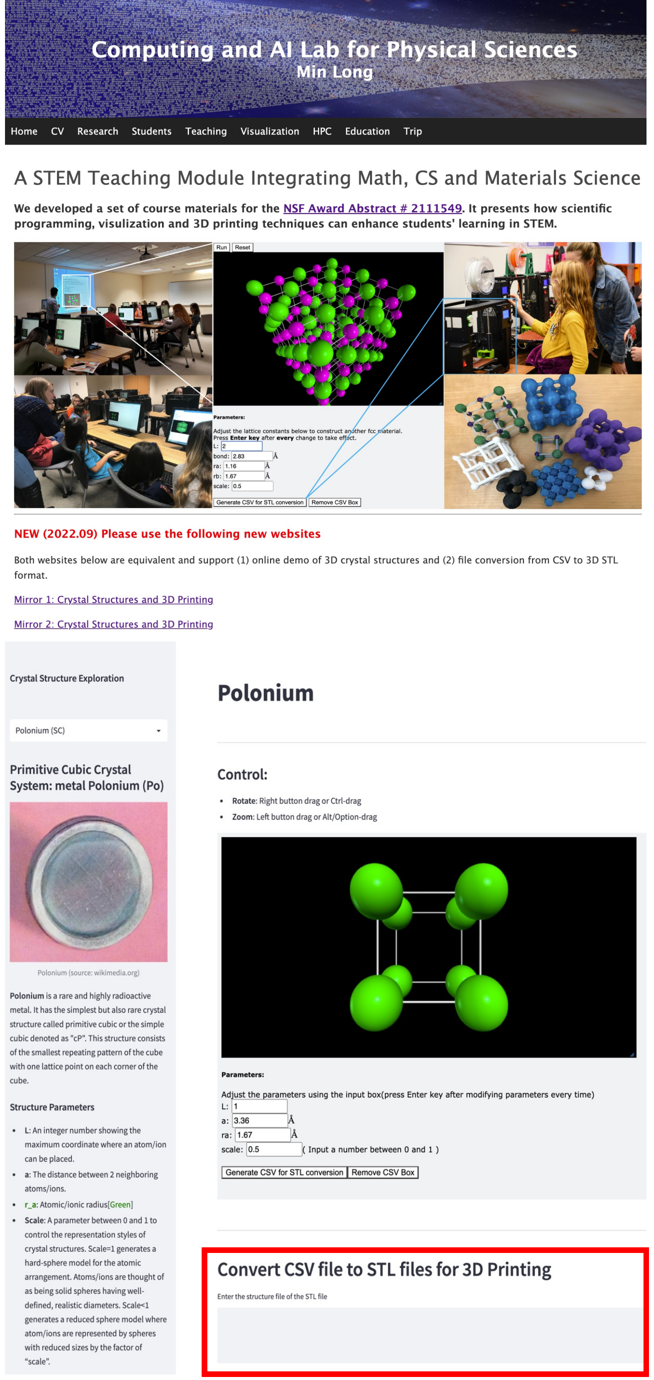
Training Materials: Exploring Math through Programming and Visualization of Crystal Structures

Min Long, Andy Lau
Department of Computer Science
Boise State University

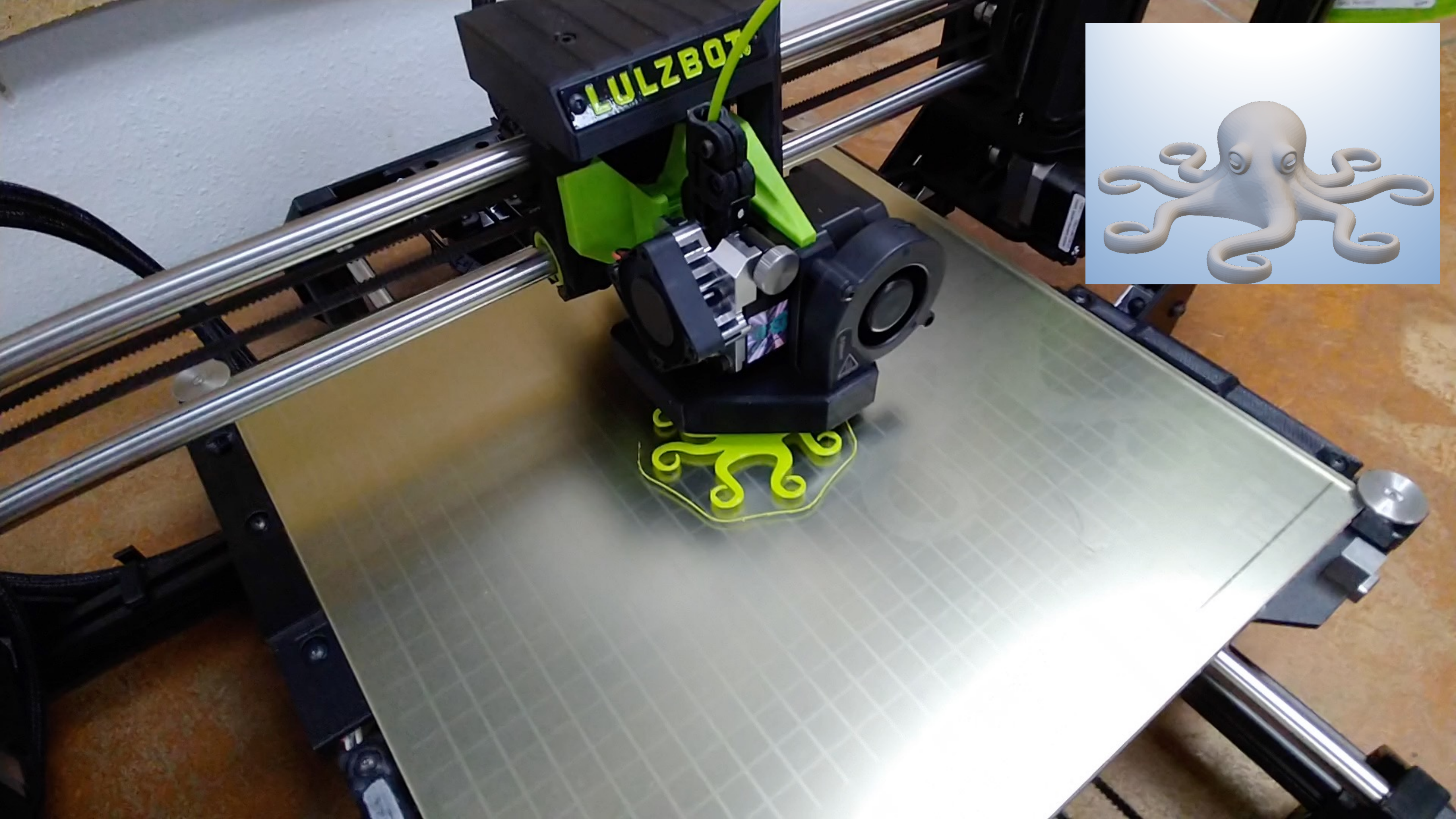
Websites for Resources

- Main Websites:
  - Toolkit, tables of data, 3D printer manuals...
  - https://cs.boisestate.edu/~mlong/education.html
  - https://minlong1.github.io/education.html
- Converting structure files (CSV) to 3D STL files:
  - Toolkit and converting tool
  - https://minlong1-csv2stl-streamlit-app-1nkv76.streamlitapp.com/
  - https://laumiulun-csv2stl-streamlit-app-lcc7hm.streamlitapp.com/



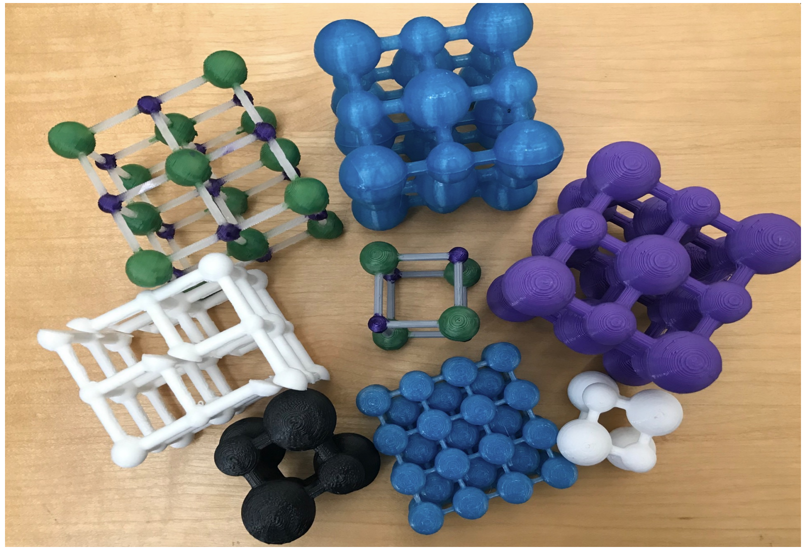
Training Materials

- Overview and Objectives
- Lecture 1: Introduction to Online Toolkits and STEM Concepts (For instructors)
- Lecture 2: Introduction to 3D Printing
- Lecture 3: Design and Print SC and FCC Materials
- Lecture 4: Design BCC and Perovskite Materials
- Note: In-class activities can start from Lecture 2


LULZBOT

Objective

- Enhance Student’s learning in STEM context using scientific Programing, visualization and 3D printing techniques.



