

Computational Materials Science: Hands-on

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

Day 4:
YALE PATHWAYS TO
SCIENCE SUMMER
WORKSHOP 2021

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HANDS-ON SESSION

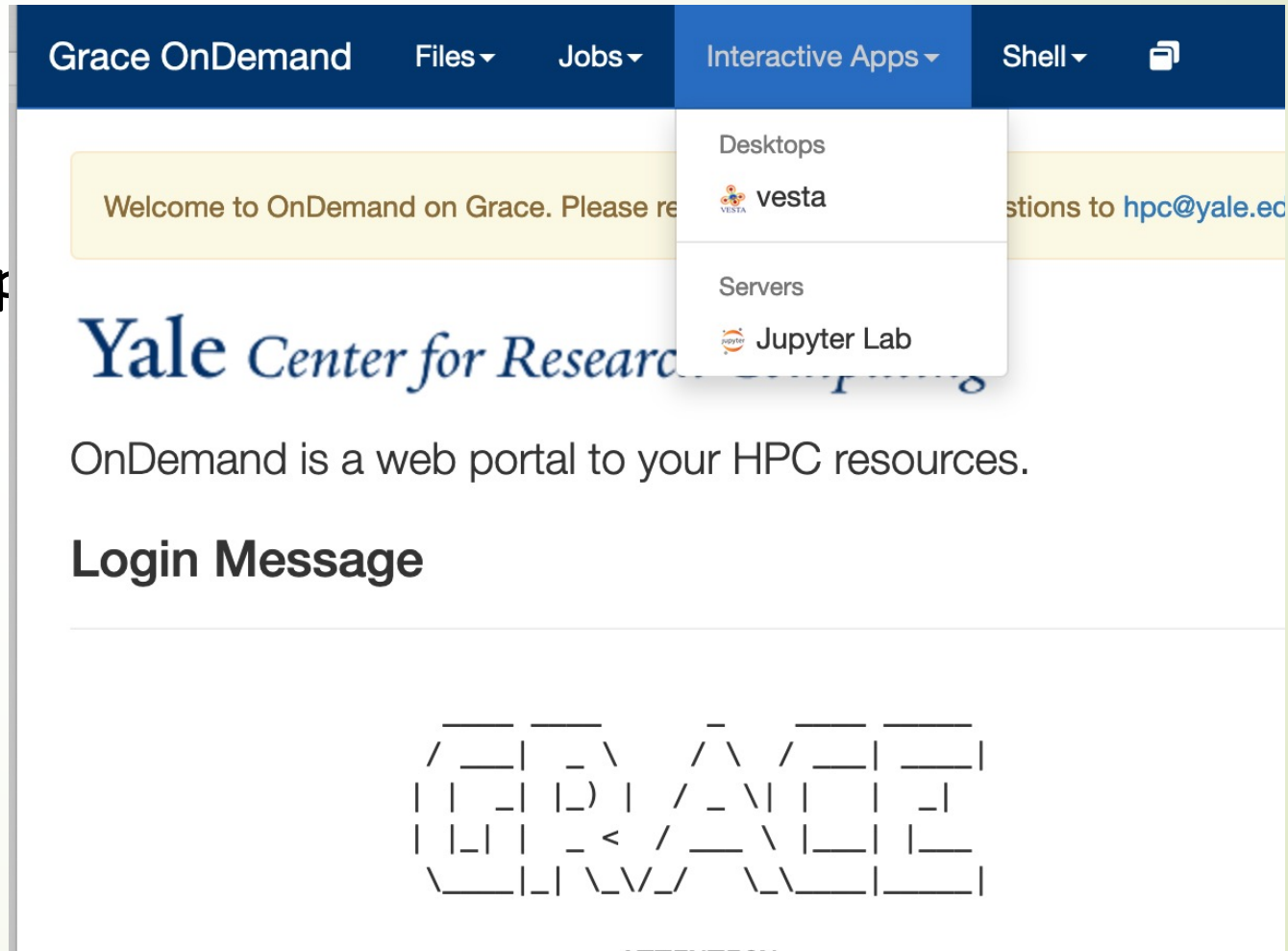
- ▶ Quantum Espresso - Software to calculate the energies of structures
- ▶ Finding the lowest-energy structure of Au, Fe and NaCl
- ▶ Lattice parameters of the lowest-energy structures and comparison with earlier experimental data

