- 1. Determine the basis vectors of the primitive unit cell of the GaN 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 GaN lattice (use https://www.cryst.ehu.es/). Calculate the volume of a primitive elementary cell.
- 2. Vibration of 3D lattices. Equation of motion and its solution in harmonic approximation. Dynamical matrix (explanation). Dispersion relations for frequency of vibrations. Optical and Acoustic vibrations. Calculation of energy of vibration (quantum mechanical approach).
- 3. Weak potential approximation for almost free electrons. The band-gap formation. Dependence of conducting properties of materials on the type of electron energy spectrum. Band gap width dependence on external pressure.
- 4. Don't forget to include the results of the VASP calculation.