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Lecture 1

- Overview of STEM Concepts
  - Math Concepts
  - Materials Concepts
  - Computer Science Concepts
- Online Toolkit: Learning Math in STEM Context
- Design Simple Cubic (SC) and Face-center Cubic (FCC) Materials

STEM Concepts

Mathematics

- Polygon (2D)
- Polyhedron and Platonic solids (3D)
- Measurement
- Symmetry (Rotation, Translation, Reflection)
- Coordinates
- Ratio
- Similarity

Computer Science: Programming

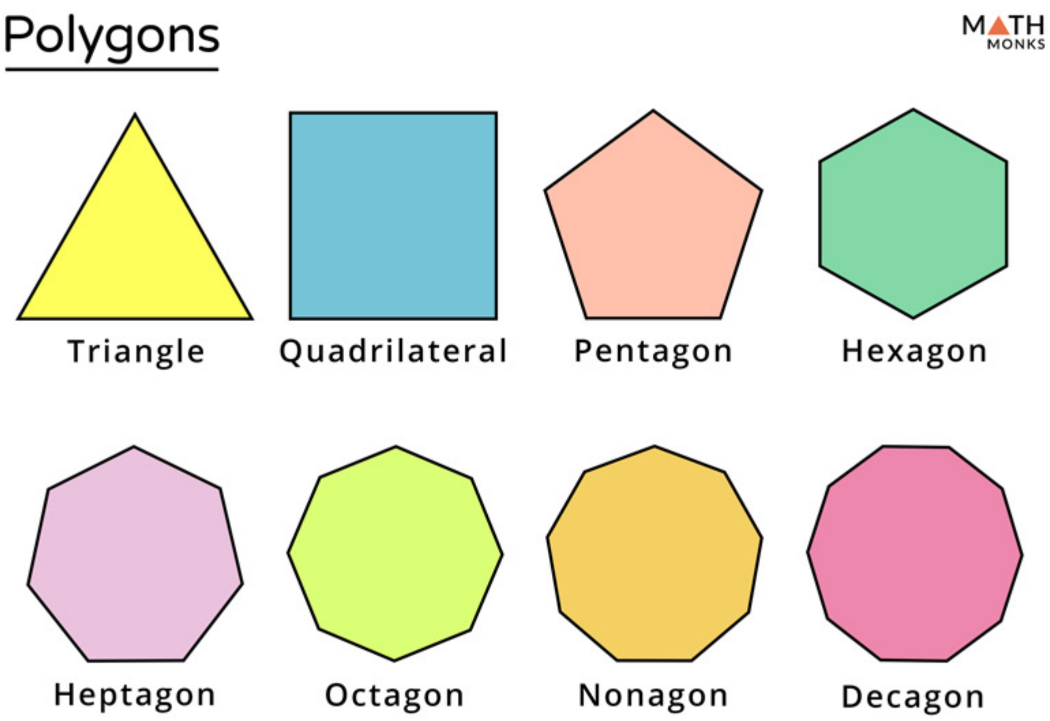
- Class
- Object

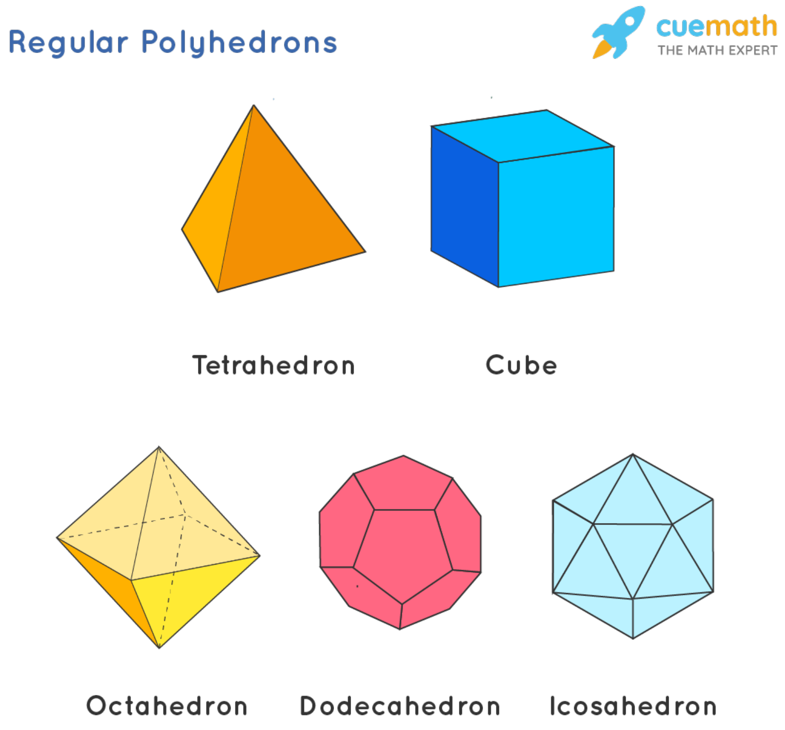
Material Science & Engineering

- Crystal Structure
- Lattice
- Materials
- 3D Printing

Math Concepts

- Polygon (2D)
- Polyhedron and Platonic solids (3D)
- Measurement
- Coordinates
- Symmetry
- Ratio
- Similarity





Materials Concepts

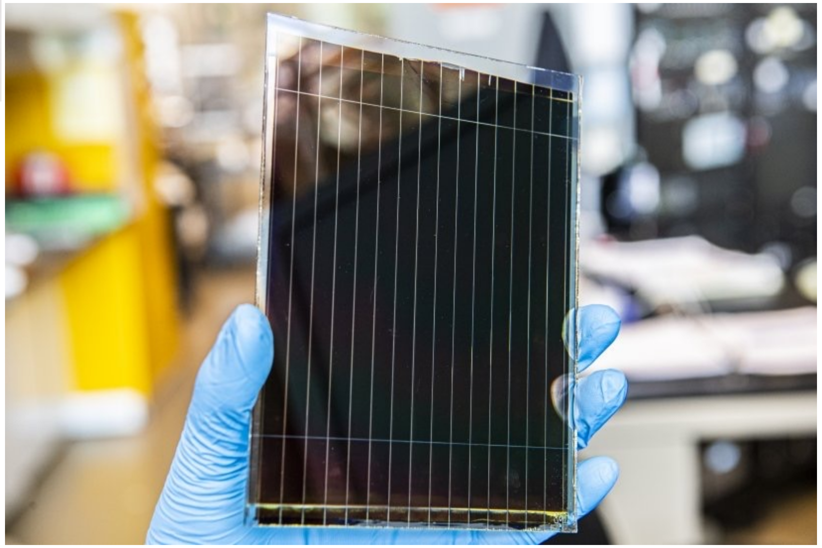
- Crystalline
  - A material in which the atoms are situated in a repeating or periodic array
  - Atoms will position themselves in a repetitive 3D pattern.
  - All metals, many ceramics and certain polymers.

