Problem 3: Band structure of Arsenic

Elemental arsenic is a metal with a rhombohedral unit cell and two atoms per cell. In this exercise we plot the electronic band structure of metallic arsenic using the empirical pseudopotential method of Cohen and Bergstresser (CB).

The arsenic structure can be described in comparison with the diamond structure. Starting from the fcc lattice of diamond where the side of the conventional cubic cell is a_{fcc} and stretching the cube along a diagonal we obtain a rhombohedral lattice described by the primitive vectors:

$$\begin{aligned} \mathbf{a}_1 &= a_0(\epsilon, 1, 1), \\ \mathbf{a}_2 &= a_0(1, \epsilon, 1), \\ \mathbf{a}_3 &= a_0(1, 1, \epsilon). \end{aligned}$$

When $\epsilon = 0$ and $a_0 = a_{fcc}/2$ we have the fcc lattice of diamond. In arsenic $\epsilon \neq 0$ and $a_0 = 5.510$ a.u.. The positions of the atoms in the unit cell are $\mathbf{d}_{1,2} = \pm u\mathbf{d}$ where $\mathbf{d} = \mathbf{a}_1 + \mathbf{a}_2 + \mathbf{a}_3$. In diamond $u = 1/8$ while in arsenic $u = 0.226$.

In order to apply the empirical pseudopotential method we need the form factors for arbitrary values of the reciprocal lattice vectors $|\mathbf{G}|^2$ and we can use the function:

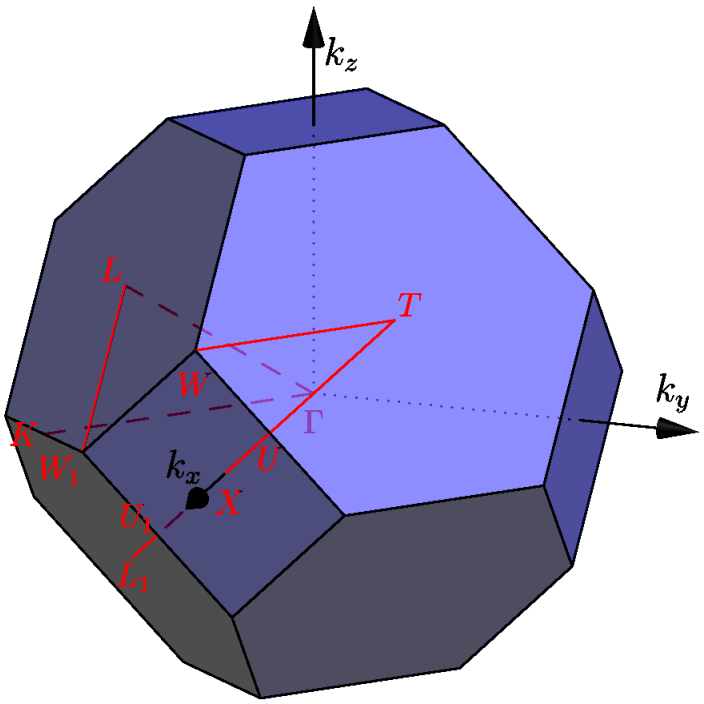
$$U(|\mathbf{G}|^2) = \frac{A_1(|\mathbf{G}|^2 - A_2)}{e^{A_3(|\mathbf{G}|^2 - A_4)} + 1} \tag{1}$$

with $A_1 = 0.0655$, $A_2 = 2.78$, $A_3 = 2.38$, $A_4 = 3.70$. With these values of the parameters and $\mathbf{G}$ in atomic units (1/bohr) the form factors are in Hartree.

1. Determine the value of ϵ using the experimental value of the angle between two direct lattice vectors: $\alpha = 54.167°$.

2. Modify the CB program in order to use Eq. 1 and to introduce the positions of the atoms inside the unit cell of arsenic.

3. Modify the CB program and generate the reciprocal lattice vectors of the rhombohedral lattice of arsenic. The Brillouin zone of this lattice is shown in the figure. Find the coordinates of the points Γ, X, L, L_1, T, W, W_1 U, U_1 and K:



(Hint: The coordinates of each vertex of the BZ can be determined analytically as the solution of a 3×3 linear system, but you can also solve the linear system numerically using, for instance, the `Lapack` routine `DGESV`).

4. Show that only the hexagonal faces perpendicular to the vector $(1, 1, 1)$ are regular, the sides of the other hexagonal faces have two different lengths that are also the sides of the six rectangles. Find these two lengths.

5. To the points found at previous point, add the point $X_1 = (0.5153, -0.5153, 0.0)$. Plot the band structure of arsenic along the lines $X_1 - K - \Gamma - T - W \equiv W_1 - L$ and along the lines $U - X - \Gamma - L_1 - U_1 \equiv U - T$.

6. An approximate value for the Fermi energy is 0.540 Ha. Put the level on the band plot and describe qualitatively the Fermi surface of arsenic.

7. Compare your bands with Fig. 2 of Phys. Rev. **137**, A871 (1965).