Day 3:
YALE PATHWAYS TO SCIENCE SUMMER WORKSHOP 2021

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Introduction to Materials Science: Hands-on

DESIGN OF NEW MATERIALS USING SUPERCOMPUTERS

LEARNING GOALS

- Use VESTA to load structures of Au, Fe and NaCl
- Measure lattice parameters, nearest-neighbor distances
- Create new structures files that contain defects (vacancies, interstitials, antisites)

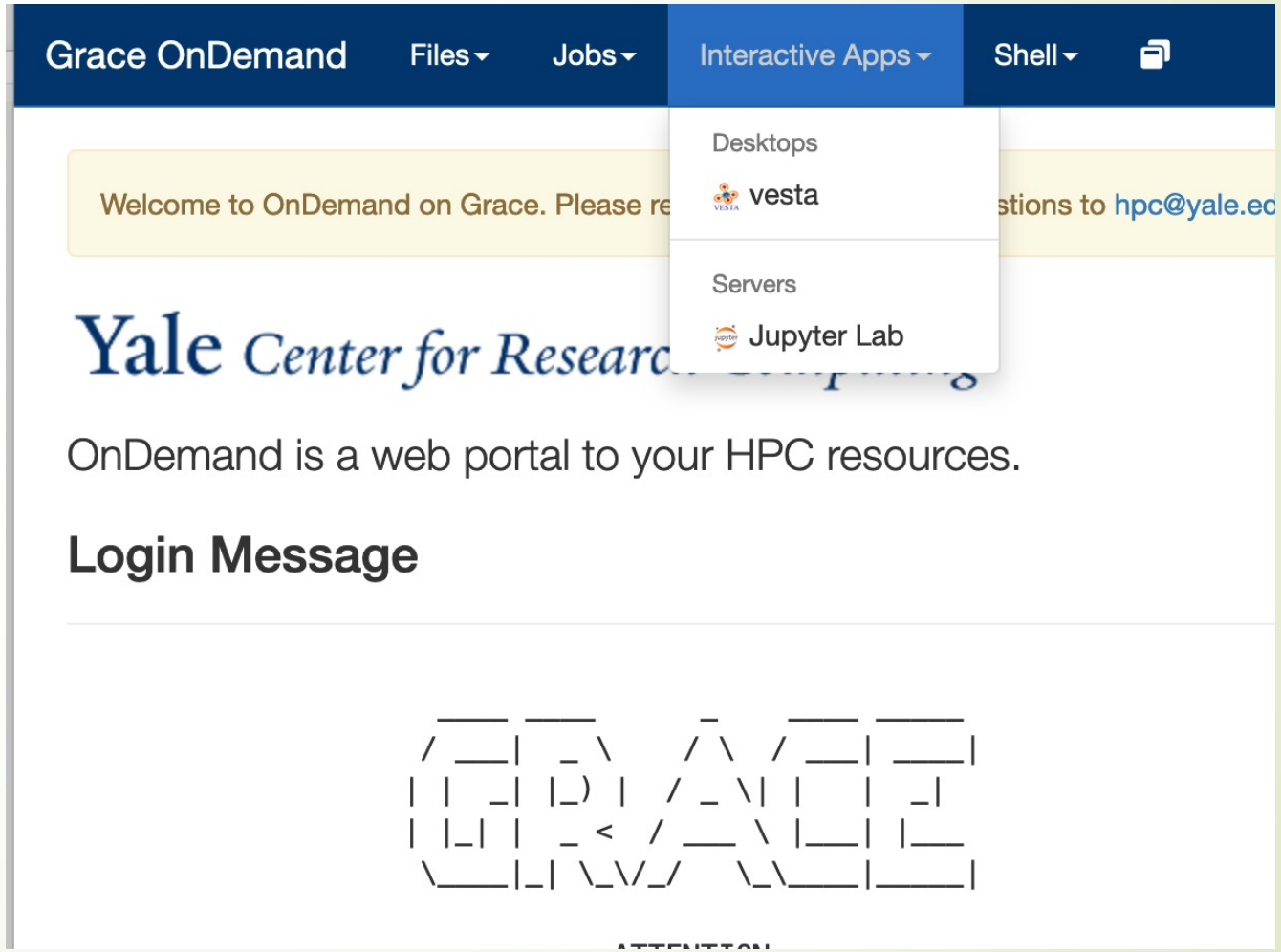
VESTA TO VIEW STRUCTURES

- We will use VESTA to visualize the structures!

