Day 4:
YALE PATHWAYS TO SCIENCE SUMMER WORKSHOP 2021

Aakash Kumar
aakash.kumar@yale.edu

Computational Materials Science: Hands-on

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

HANDS-ON SESSION

- Quantum Espresso – Software to calculate the energies of structures
- Finding the lowest-energy structure of Au, Fe and NaCl
- Lattice parameters of the lowest-energy structures and comparison with earlier experimental data

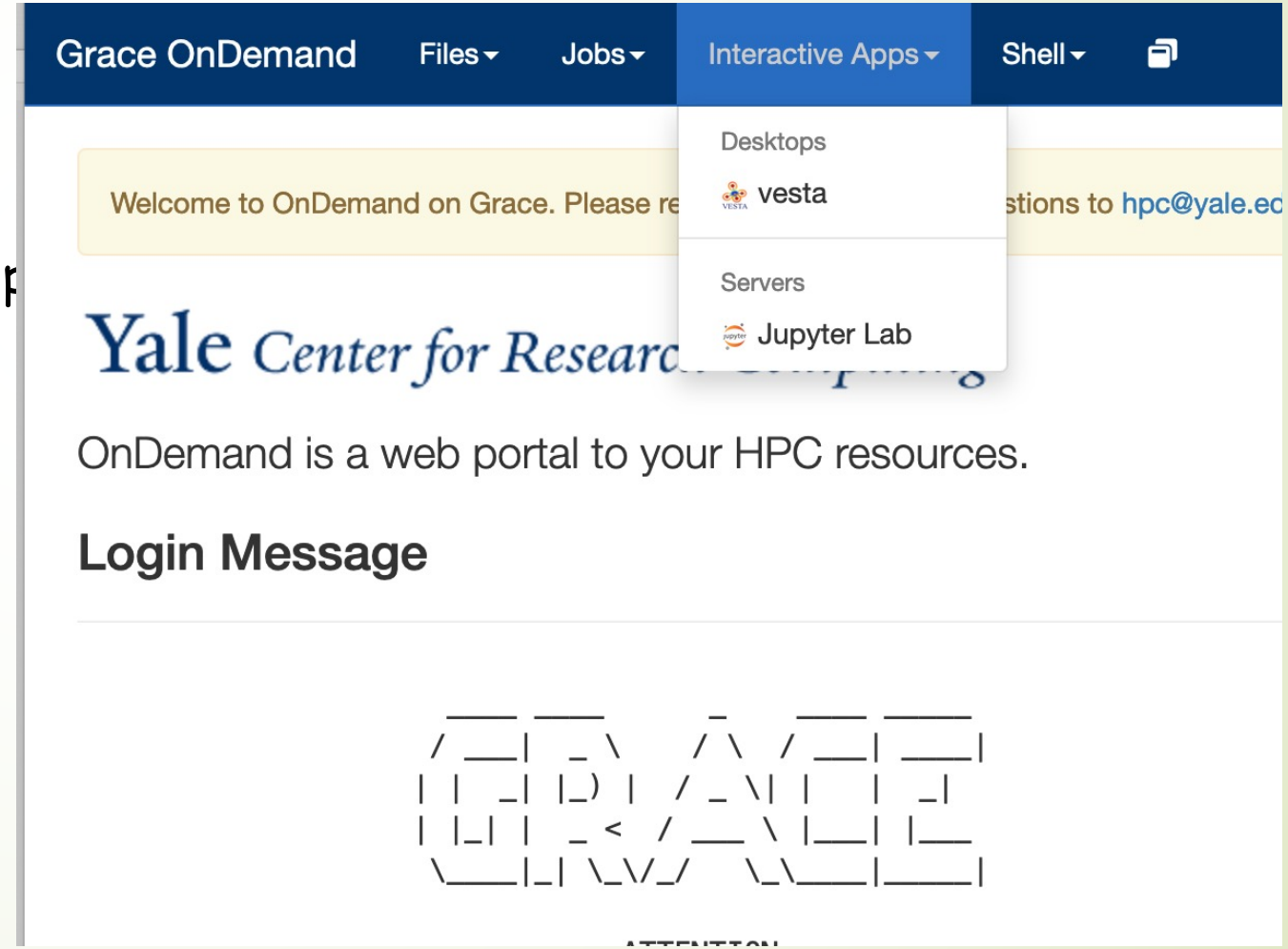
Day 4

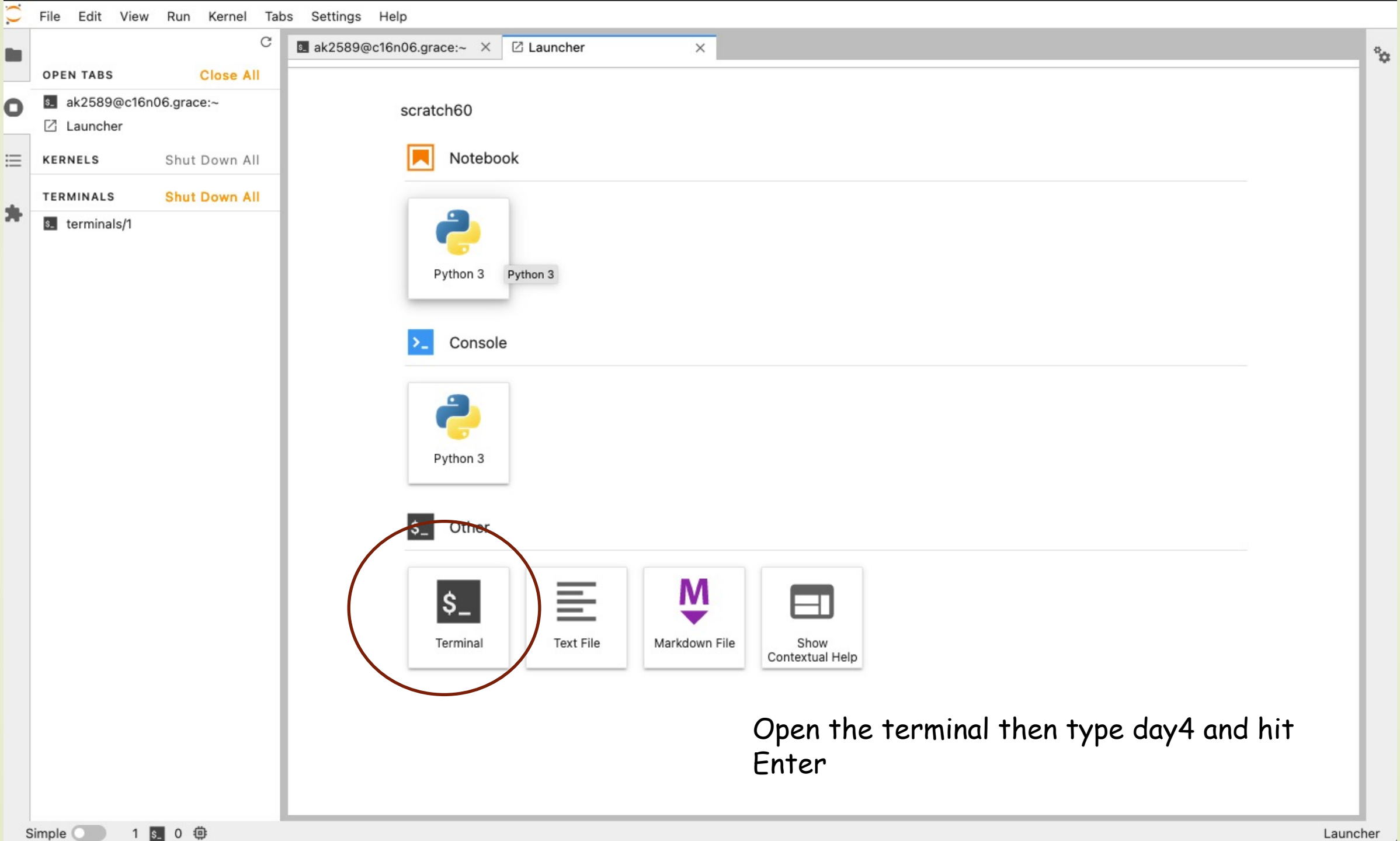
- We will use Quantum Espresso to do the energy calculations using Density Functional Theory (DFT).

