

1. Determine the basis vectors of the primitive unit cell of the CuCl crystal. What Bravais lattice underlies this lattice? Specify the Cartesian coordinates of the basis vectors and all atoms inside the primitive elementary cell. Determine the space group number for the CuCl lattice (use <https://www.cryst.ehu.es/>). Calculate the volume of a primitive elementary cell.
2. Ionic chemical bond - explanation. Potential energy for ionic interaction. Long-range Coulomb attraction, formulas for calculation. Madelung constant and energy. The nature of the repulsive forces, the formula for calculation. Ionicity of the chemical bond.
3. Adiabatic approximation. Explanation and corresponding mathematical apparatus.
4. Don't forget to include the results of the VASP calculation.