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 Apps
- Go to **Day 4** directory inside the **Pathways_workshop** directory



The screenshot shows the Grace OnDemand web portal. The top navigation bar includes 'Grace OnDemand', 'Files', 'Jobs', 'Interactive Apps', and 'Shell'. A dropdown menu is open under 'Interactive Apps', showing options for 'Desktops', 'Servers', and 'Jupyter Lab'. The main content area features a welcome message, the Yale Center for Research Computing logo, and a 'Login Message' section. At the bottom, there is a large graphic of a molecular structure.

ak2589@c16n06.grace:~ x Launcher x

scratch60

Notebook

Python 3 Python 3

Console

Python 3

Other

Terminal Text File Markdown File Show Contextual Help

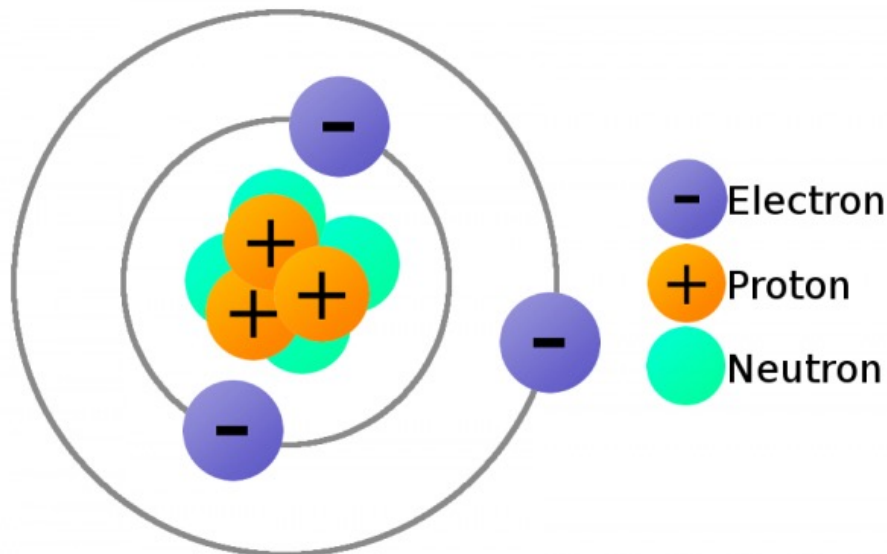
Open the terminal then type day4 and hit Enter

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.



NEWS

07.04.21

QUANTUM ESPRESSO E-SCHOOL

Applications are open for the MaX e-School on Advanced Materials and Molecular Modelling with Quantu...

30.11.20

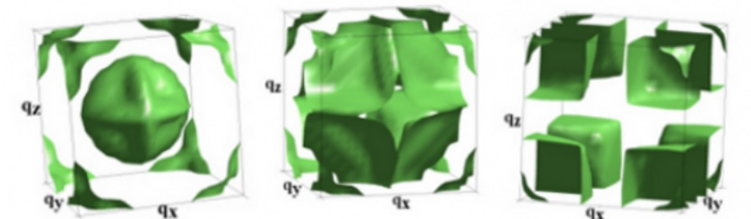
QUANTUM ESPRESSO V.6.7

The 6.7 version of QUANTUM ESPRESSO is available for download. For more information please see the...

05.08.20

QUANTUM ESPRESSO V.6.6

The 6.6 version of QUANTUM ESPRESSO is available for download. For more information please see the...



Phonons of SrTiO₃ under strain, zero-frequency isosurface, Phys. Rev. Lett. 107, 257602 (2011) courtesy of T. Birol.

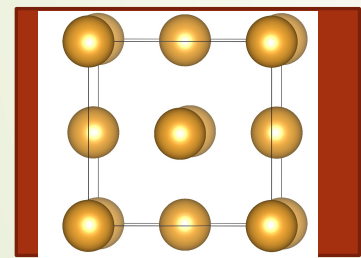
QUANTUM ESPRESSO

is an integrated suite of Open-Source computer codes for electronic-structure calculations and materials modeling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials.