Go to:

- https://pathways.ycrc.yale.edu
- Click on Jupyter Lab under interactive App

- Go to Day 4 directory inside the Pathways_workshop directory





Open the terminal then type day4 and hit Enter

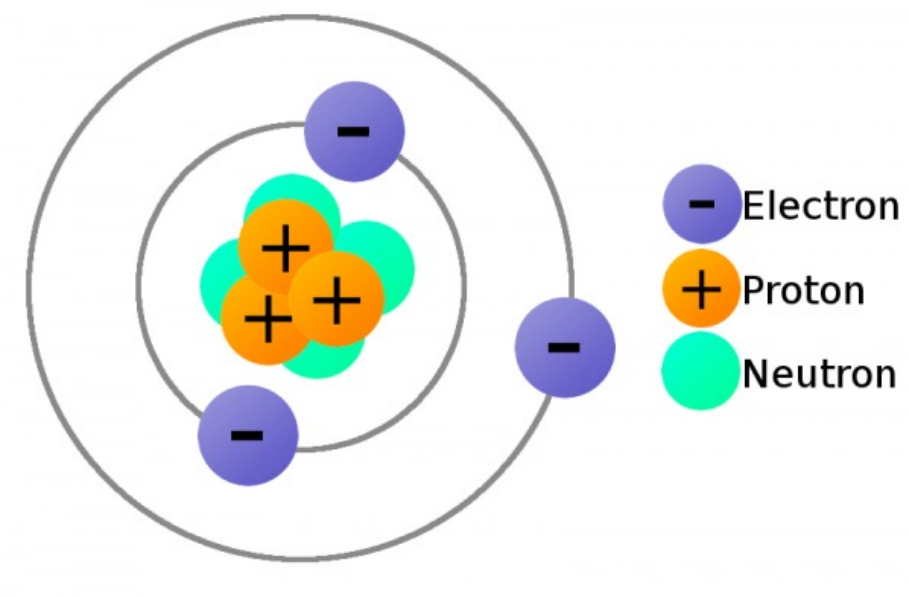
QUANTUM ESPRESSO (QE)

- Quantum Espresso is a software to calculate the energies, forces, …. of a structure made of atoms.

https://www.quantum-espresso.org/

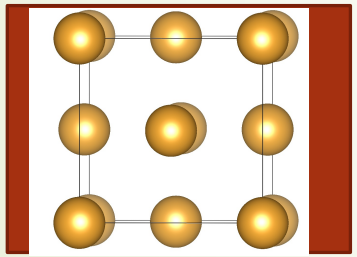
- open-source (free to use!)

- focus on valence electrons of atoms.



QE BASIC WORKFLOW

1. Provide the structure to QE
2. QE calculates the energy of the input structure based on the settings
3. Move the atoms such that the energy decreases (our goal is to find the minimum energy)
4. We continue Steps 2 and 3 until convergence is reached (energy and force on atoms don't change much)



Input structure

Quantum Espresso (QE)

pw.x

Energy

Energies, forces, lattice parameter

QE INPUT FILE

https://www.quantum-espresso.org/Doc/INPUT_PW.html

- Different sections separated by &…. /

```
&control
   prefix = 'gold'                  ! prefix for the generated files
   calculation = 'relax'            ! type of calculation, relax the atoms
   restart_mode = 'from_scratch'    ! fresh calculation
   tstress = .true.                 ! calculate the stress
   tprnfor = .true.                 ! calculate the forces
   pseudo_dir = './'                ! directory containing the potential file
   etot_conv_thr = 1.0d-4           ! energy convergence threshold
   forc_conv_thr = 1.0d-3           ! force convergence threshold
/
&system
   ntype = 1                        ! types of atoms
   nat   = 4                        ! number of atoms
   ibrav = 0                        ! related to crystal structure
   ecutwfc = 40                     ! convergence parameter
   occupations = 'smearing'
   smearing = 'gaussian'              ! settings for metals
   degauss = 5d-3
/
```

QE INPUT FILE- STRUCTURE

https://www.quantum-espresso.org/Doc/INPUT_PW.html

- Structure data includes lattice parameters and atom positions

```
CELL_PARAMETERS angstrom
4.100000   0.000000  0.000000
0.000000   4.100000  0.000000
0.000000   0.000000  4.100000
ATOMIC_SPECIES
Au 196.970 Au.potential.UPF (core electrons)
ATOMIC_POSITIONS crystal
Au  0.000000    0.00000  0.000000
Au  0.500000    0.50000  0.000000
Au  0.000000    0.50000  0.500000
Au  0.500000    0.00000  0.500000
```

- Does this look familiar?

```
Au
1.0
4.078200 0.00000 0.000000
0.000000 4.07820 0.000000
0.000000 0.00000 4.078200
Au
4
direct
0.000000 0.000000 0.000000 Au
0.500000 0.500000 0.000000 Au
0.000000 0.500000 0.500000 Au
0.500000 0.000000 0.500000 Au
```

our POSCAR file for Au

SOME CONVERGENCE TIPS

https://www.quantum-espresso.org/Doc/INPUT_PW.html

```
&system
    ….
    ecutwfc = 40                    ! increase this value systematically
    ….
/

K_POINTS automatic                  ! points to sample on the lattice
4 4 4 0 0 0                         ! increase this systematically
```

