Theoretical Methods for Simulation of Materials

Home work: Quantum Espresso

For the system assigned in the table below, compute for both phases 2H and 1T:

1- The lattice parameter and the position of the unit cell atoms after the geometry optimization.
2- The density of states.
3- The band structure.

Make brief report including inputs data, optimized cell parameters, atom position in cartesian coordinate, density of states plots, and ban structure plots. Maximum length 6 pages.

System (phases: 2H and 1T)