[READ MORE >](#)

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)

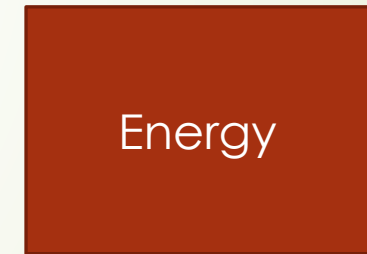


Input structure



Quantum Espresso (QE)

pw.x



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

```
nstype = 1                ! types of atoms
nat      = 4               ! number of atoms
ibrav    = 0               ! related to crystal structure
ecutwfc  = 40              ! convergence parameter
```

```
occupations = 'smearing'
smearing    = 'gaussian'
degauss     = 5d-3
```

} ! settings for metals

/

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  0.000000  0.000000
Au 0.500000  0.500000  0.000000
Au 0.000000  0.500000  0.500000
Au 0.500000  0.000000  0.500000
```

- Does this look familiar?

```
Au
1.0
4.078200  0.000000  0.000000
0.000000  4.078200  0.000000
0.000000  0.000000  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  
4 4 4 0 0 0
```

! points to sample on the lattice
! 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

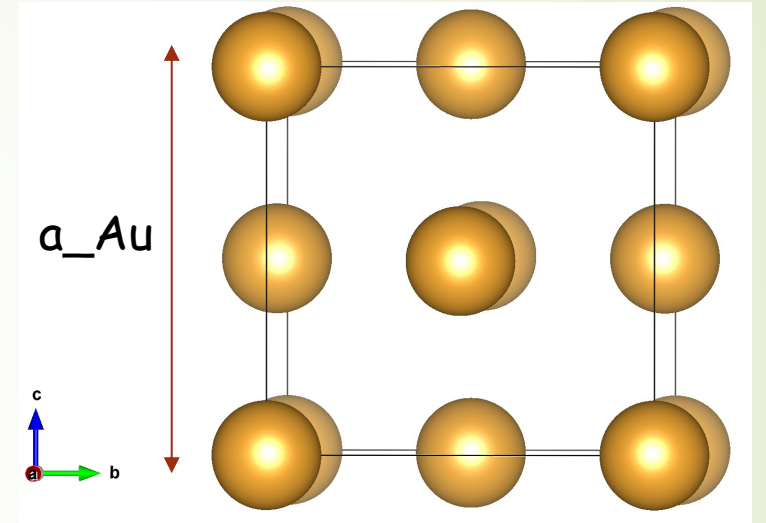
► Remember, lattice parameter

$$a_{\text{Au}} = 4.08 \text{ \AA}$$

► 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

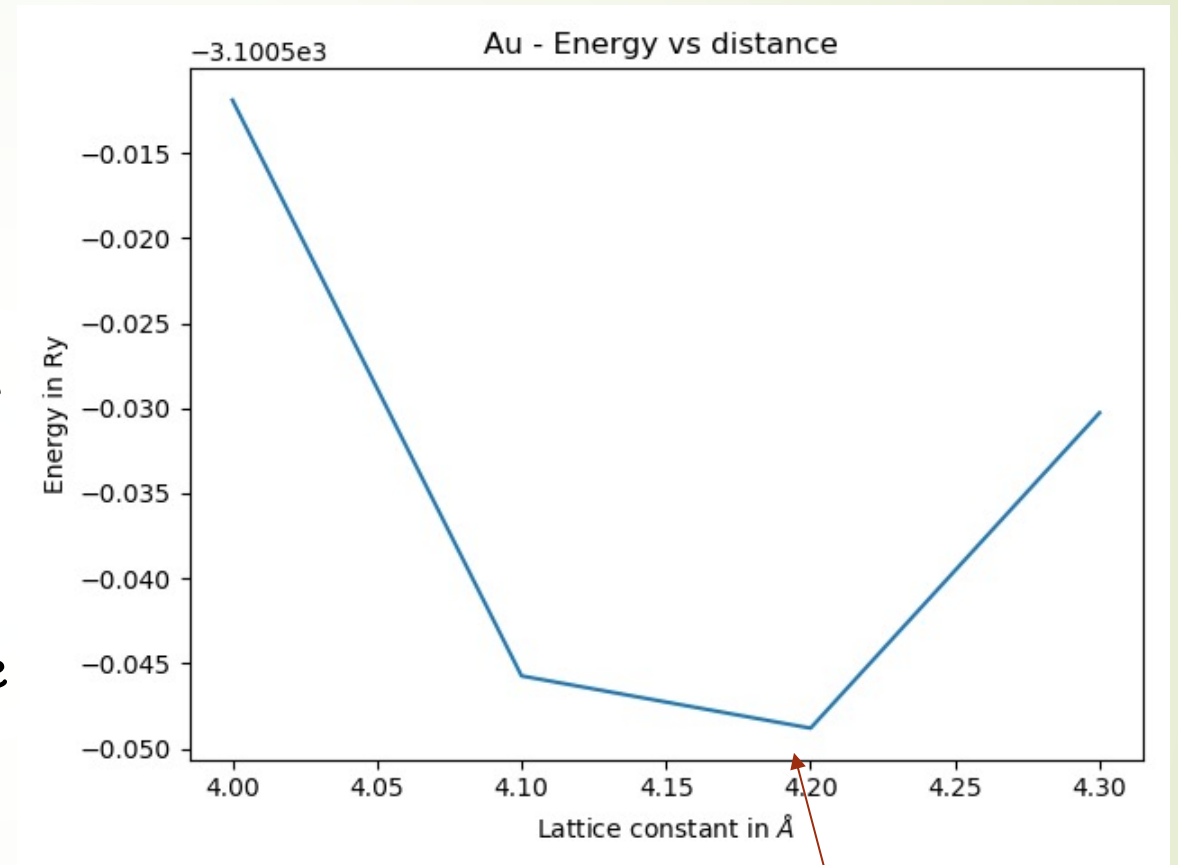
$$a_{\text{Au}} = 4.08 \text{ \AA}$$

➤ 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

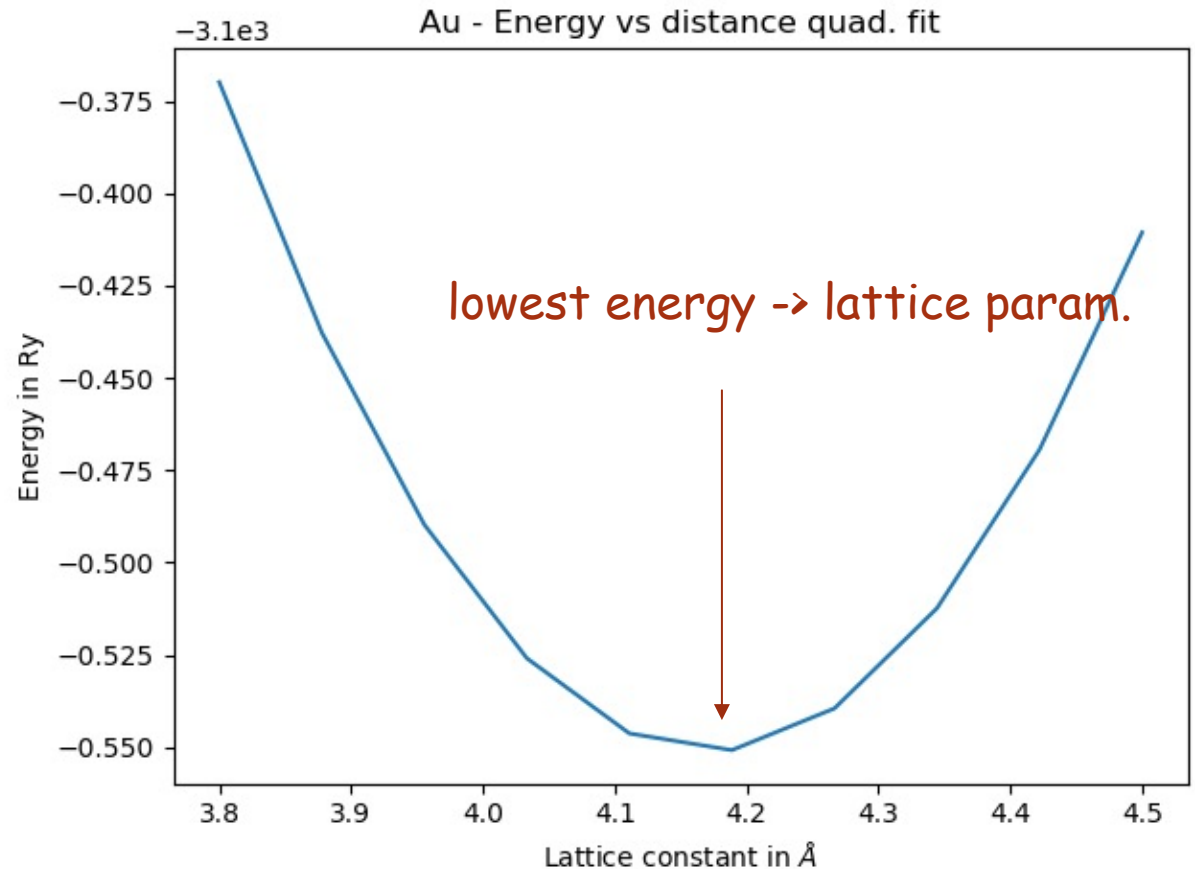
➤ We can plot the **energy vs distance** to find the energy minimum (`plt_energy_dist.py`)



lowest energy -> lattice param.

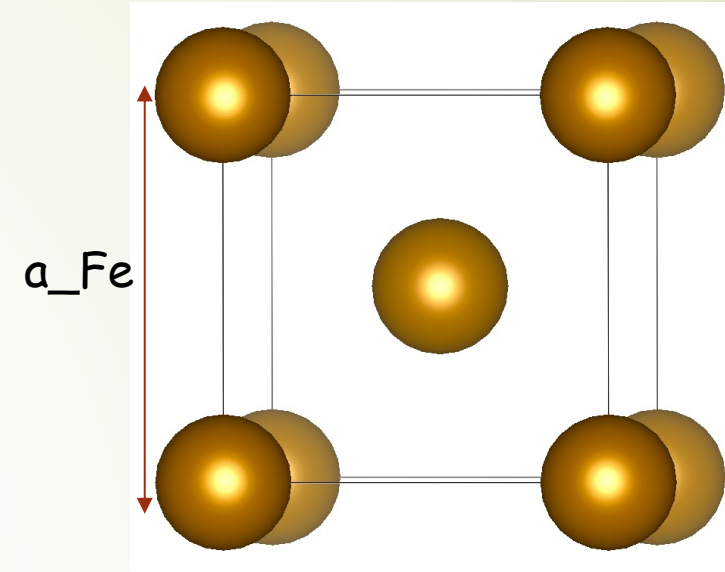
EXERCISE 2- Au

- ▶ The **lowest energy structure** gives us the lattice parameter
- ▶ We can plot the **energy vs distance** to find the energy minimum