- ecutwfc is the energy cut-off of functions that we use to represent atoms
- K-points are point on the lattice where we calculate the energies

EXERCISE 1- Au

- Remember, lattice parameter

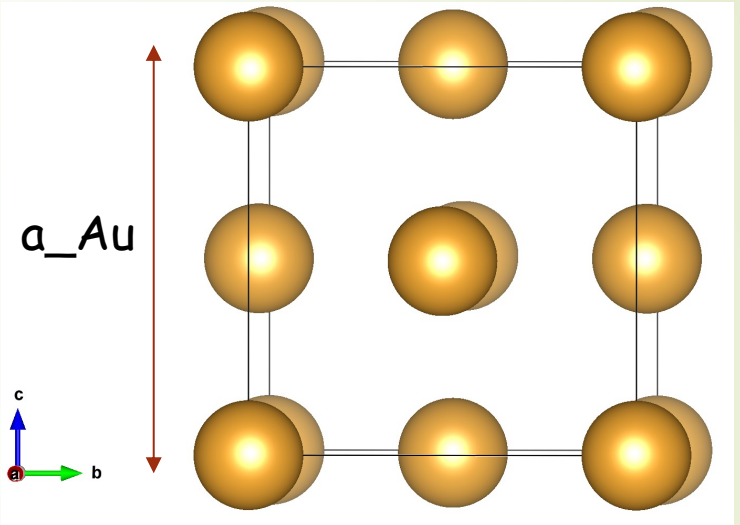
a_Au = 4.08 Å

- Here, we will change this to different values

4, 4.1, 4.2 and 4.3

- We will calculate the energy of Au structure at each

lattice parameter value using QE



EXERCISE 1- Au

- Remember, lattice parameter

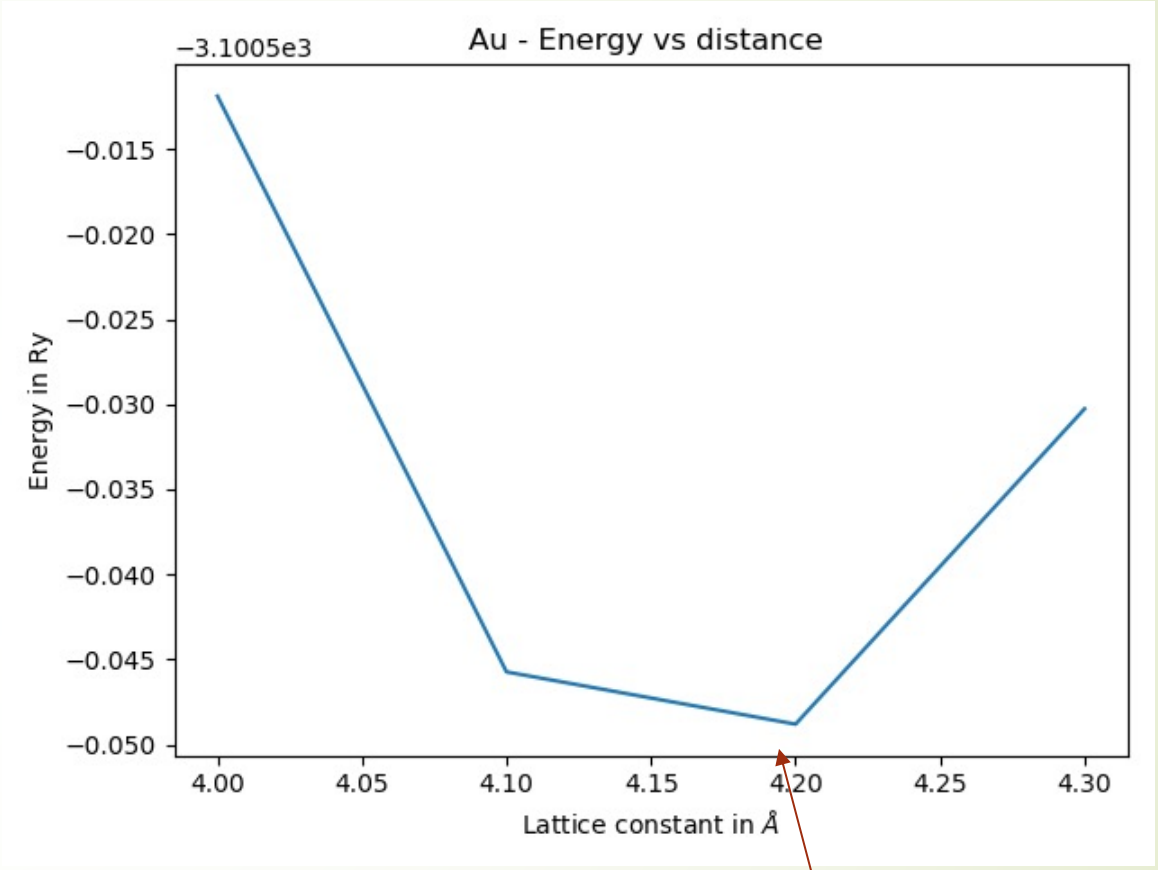
a_Au = 4.08 Å

- Here, we will change this to different values