Salt Crystal

Hope diamond



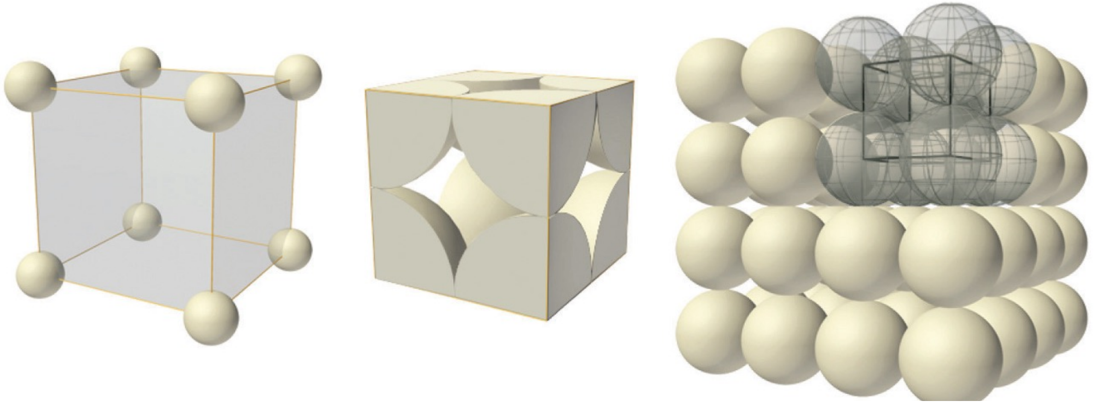
Iron

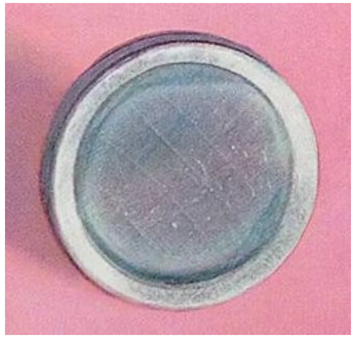
Perovskite Solar Cell


Crystal Structures

- Many…

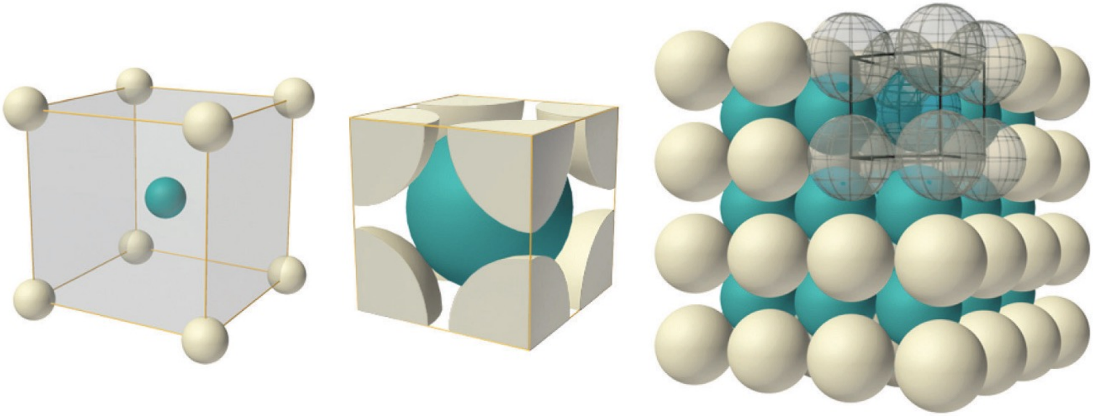
Simple Cubic





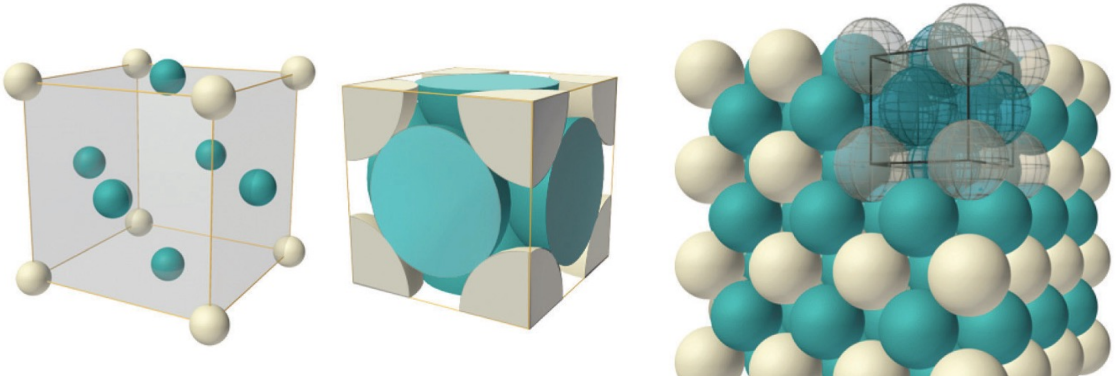
Polonium

Body-centered Cubic (bcc)



Iron

Face-centered Cubic (fcc)

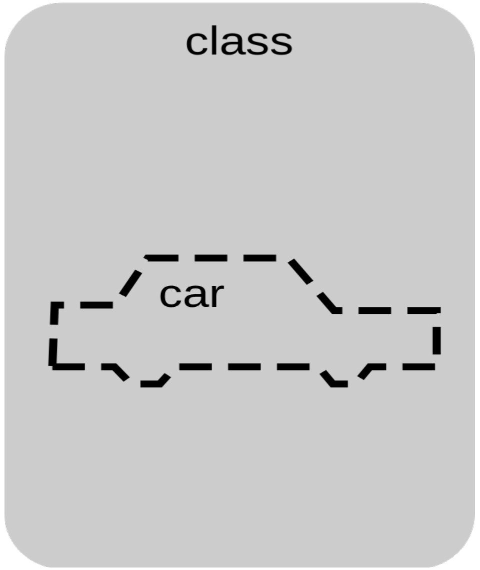


“Unit Cell”

Computer Science: Programming

- **Class**: A user-defined type specifying attributes
- **Object**: an instance of a class, showing a run-time entity

Car
Attribute:
Color
Brand
Model



Objects
Color: Silver
Brand: Toyota
Model: Camry

Objects
Color:
Brand:
Model:

"blueprint"

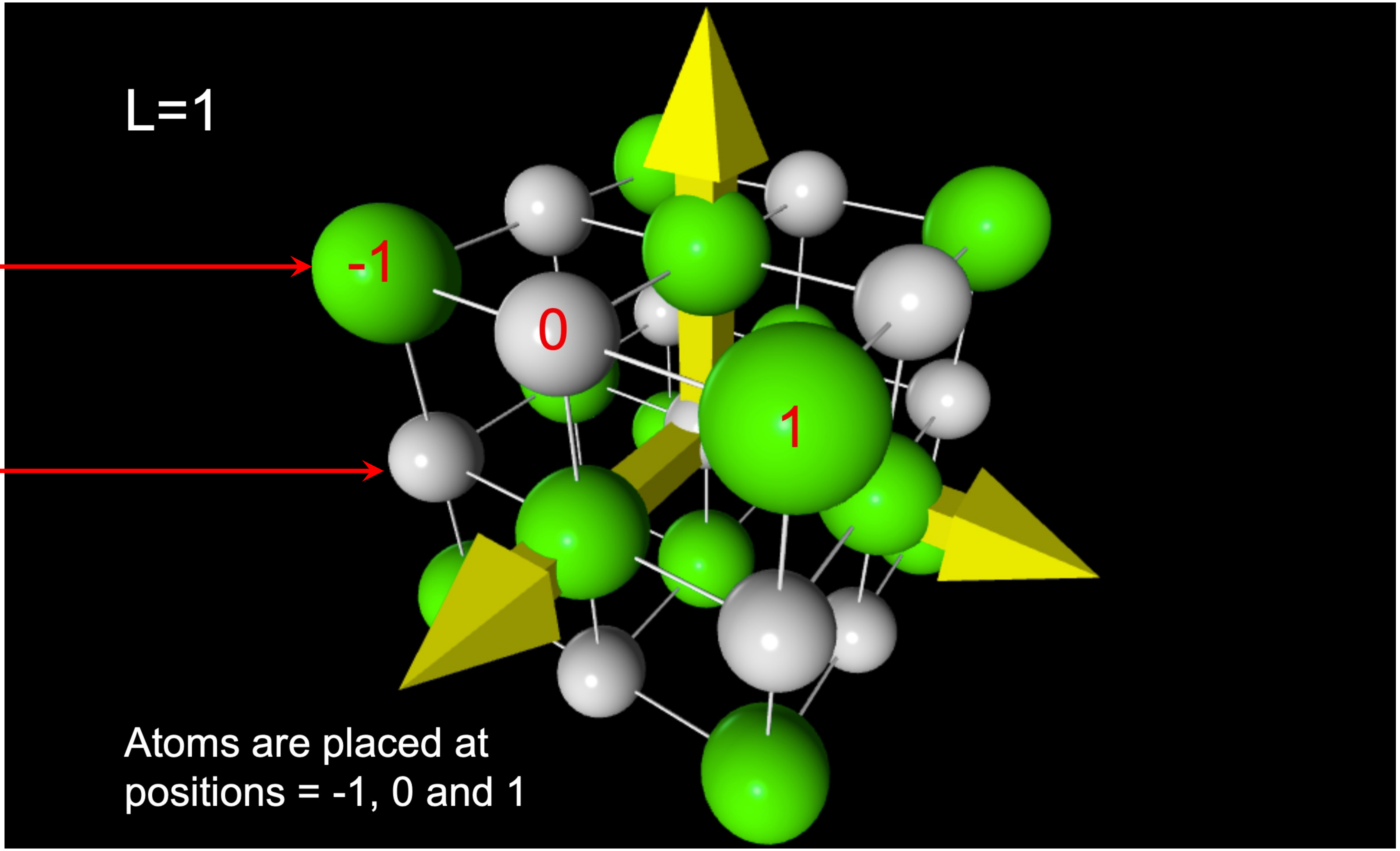
"realization"

Programming Concepts

- Build a number of objects using the same class

Class:
Sodium atom
Object:
Many Spheres
Attributes:
Color: Green
Size: 1.67
Position: X, Y, Z

Class:
Chloride atom
Object:
Many Spheres
Attributes:
Color: Silver
Size: 1.16
Position: X, Y, Z

