Lab 06 – Stability

1. **Structure Optimization and Electronic DOS of Cubic BaTiO3.**
   1. BaTiO3 undergoes a series of phase transitions, starting out at high temperatures with a cubic lattice and all atoms in high symmetry positions before gradually breaking symmetry as its temperature is lowered. It is often beneficial to use the high temperature phase as a reference for the lower temperature phases, so we will begin today by considering the cubic phase of BaTiO3.
   2. Use the “BTO.relaxHS.in” file to run a relaxation where the only degree of freedom being changed is the volume.
      1. What is the new lattice parameter?
      2. How long did your calculation take? Why does it take so much more time than an scf calculation?
      3. Try using “grep” to find the total energy from the BTO.relaxHS.out file. What do you see, and how is it different from a typical calculation?
   3. Once relaxed, use the output lattice parameter to compute the electronic density of states. This involves three steps:
      1. Run a scf calculation (BTO.dos-scf.in)
      2. Run a nscf calculation (BTO.dos-nscf.in)
      3. Prepare the dos (BTO.dos.in)
   4. Plot the density of states using python, an example script is provided.
   5. Deliverables:
      1. Electronic DOS plot
      2. Answers to all questions
2. **Structure Optimization and Electronic DOS of Tetragonal BaTiO3.**
   1. Next, we’ll look at the Tetragonal phase of BaTiO3. To do this, start by repeating your relaxation, only this time change the “cell\_dofree” to “all” and shift one of the coordinates of the Ti atom by .05, then answer the following:
      1. How long did this calculation take? How did it compare to your previous relaxation? Explain any differences.
      2. Again use “grep” to find the total energy from the BTO.relaxHS.out file. How does it compare to the previous relaxation?
      3. Provide the new lattice parameter(s) and atomic positions below:
      4. You should that the type of lattice has changed. If it was cubic before, what is it now?
   2. Next, repeat the steps to produce a density of states plot. NOTE, because of the change in lattice, you will want to change “ibrav” to 0, and add a section just above the atomic positions titled “CELL PARAMETERS”, in BOTH the scf and nscf input files. See the [QE documentation](https://www.quantum-espresso.org/Doc/INPUT_PW.html#CELL_PARAMETERS) for more information.
      1. Run a scf calculation (BTO.dos-scf.in)
      2. Run a nscf calculation (BTO.dos-nscf.in)
      3. Prepare the dos (BTO.dos.in)
   3. Plot the density of states using python.
      1. Compare and contrast the cubic DOS and the tetragonal DOS. The differences are small, but should be present. Thinking about molecular orbitals, try to explain the change(s).
   4. Deliverables:
      1. DOS plot
      2. Answers to all questions