4, 4.1, 4.2 and 4.3

- We will calculate the energy of Au structure

lattice parameter value using QE



- The lowest energy structure gives us the lattice parameter
- We can plot the energy vs distance to find the energy minimum (plt_energy_dist.py)

lowest energy -> lattice param

EXERCISE 2- Au

- The lowest energy structure gives us the lattice parameter
- We can plot the energy vs distance to find the energy mimimum

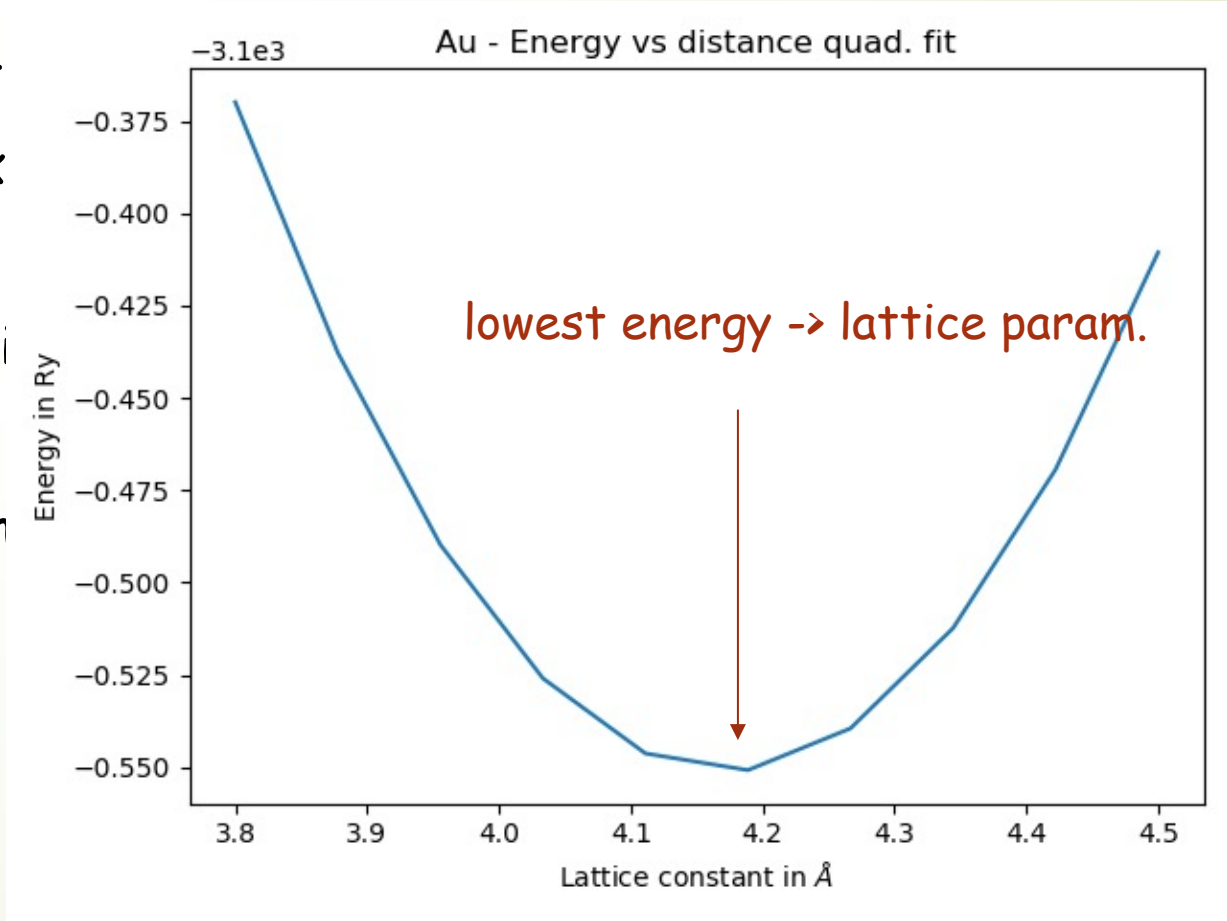
- We will learn how to use the energies to fit