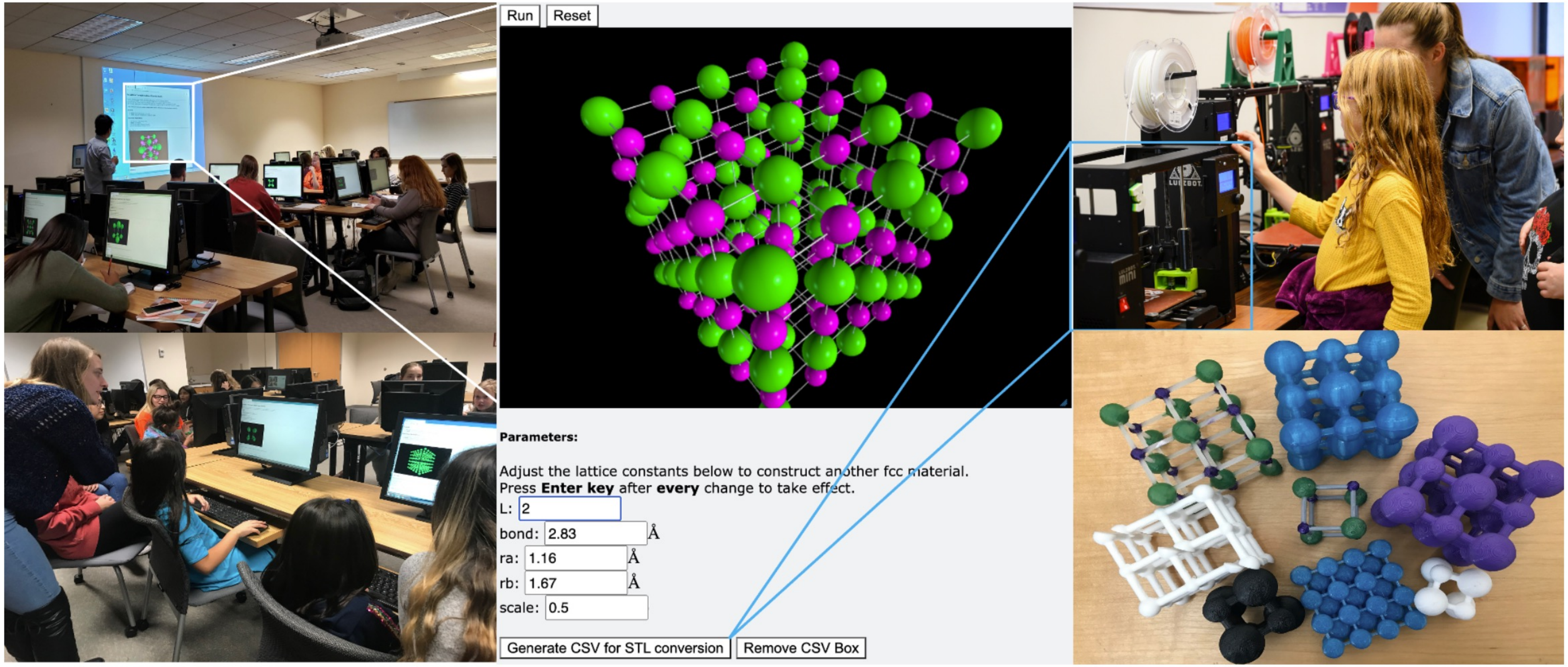


Online Toolkit: Learning Math in STEM

- https://cs.boisestate.edu/~mlong/education.html

A STEM Teaching Module Integrating Math, CS and Materials Science

We developed a set of course materials for the NSF Award Abstract # 2111549. It presents how scientific programming, visulization and 3D printing techniques can enhance students' learning in STEM.



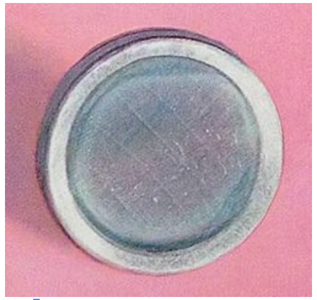
Summary of STEM Concepts

- Math
  - Polygon (2D)
  - Polyhedron and Platonic solids (3D) • Measurement
  - Coordinates
  - Symmetry
  - Ratio
  - Similarity
- Materials
  - Atoms
  - Crystal Structures
  - Crystalline
- Programming
  - Class
  - Object
  - Attribute

Before the class: Look through these concepts

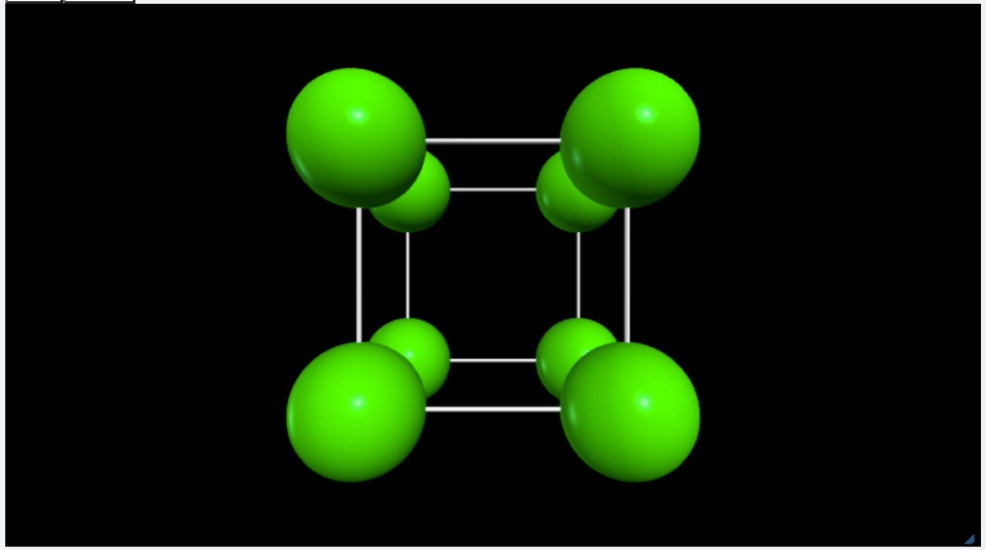
Applications: Design simple cubic and face-center cubic materials

Ex1 - Simple Cubic: Metal Polonium (Po)



- **Polonium** is a rare and highly radioactive metal.
- This structure consists of the smallest repeating pattern of the cube with one lattice point on each corner of the cube.

Run Reset



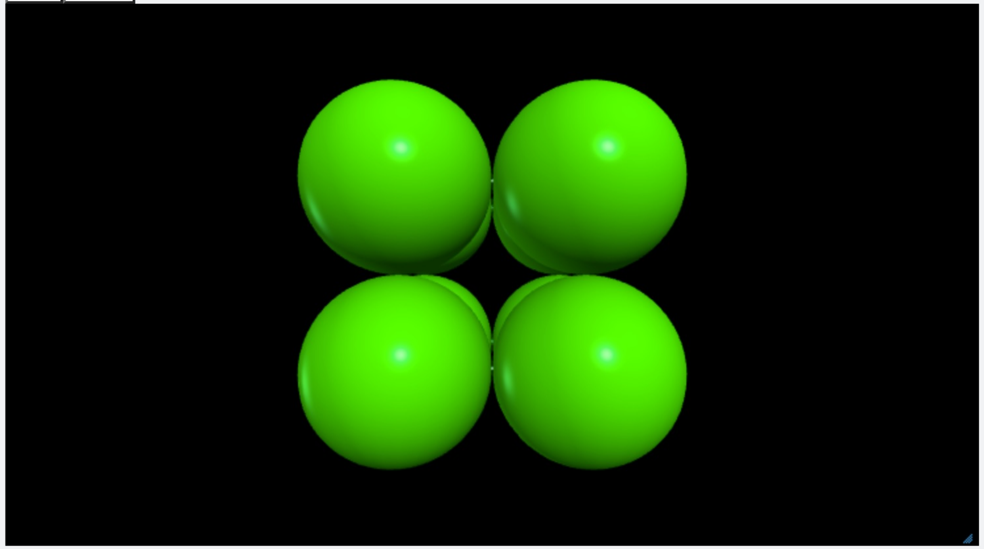
Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

Parameters:

Adjust the parameters using the input box(press Enter key after modifying parameters every time)
U: 1
a: 3.34 Å
ra: 1.67 Å
scale: 0.5 (Input a number between 0 and 1)

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

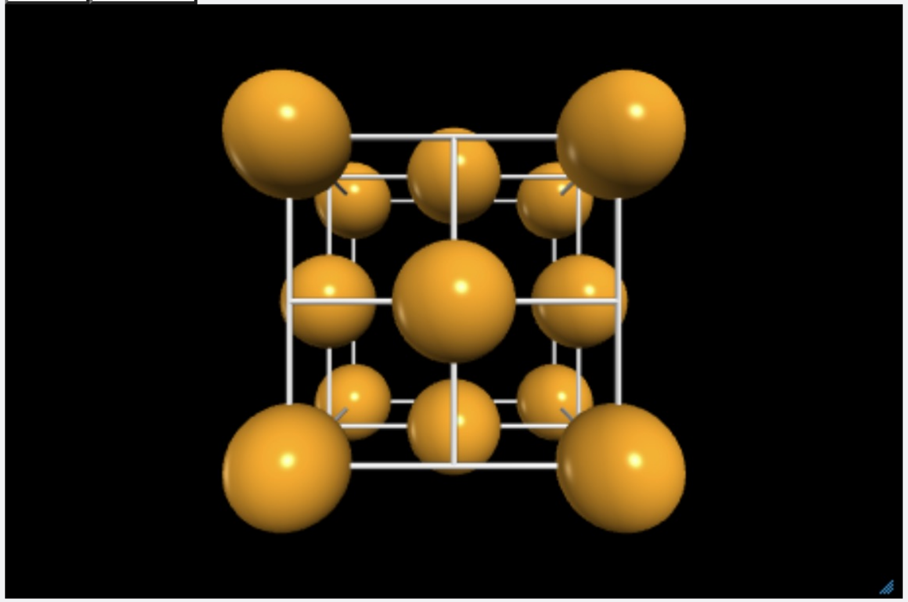
Parameters:

Adjust the parameters using the input box(press Enter key after modifying parameters every time)
U: 1
a: 3.34 Å
ra: 1.67 Å
scale: 1 (Input a number between 0 and 1)

Ex2 - Face-centered Cubic: Copper Cu

- **Solid copper** is used for wiring in daily life.
- Atoms are placed in corner of the cube and center of the faces

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

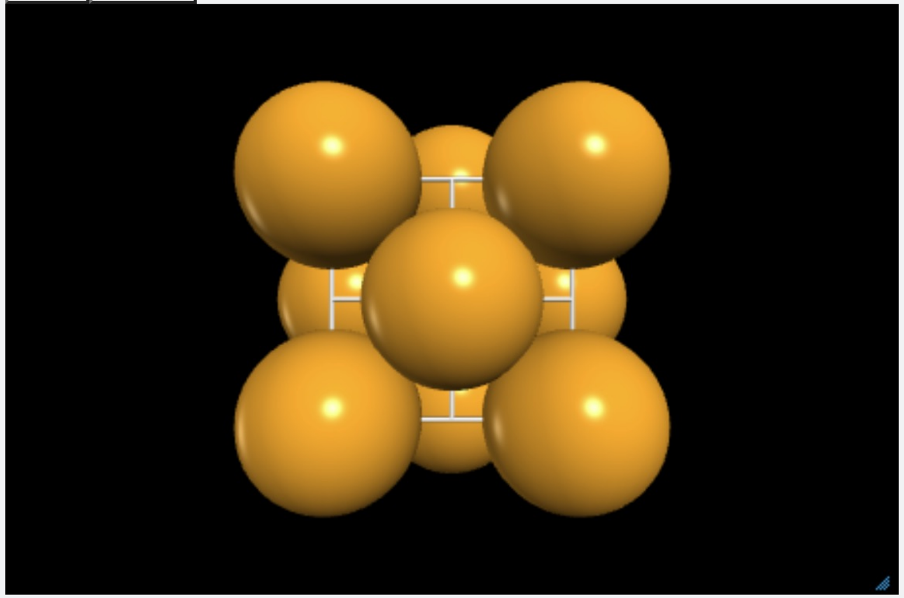
L: 1

a: 3.597 Å

ra: 1.35 Å

scale: 0.5 (Input a number between 0 and 1)

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

L: 1

a: 3.597 Å

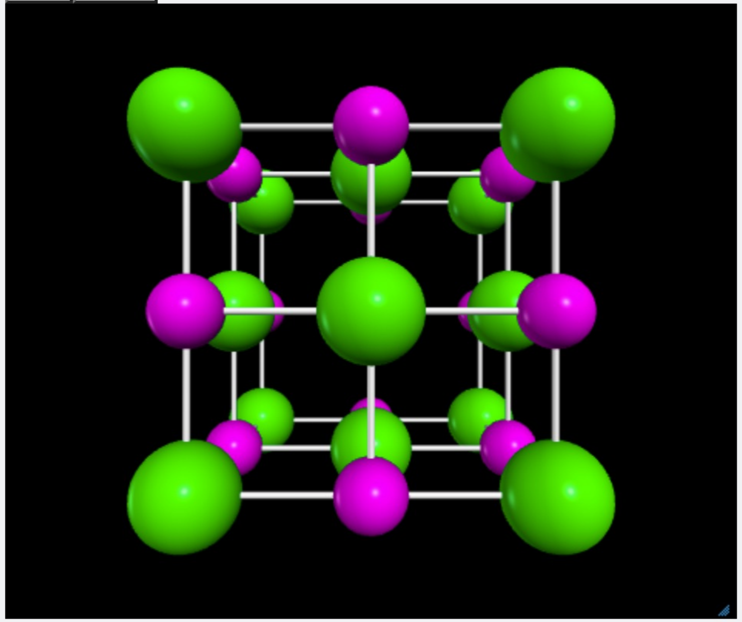
ra: 1.35 Å

scale: 1 (Input a number between 0 and 1)

Ex3 - Face-centered Cubic: NaCl

- Salt consists sodium ions and chloride ions
  - They alternate with each other in each of the three dimensions.
  - The repeating pattern is still a cube with lattice points on the faces of the cube.

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

L: 1

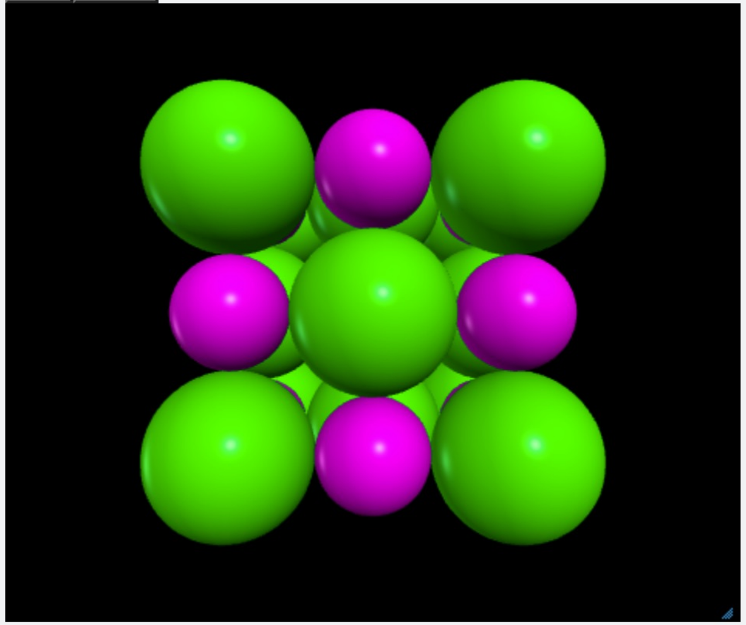
a: 5.64 Å

ra: 1.16 Å

rb: 1.67 Å

scale: 0.5 (Input a number between 0 and 1)

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

L: 1

a: 5.64 Å

ra: 1.16 Å

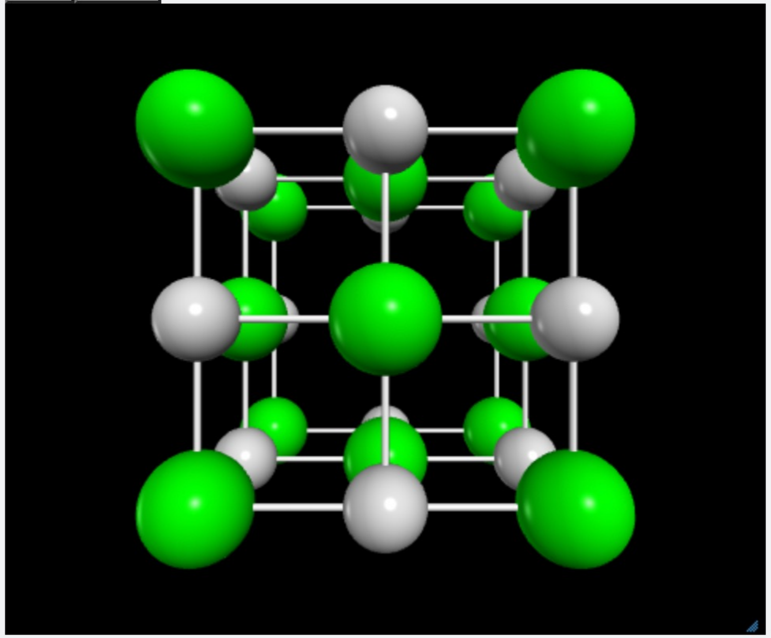
rb: 1.67 Å

scale: 1 (Input a number between 0 and 1)

Ex4 - Face-centered Cubic: AgCl

- The solid adopts the fcc NaCl structure
  - But Ag+ ions replace Na+ ions

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

L: 1

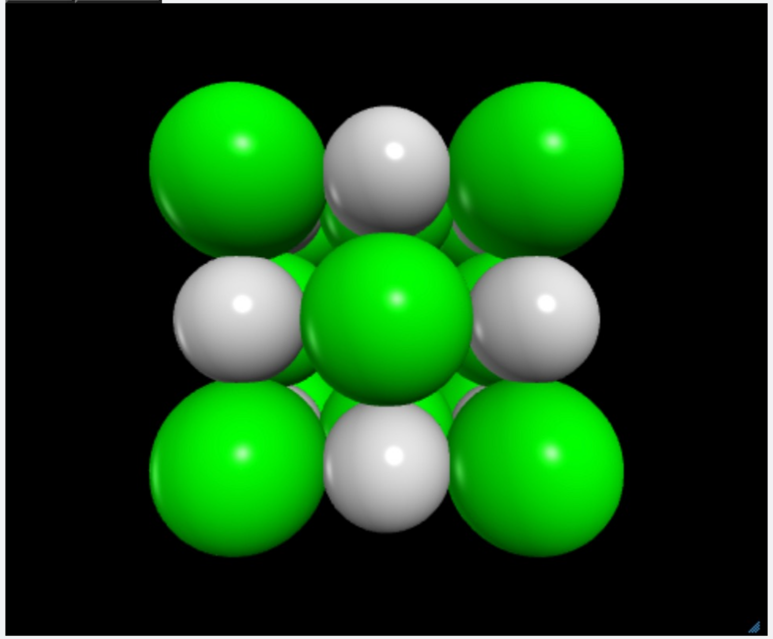
a: 5.55 (Å)

ra: 1.26 (Å)

rb: 1.67 (Å)

scale: 0.5 (Input a number between 0 and 1)