- ▶ We will learn how to use the energies to fit $ax^2 + bx$
- ▶ Then, we will plot the **energy vs distance** using `plt_parabola.py`
- ▶ This is closer to the real energy variation in



EXERCISE 3- Fe

- ▶ We will repeat the previous exercises for Fe
- ▶ Since for Fe, lattice parameter, $a_{\text{Fe}} = 2.87 \text{ \AA}$
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

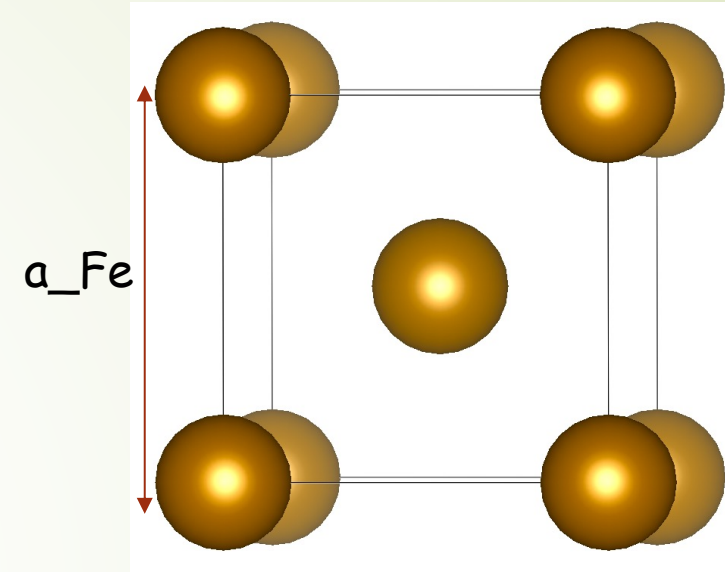
➤ For NaCl, lattice parameter, $a_{\text{NaCl}} = 5.64 \text{ \AA}$

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 $a(\text{\AA})$	Measured $d\text{-1NN} (\text{\AA})$	Experimental $a(\text{\AA})^*$	DFT calculated lattice parameter $a(\text{\AA})$
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 $a (\text{\AA})$

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