Problem 6: Density of electronic states and charge density of MgO

MgO is a ionic solid with the rocksalt structure (i.e. the NaCl structure). It can be described by an fcc lattice with $a = 4.21$ Å and two atoms in the unit cell:

$$\begin{aligned} \mathbf{d}_{Mg} &= a(0,0,0), \\ \mathbf{d}_{O} &= a(1/2,1/2,1/2). \end{aligned} \tag{1}$$

The form factors for Mg and O in the rocksalt structure are given in Phys. Rev. **155**, 992 (1967).

1. Modify the CB program in order to deal with the rocksalt structure of MgO and to use the form factors given in the above reference.

2. Plot the band structure of MgO and compare with Fig.2 of the above reference.

3. Modify the CB program in order to calculate the density of states of MgO. Check the convergence of your results with respect to the mesh of $\mathbf{k}$ points and of the smearing σ of the gaussian function used to represent $\delta(x)$.

4. Compute the charge density of MgO along the diagonal of the cubic cell and plot it.