Go to:

- https://pathways.ycrc.yale.edu
- Click on vesta under interactive Apps

- Go to Day 3 directory inside the Pathways_workshop directory



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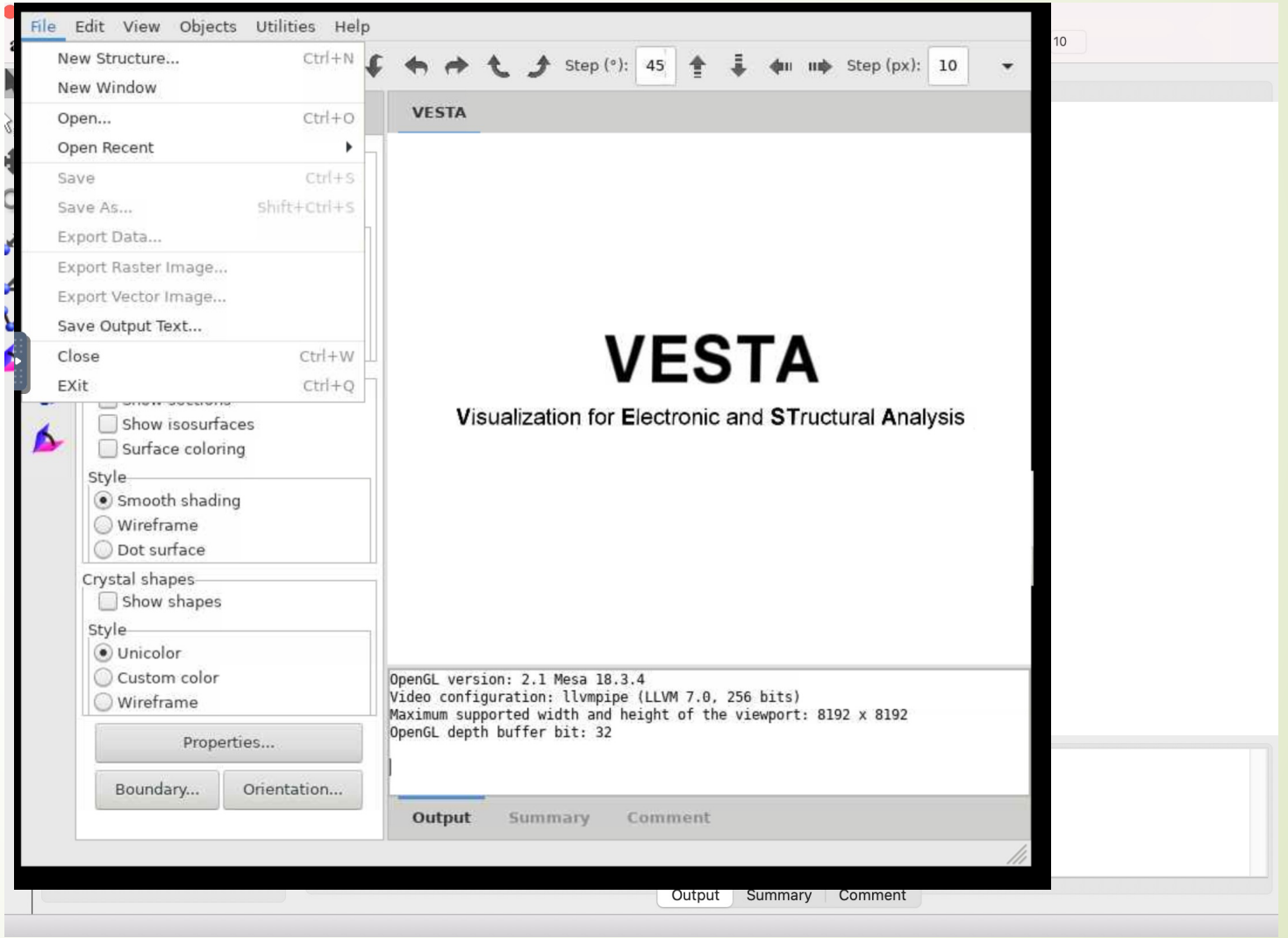
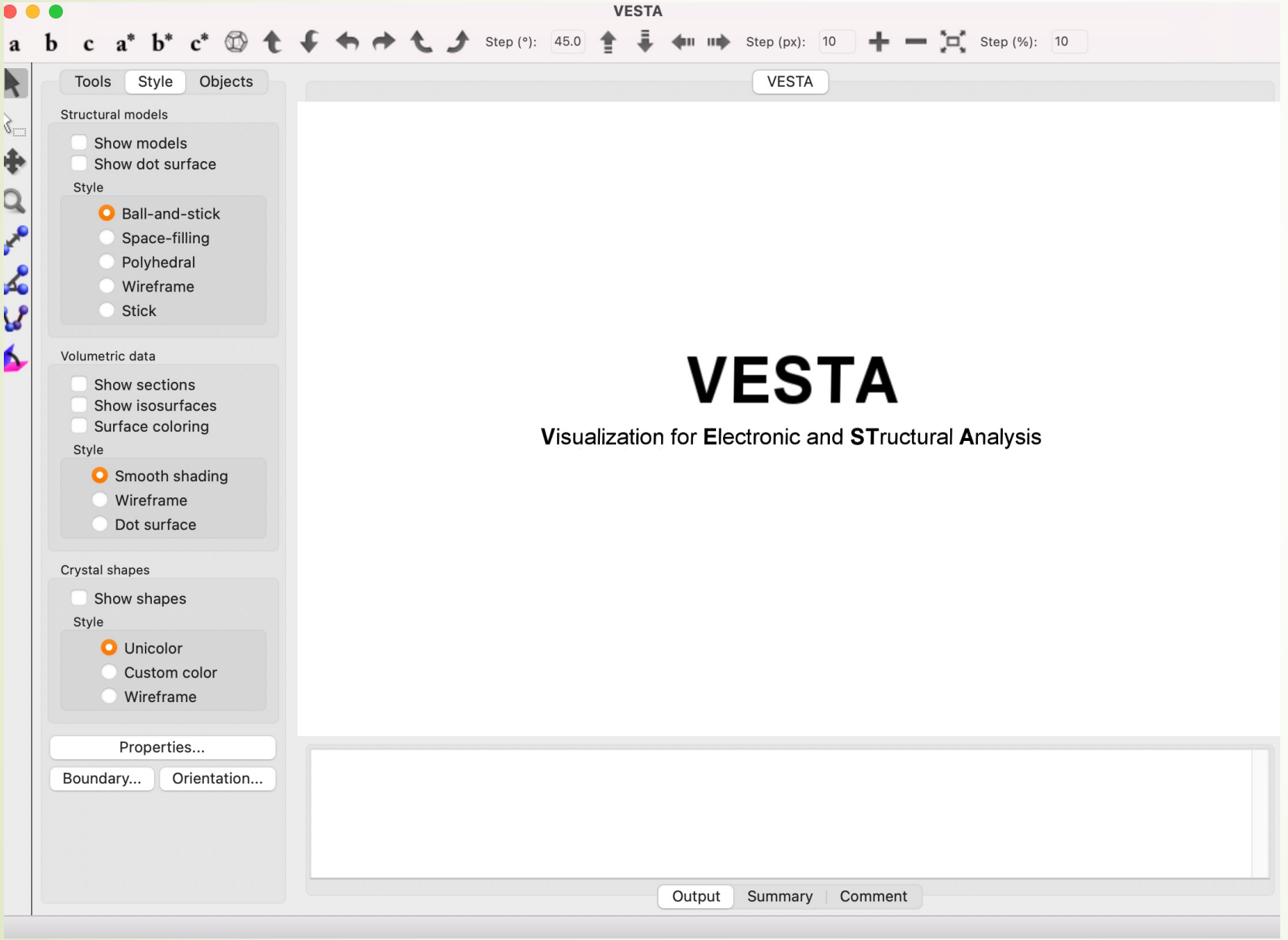
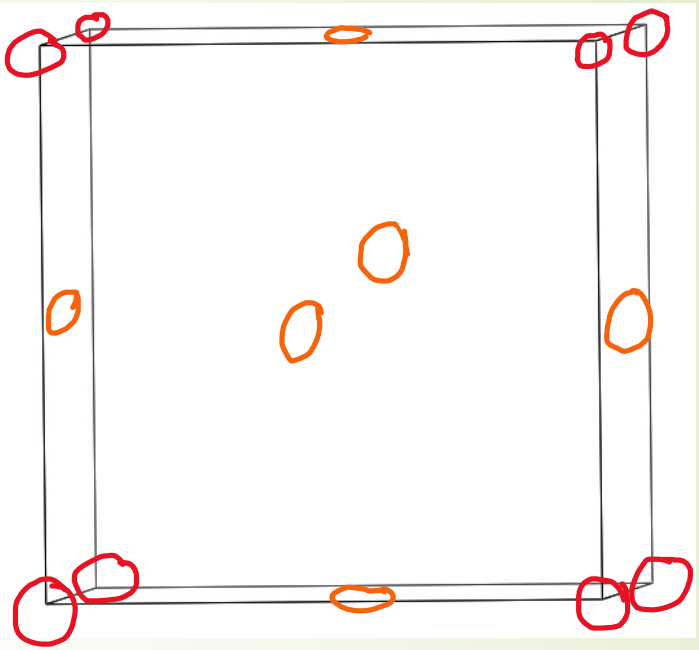
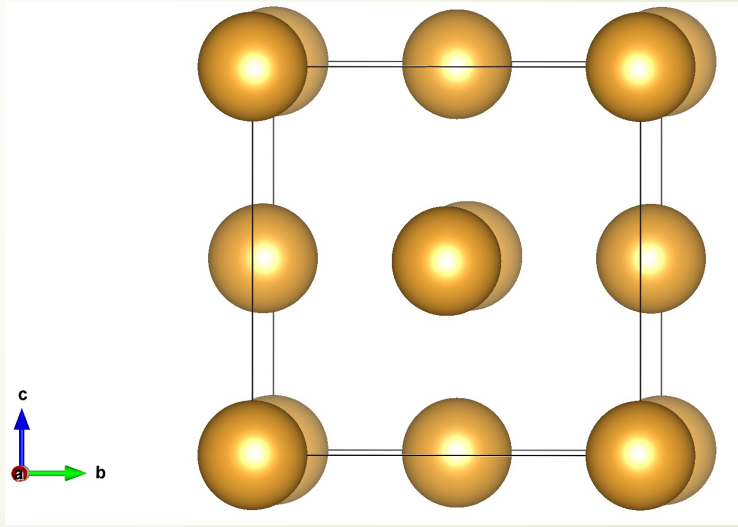