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

L: 1

a: 5.55 (Å)

ra: 1.26 (Å)

rb: 1.67 (Å)

scale: 1 (Input a number between 0 and 1)

Lattice Constants at 300K

- Other FCC Materials (Simple Substance)

Material	a (Å)	ra(Å)
Al	4.046	1.25
Ni	3.499	1.35
Cu	3.597	1.35
Pd	3.859	1.40
Ag	4.079	1.60
Pt	3.912	1.35
Au	4.065	1.35
Pb	4.920	1.80

- https://en.wikipedia.org/wiki/Atomic_radii_of_the_elements_(data_page)

Lattice Constants at 300K

- Other FCC Materials (Compounds, "crystal ionic radii" are used)

Material	a (A)	Ionic ra(Å)	ionic rb(Å)
MgO	3.0399	0.86	1.26
ZnO	4.580	0.88	1.26
PbS	5.9362	1.33	1.70
PbTe	6.4620	1.33	2.07
LiF	4.03	0.90	1.19
LiCl	5.14	0.90	1.67
LiBr	5.50	0.90	1.82
LiI	6.01	0.90	2.06
NaF	4.63	1.16	1.19
NaCl	5.64	1.16	1.67
NaBr	5.97	1.16	1.82
NaI	6.47	1.16	2.06

Material	a (A)	Ionic ra(Å)	Ionic rb(Å)
KF	5.34	1.52	1.19
KCl	6.29	1.52	1.67
KBr	6.60	1.52	1.82
KI	7.07	1.52	2.06
RbF	5.65	1.66	1.19
RbCl	6.59	1.66	1.67
RbBr	6.89	1.66	1.82
RbI	7.35	1.66	2.06
CsF	6.02	1.81	1.19
AgF	4.92	1.29	1.19
AgCl	5.55	1.29	1.67
AgBr	5.77	1.29	1.82

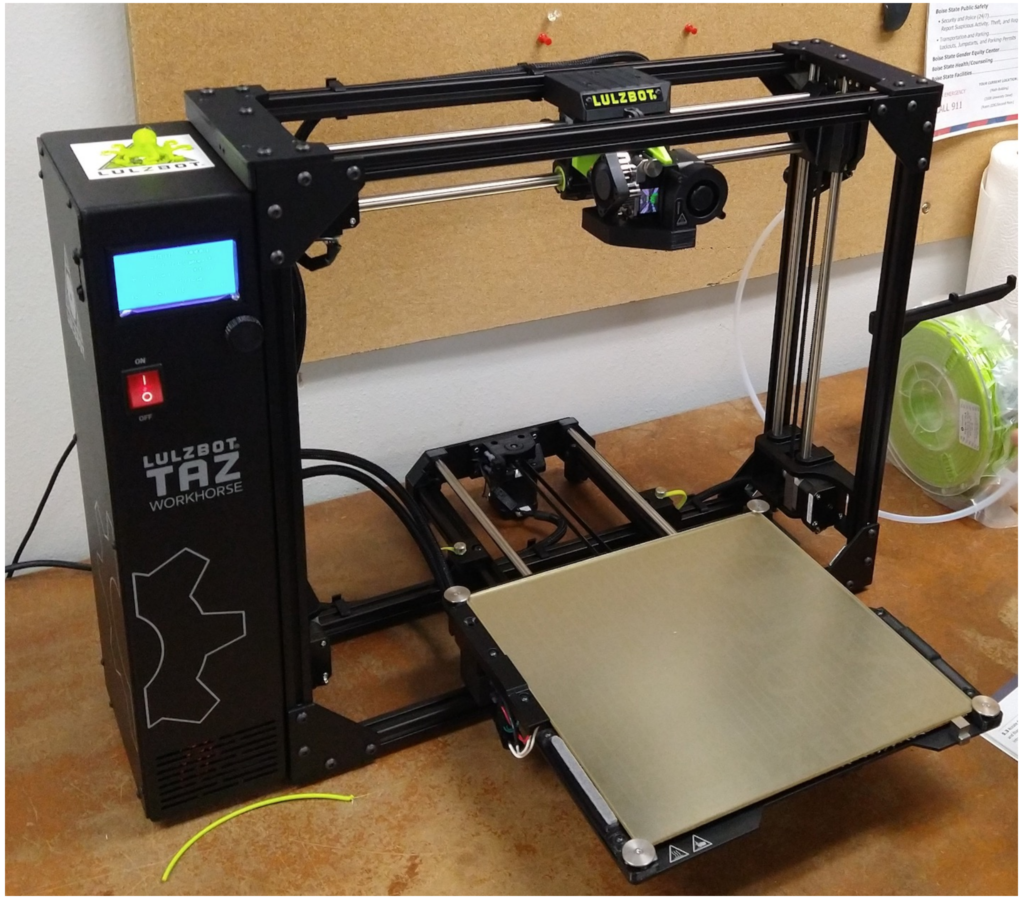
Lattice Constants at 300K

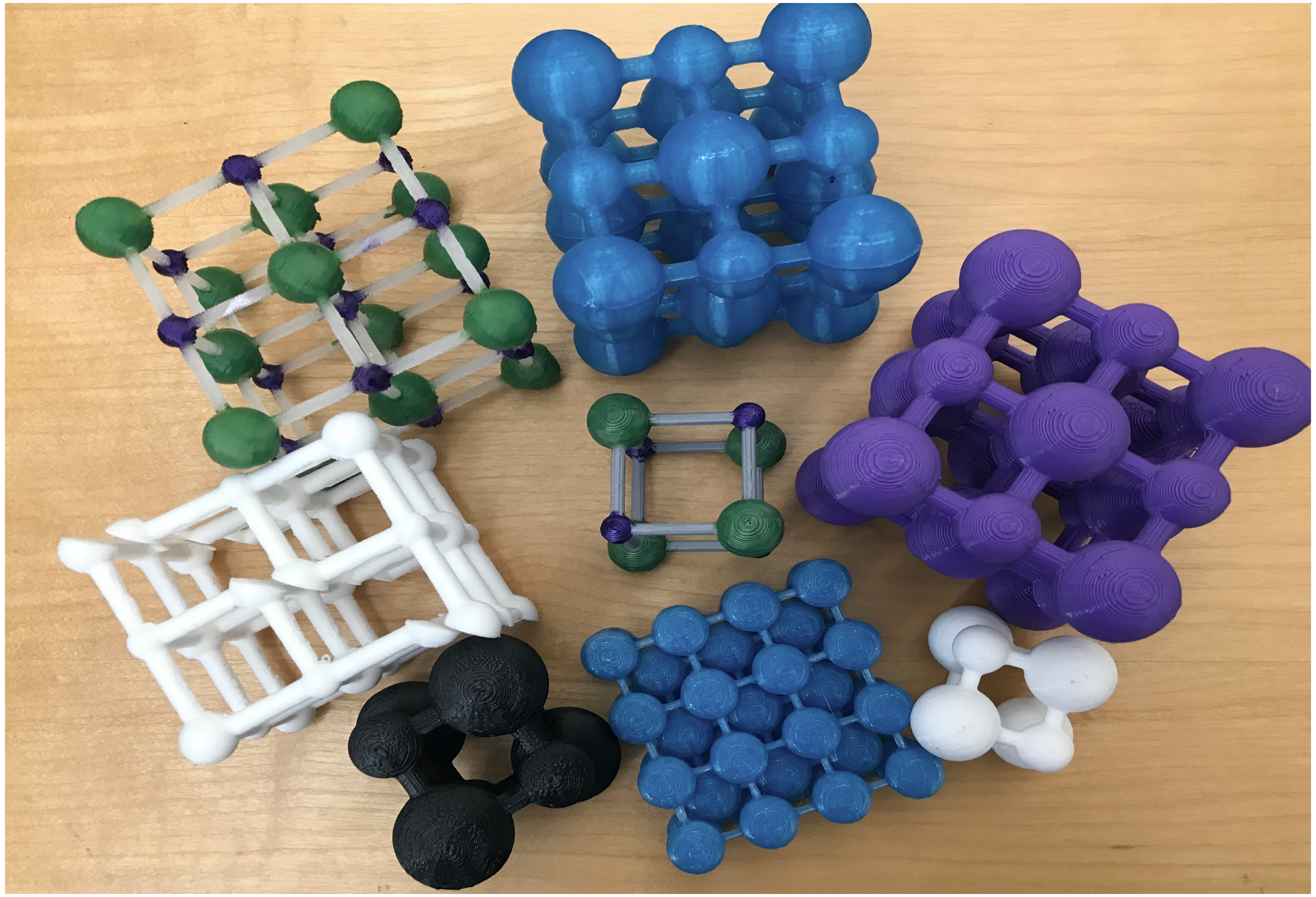
- Simple substance + compounds

Material	a (Å)	ra (Å)	Material	a (A)	Ionic ra(Å)	ionic rb(Å)	Material	a (A)	Ionic ra(Å)	Ionic rb(Å)
Al	4.046	1.25	MgO	3.0399	0.86	1.26	KF	5.34	1.52	1.19
Ni	3.499	1.35	ZnO	4.580	0.88	1.26	KCl	6.29	1.52	1.67
Cu	3.597	1.35	PbS	5.9362	1.33	1.70	KBr	6.60	1.52	1.82
Pd	3.859	1.40	PbTe	6.4620	1.33	2.07	KI	7.07	1.52	2.06
Ag	4.079	1.60	LiF	4.03	0.90	1.19	RbF	5.65	1.66	1.19
Pt	3.912	1.35	LiCl	5.14	0.90	1.67	RbCl	6.59	1.66	1.67
Au	4.065	1.35	LiBr	5.50	0.90	1.82	RbBr	6.89	1.66	1.82
Pb	4.920	1.80	LiI	6.01	0.90	2.06	RbI	7.35	1.66	2.06
			NaF	4.63	1.16	1.19	CsF	6.02	1.81	1.19
			NaCl	5.64	1.16	1.67	AgF	4.92	1.29	1.19
			NaBr	5.97	1.16	1.82	AgCl	5.55	1.29	1.67
			NaI	6.47	1.16	2.06	AgBr	5.77	1.29	1.82

Print it!