$ax^2 + bx$

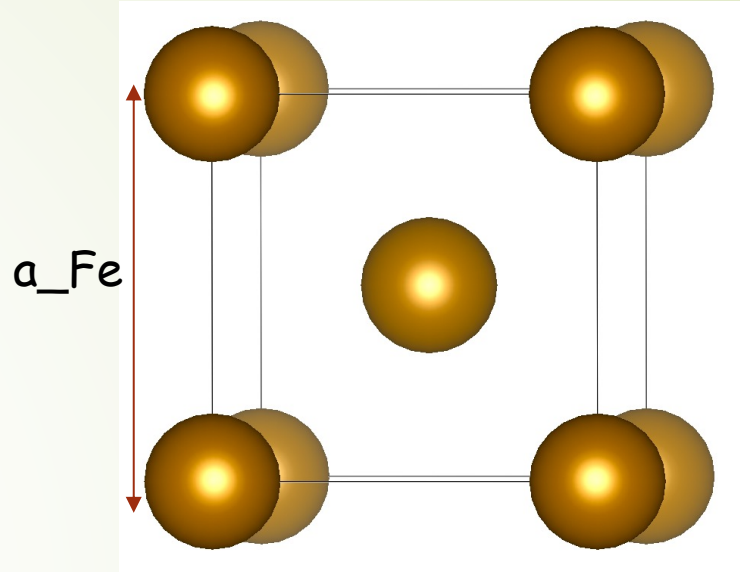
- Then, we will plot the energy vs distance usi

plt_parabola.py

- This is closer to the real energy variation ir



EXERCISE 3- Fe



- We will repeat the previous exercises for Fe
- Since for Fe, lattice parameter, a_Fe = 2.87 Å

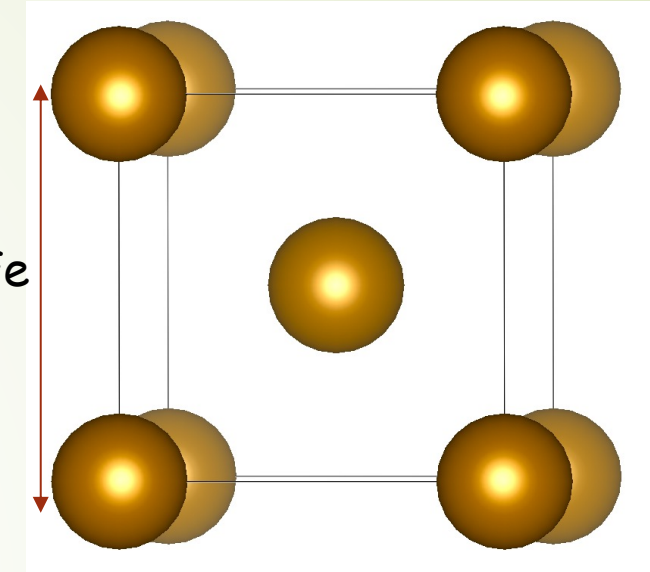
We will change this to different values

2.7, 2.8, 2.9 and 3.0

- We will calculate the energy of these structures individually using QE

- Next, we plot the energy vs distance curve using both linear and quadratic fits

EXERCISE 4- NaCl



- We will repeat the previous exercises for NaCl
- For NaCl, lattice parameter, a_NaCl = 5.64 Å

We will change this to different values

5.6, 5.7, 5.8 and 5.9

- We will calculate the energy of these structures individually using QE

- Next, we plot the energy vs distance curve using both linear and quadratic fits

SUMMARY OF ALL RESULTS

- Fill out the following table after measuring the distances in VESTA

	Measured lattice parameter a(Å)	Measured d-1NN (Å)	Experimental a(A)*	DFT calculated lattice parameter a(Å)
Au	4.08	2.88	4.08	
Fe	2.87	2.48	2.87	
NaCl	5.69	2.85	5.64	

- Using the results of your DFT parabolic (quadratic) fit, enter the lattice parameter values a (Å)

* Google search lattice parameter of gold/Fe/NaCl and fill in the value