$  vs.  $\varepsilon$ . How does this density of states differ from the one with the same lattice constant calculated above for 8 atoms?
4. Consider the eigenenergies for 64 atoms and the bulk Si lattice constant,  $LCNS = 1 \times 10.2622$  au. Determine the Fermi distribution,

$$f(\varepsilon_v) = \frac{2}{\exp((\varepsilon_v - \mu)/T) + 1},$$

for all the 256 eigenenergies, where  $T = 0.2$  eV/ $k_B$  ( $k_B$  is the Boltzmann constant)  $= 0.2 \times 11604.5$  K  $= 2320.9$  K is the temperature and  $\mu$  is the chemical potential to satisfy

$$\sum_v f(\varepsilon_v) = 4N = 256.$$

(Note that there are 4 valence electrons from each of the 64 Si atoms). Plot  $f(\varepsilon_v)$  vs.  $\varepsilon_v$ .