- 3D Printing





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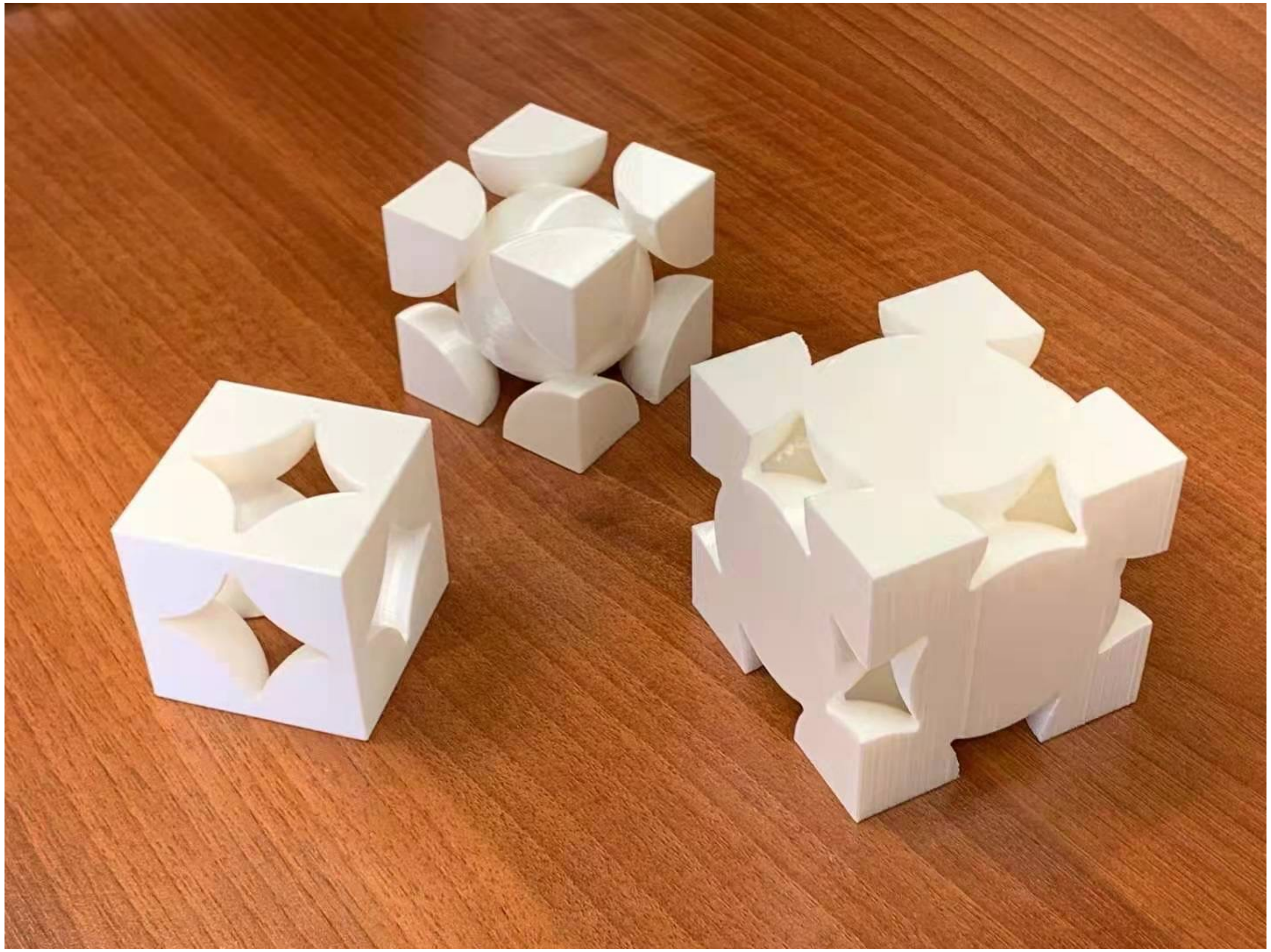
- 3D Printing



Summary: Geometrical Concepts

- Polygon (2D)
  - A plane shape consisting of a finite number of line segments.
- Polyhedron and Platonic solids (3D)
  - (Regular) Tetrahedron has 4 triangular faces, with 3 meeting at each vertex, 6 straight edges, and 4 vertices.
  - Cube has 6 squares, with 3 meeting at each vertex, 12 straight edges and 8 vertices.
  - (Regular) Octahedron has 8 equilateral triangles, with 4 meeting at each vertex, 12 edges, and 6 vertices.
- Measurement
  - A comparison with a fixed reference amount of a quantity. The reference amount is called unit.
- Coordinates
  - A system using numbers (e.g., x, y, z) to determine positions of geometrical elements
- Symmetry
  - Translation: A shape or design if there is a translation of the plane such that the design or pattern as a whole occupies the same place in the plan both before and after translation.
  - Rotation: A shape or a design in a plan, if there is a rotation of the plane of more than 0 degrees but less than 360 degrees, such that the shape or design as a whole occupies the same points in the plan both before and after rotation.
  - Reflection: A shape or a design in a plan, if there is a line in the plane such that there are matching parts when the shape or design is folded along the line. Coordinates
- Ratio
  - Two quantities are in ratio A to B if there are N x A units of the first quantity, N x B units of the second quantity.
- Similarity
  - Two objects are similar if every point on one object corresponds to a point on the other object and there is a positive K, such that the distance between any two points on the second object is K times as long as the distance between the corresponding points on the first object.

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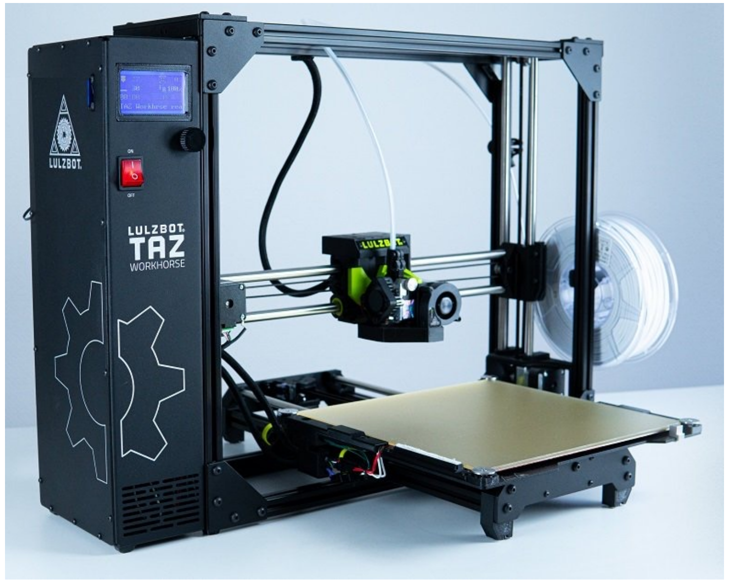
Outline

- What is 3D Printing
- Anatomy of 3D Printer
- 3D Printing Steps



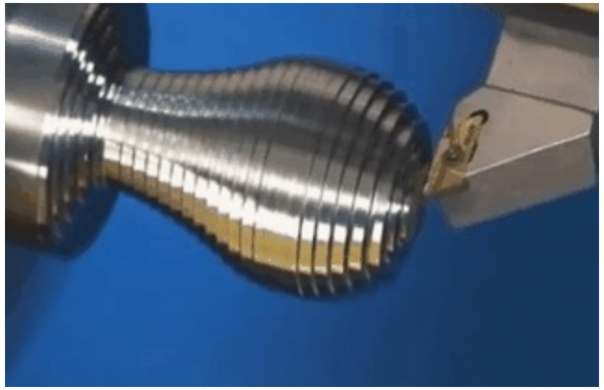
Lulzbot Workhorse

Prusa i3 MK3S+

3D Printing

- Traditional manufacturing: material is subtracted during the manufacturing process
- Additive manufacturing: material is *additively* deposited, joined or solidified under computer control to create a 3D object typically layer by layer using a deposited nozzle.

