Lab 1: Electronic structure and lattice constant of fcc diamond (MSE760)
Due date (Oct. 8, 2024)

1. build the structure of diamond (similar to fcc silicon, only different lattice constant)

2. total energy convergence as a function of k-point and wavefunction cutoff individually
for now you can use the norm conserving poseudopotentials here
(UPF format and find the carbon one-- attached also)
(http://www.quantum-simulation.org/potentials/sg15_oncv/)

You can learn how to write a script to speed up your calculations.
e.g. http://tldp.org/HOWTO/Bash-Prog-Intro-HOWTO.html

3. optimize the lattice constant by total energy fitting to Murnaghan equation of state
https://en.wikipedia.org/wiki/Murnaghan_equation_of_state

For this, you can write a Fortran code or use other programs on line for the fittings.

You can see visually if the equilibrium lattice constant/volume sits at the energy minimum of the parabolic energy surface.

4. (optional) Alternatively, you can optimize the lattice constant by varicell optimization

5. find experimental results of diamond structure and compare

6. compute band structure of diamond and compare with experimental band structure

7. compute the density of states of diamond

8. write a lab report including the details of your calculations

The information about the lab report:

1. abstract: summary of the project

2. introduction and methods

we always separate introduction and method in a real paper; but here for simplicity you can put them together

mention what method you used and computational details (e.g. kpoints, wavefunction cutoff, norm-conserving or ultrasoft posedopotential, which functional? (LDA or PBE)

See computational papers on first principles calculations as examples.

3. results and discussions

write your results in the step by step order. And put your results with pictures and tables you need.

Discuss the results you got:
e.g. the calculations converge at which parameters;

what's the fitted lattice constant and how it compared with experimental data and other computational data;

what is your band gap; it's direct or indirect; how it compares with experiments

4. conclusion
Conclude your results and mention open questions in your calculations

5. references
list the experimental and other computational references