

DOS and PDOS of bulk silicon

- **Calculate the density of states (DOS) using the tetrahedron method**
 1. Run the SCF with pw.x
 2. Run the NSCF (tetrahedron occupations & dense grid) with pw.x
 3. DOS post-processing with dos.x
 4. Plot the DOS with gnuplot
 5. Projected DOS (PDOS) post-processing over s-orbitals and p-orbitals with projwfc.x
 6. Plot the PDOS with gnuplot for s and p orbitals.

Input files available at

https://github.com/AntimoMarrazzo/DFT_course_UniTS/tree/main/pdos