To begin, I found that I have issues trying to work with the native python (the original system python). Thus, I chose to install Anaconda and use this version of python. To do so, you can install it for Mac from the following website: <https://www.continuum.io/downloads>.

ASE

1. Find a location to install the Atomic Simulation Environment (ASE) package. You can go to the following page to look at the repository: <https://gitlab.com/ase/ase>. I suggest installing under the software directory:
   1. cd ~/software
   2. git clone <https://gitlab.com/ase/ase.git>
   3. cd ase

If you do not have git, don’t worry. You can use the following:

sudo easy\_install <software>

1. Then, we need to allow python to find ASE. Go to your home directory and we need to add location to look in the bashrc file:
   1. cd ~
   2. Edit the .bashrc file (or make one) and add these lines:

# ASE

export ASE\_PATH="$HOME/software/ase"

export PYTHONPATH="$PYTHONPATH:$ASE\_PATH"

export PATH="$PATH:$ASE\_PATH/tools"

* 1. Then, you need to re-run your bashrc file to take these changes

. .bashrc

* 1. Now, you should be able to test ASE in python. You can use either python or ipython (I suggest IPython, so much nicer….). First, lauch either
     1. python or ipython
     2. import ase

If there are no errors, you should be good to go with ASE.

ASE-Espresso

To install the Quantum Espresso plugin for ASE, we will use a Git repository located on GitHub from the following: https://github.com/marshallmcdonnell/ase-espresso

1. Go to your software directory and download the git repository:
   1. cd ~software
   2. git clone https://github.com/marshallmcdonnell/ase-espresso.git
2. Install
   1. pip install ase-espresso
3. Test installation. First, launch Python (or IPython) and try the following import:
   1. from espresso import Espresso

If no errors, ase-espresso should be installed now as well.

SnO2 ASE-Espresso examples

Now that you have these installed, you should be good to go with the SnO2 examples I have created. It is a Git repository on GitHub at the following: <https://github.com/marshallmcdonnell/sno2_ase_espresso>.

1. Go to a directory you want to download and test the project. I chose ‘projects’ as a place to use but use whatever you like:
   1. cd ~
   2. mkdir projects
   3. cd projects
   4. git clone https://github.com/marshallmcdonnell/sno2\_ase\_espresso.git
   5. cd sno2\_ase\_espresso
2. From here, you can enter the directories one by one and run the python scripts to make sure everything works. The order they should be run in is:
   1. ecut
   2. kpts
   3. surfaces

Run the scripts via python <python script which are \*.py files> <json input which are \*.json files>. Thus, for ecut the example is:

python test\_ecut\_sno2.py input.json

From here on, these scripts can be used to show how to build systems, including surfaces, and then run convergence testing for the energy cutoff (basis set size) and number of k-points for the reciprocal space integration mesh needed.