Au CRYSTAL STRUCTURE





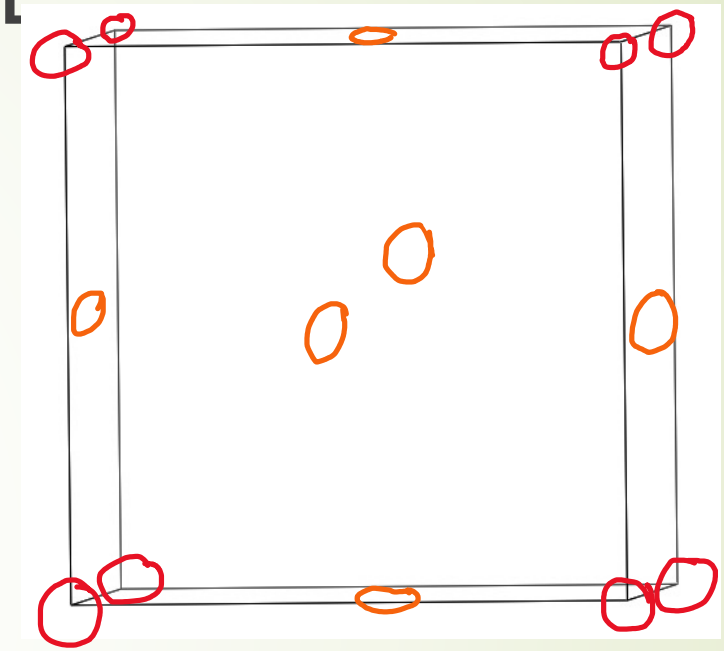


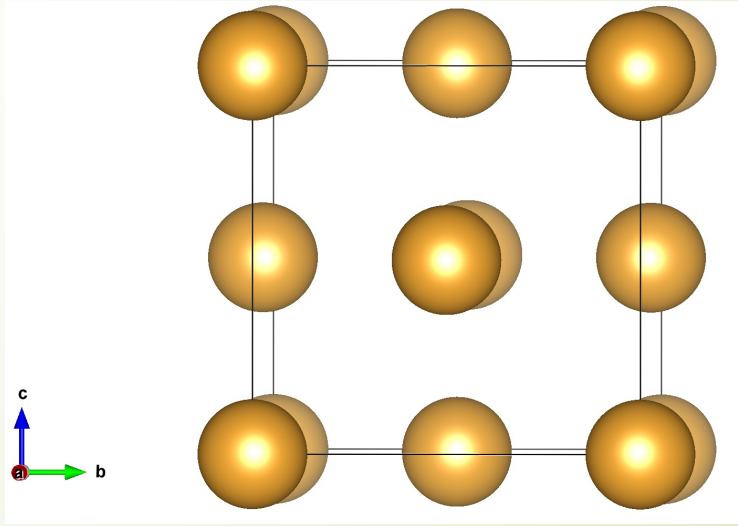
Au CRYSTAL STRUCTURE

- Open the POSCAR_Au.vasp in Jupyterlab editor.
- POSCAR file contains the structure

```
Au                                          Name
1.0                                         Scaling Factor – leave it as 1
4.078200 0.00000 0.000000                   a crystal lattice vector -> x axis
0.000000 4.07820 0.000000                   b crystal lattice vector -> y axis
0.000000 0.00000 4.078200                   c crystal lattice vector -> z axis
Au          Chemical Symbol(s) in the same order as their count below
4           Number of atoms of each type
direct      positions with respect to a cell of length 1
0.000000 0.000000 0.000000 Au               x, y and z
0.500000 0.500000 0.000000 Au               coordinates
0.000000 0.500000 0.500000 Au               of each atom
0.500000 0.000000 0.500000 Au
```

- Let's go to zoom whiteboard!





NaCl Crystal Structure

- Open the POSCAR_NaCl.vasp in Jupyterlab editor.

```
Na4 Cl4
1.0
5.691694 0.000000 0.000000
0.000000 5.691694 0.000000
0.000000 0.000000 5.691694
Na Cl
4 4
direct
0.000000 0.000000 0.000000 Na
0.000000 0.500000 0.500000 Na
0.500000 0.000000 0.500000 Na
0.500000 0.500000 0.000000 Na
0.500000 0.000000 0.000000 Cl
0.500000 0.500000 0.500000 Cl
0.000000 0.000000 0.500000 Cl
0.000000 0.500000 0.000000 Cl
```

Chemical Symbol(s) in the same order as their count below

Number of atoms of each type

positions with respect to a cell of length 1

