GEO 421
Assignment #1
Due: 3 pm, Sep 21, 2023
(Please upload your homework at Canvas/Files tab)

1. (30%) VASP calculation on small molecule
Follow the example at https://www.vasp.at/wiki/index.php/H2O
a) Report the H-O distance and H-O-H angle in degree before and after relaxation
b) Examine the convergence with respect to ENCUT
Set ENCUT to different values, 200, 300, 400, 500, 600, and 700 eV. Plot internal energy of the system as a function of the ENCUT. Read the official guide on keyword ENCUT and comment on your results.

2. (40%) VASP calculation on condensed matter
a) Follow the example at https://www.vasp.at/wiki/index.php/Fcc_Si , reproduce the energy vs. lattice parameter plot.
b) Check out the official guide on the keyword ISIF (https://www.vasp.at/wiki/index.php/ISIF). Explain how you may modify the INCAR and find the lattice parameter using just one simulation. Perform the calculation and report the lattice parameter you find. Compare your result with that of a). The example at https://www.vasp.at/wiki/index.php/Cd_Si_relaxation may be helpful.

3. (30%) LAMMPS simulation
Check out LAMMPS movie gallery (https://www.lammps.org/movies.html). Find one with input script and reproduce the movie. Upload your movie and LAMMPS log file at your canvas account.