Lab 07 – Putting it all together: Aluminum

In this lab, you will repeat the major steps from the past few weeks for a new system: FCC Aluminum. A basic scf input file and pseudopotential have been provided. As you proceed through each step, look back at your previous calculations as a reference for how to edit the input files in each step.

1. **Energy cutoff convergence with respect to total energy.**
   1. Deliverables:
      1. Table showing converged energy cutoff
2. **Kpoint convergence with respect to total energy.**
   1. Deliverables:
      1. Table showing converged kpoint mesh
3. **Structure optimization – volume only**
   1. Deliverables:
      1. The relaxed final lattice constant
4. **Electronic density of states**
   1. Deliverables:
      1. A plot of the electronic DOS for Al
5. **Discussion:**
   1. For each of the four steps above, compare and contrast to your previous experience with these types of calculations. What is different about simulating a metal vs an insulator? (You might notice differences in convergence criteria, calculation time, density of states, etc…)
   2. Reflect on your progress this semester. We have developed many new skills and learned many new concepts. What are some of the skills that you are most proud of that you have developed since the start of the semester? How do you feel about your ability to perform a simulation of a new material in the future?