x, y and z coordinates of each atom

Recall the Au FCC

```
0.000000 0.000000 0.000000 Na
0.000000 0.500000 0.500000 Na
0.500000 0.000000 0.500000 Na
0.500000 0.500000 0.000000 Na
```

Fe BCC

```
0.500000 0.500000 0.500000 Cl
```

Cl on each axis

```
0.500000 0.000000 0.000000 Cl
0.000000 0.000000 0.500000 Cl
0.000000 0.500000 0.000000 Cl
```

EXERCISE 1

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

	Measured lattice parameter a(Å)	Measured d-1NN (Å)	Experimental a(A)*
Au			
Fe			
NaCl			

- Compare with the known value in literature from experiments.

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

EXERCISE 2

- Copy POSCAR_Au.vasp to a new file POSCAR_Au_vacancy.vasp

cp POSCAR_Au.vasp POSCAR_AU_vacancy.vasp

- Delete on Au atom and save it
- Open it in VESTA. Can you see the vacancy?

- Repeat the same for POSCAR_Fe.vasp (copy to POSCAR_Fe_vacancy.vasp)
- Delete the Fe atom at 0.5, 0.5, 0.5 and save the file
- Open in VESTA. Notice the vacancy!

- Copy POSCAR_Fe.vasp to POSCAR_Fe_Au_defect.vasp
- Change the atom type of 0.5, 0.5, 0.5 to Au
- What kind of defect did we create?

EXERCISE 3

- Copy POSCAR_Fe.vasp to POSCAR_Fe_Au_defect.vasp
- Change the atom type of 0.5, 0.5, 0.5 to Au
- What kind of defect did we create?

- Copy POSCAR_Fe.vasp to POSCAR_Fe_intersititial.vasp
- Add an additional Fe atom at 0.0, 0.0, 0.5
- Can you see the intersititial defect we created?

EXERCISE 4

- Create an antistite defect in NaCl
- Copy POSCAR_NaCl.vasp to POSCAR_NaCl_antisite.vasp

- Do you see the Na and Cl atoms swapping positions?