Subtractive manufacturing



Additive manufacturing

Anatomy of 3D Printer (LulzBot)

Control Panel

SD Card

Power Button

Print Head

Filament Spool

Build Area

LulzBot Workhorse 3D Printer

Build Plate Dimensions	Limits (mm)
X	282
Y	282
Z	286

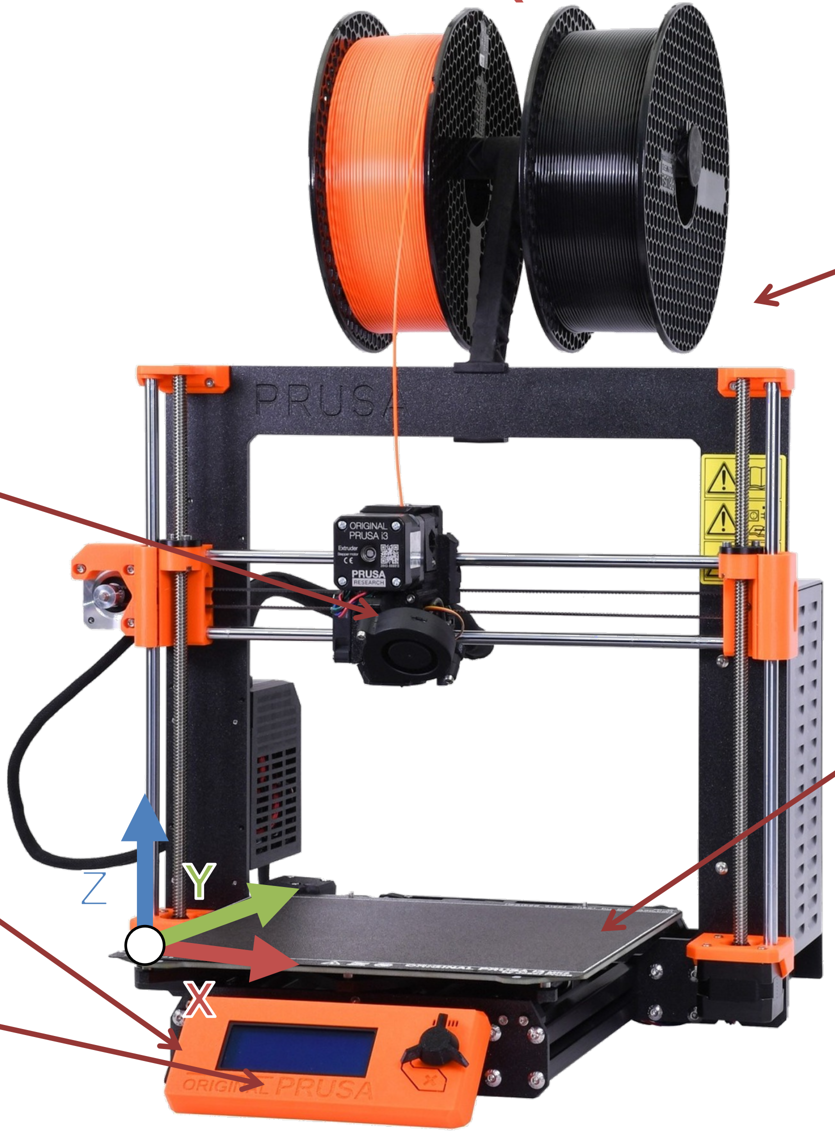
Anatomy of 3D Printer (Prusa)

Filament Spool

Print Head

Power Switch

Build Area



SD Card

Control Panel

Prusa i3 Mk3S+

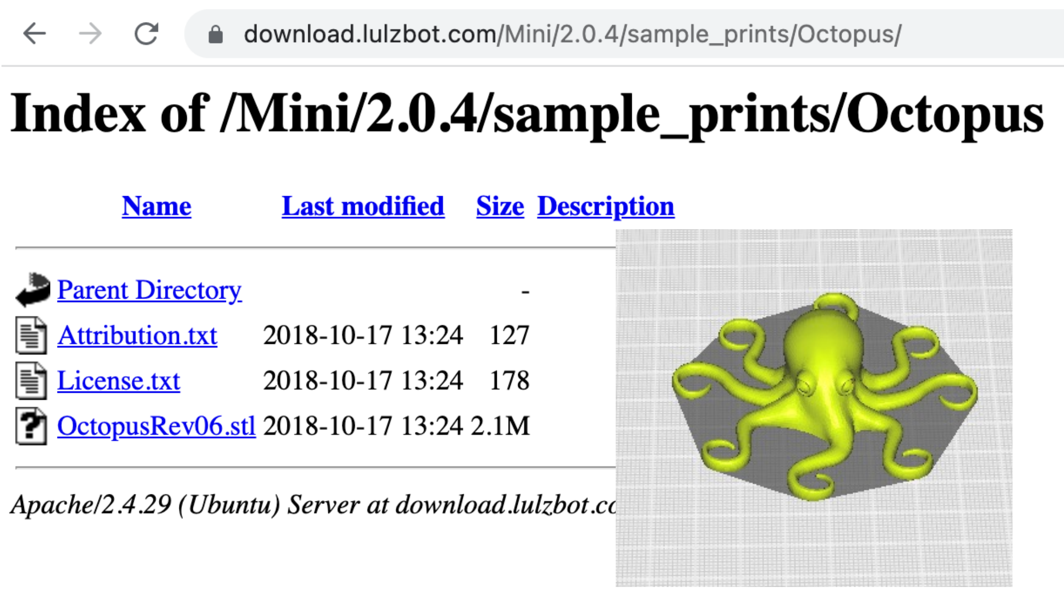
Build Plate Dimensions	Limits (mm)
X	210
Y	210
Z	250

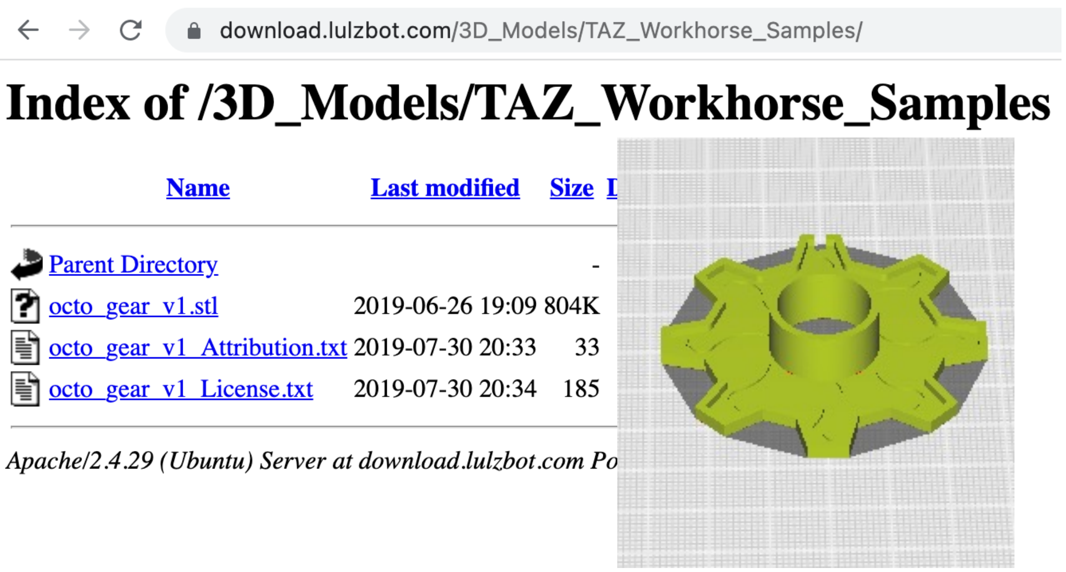
Steps to 3D Prints

1. Prepare the 3D Model file
2. Access LulzBot Cura (First Time User)
3. Prepare for 3D Printing
4. Print on 3D Printer
5. Lab Scheduling Management
6. Safety

Steps 1. Prepare a 3D Model file for print

- Your first 3D Prints using built-in 3D files
  - In lab computers, search "OctopusRev06.stl" "octo_gear_v1.stl"
  - Or
    - https://download.lulzbot.com/Mini/2.0.4/sample_prints/Octopus/
    - https://download.lulzbot.com/3D_Models/TAZ_Workhorse_Samples/
  - Or
    - http://cs.boisestate.edu/~mlong/3dprinting/octo_gear_v1.stl
    - http://cs.boisestate.edu/~mlong/3dprinting/OctopusRev06.stl





Step 2. Access Cura LulzBot (Printing Software)

- Open Cura Lulzbot on any computer in the Lab. You can also download it to your personal computer.

https://www.lulzbot.com/cura

QUICK START GUIDE (VIDEO) DOWNLOAD

Cura LulzBot Edition is a Free Software program that both prepares your files for printing (by converting your model into GCODE), and also allows you to control the operation of your LulzBot 3D printer.

The latest version features an updated user interface, more slicing options, an updated slicing engine, and better print quality than ever before. Keep Cura LulzBot Edition updated to have the latest pre-set Cura print profiles, developed and tested by the LulzBot team to ensure the best performance out of your LulzBot!

Download, Installation, and Removal Instructions

Find links and instructions based on your operating system in the tutorials below.

Current Version: **3.6.25 - 10**

CURA LulzBot Edition WINDOWS

CURA LulzBot Edition MAC OSX

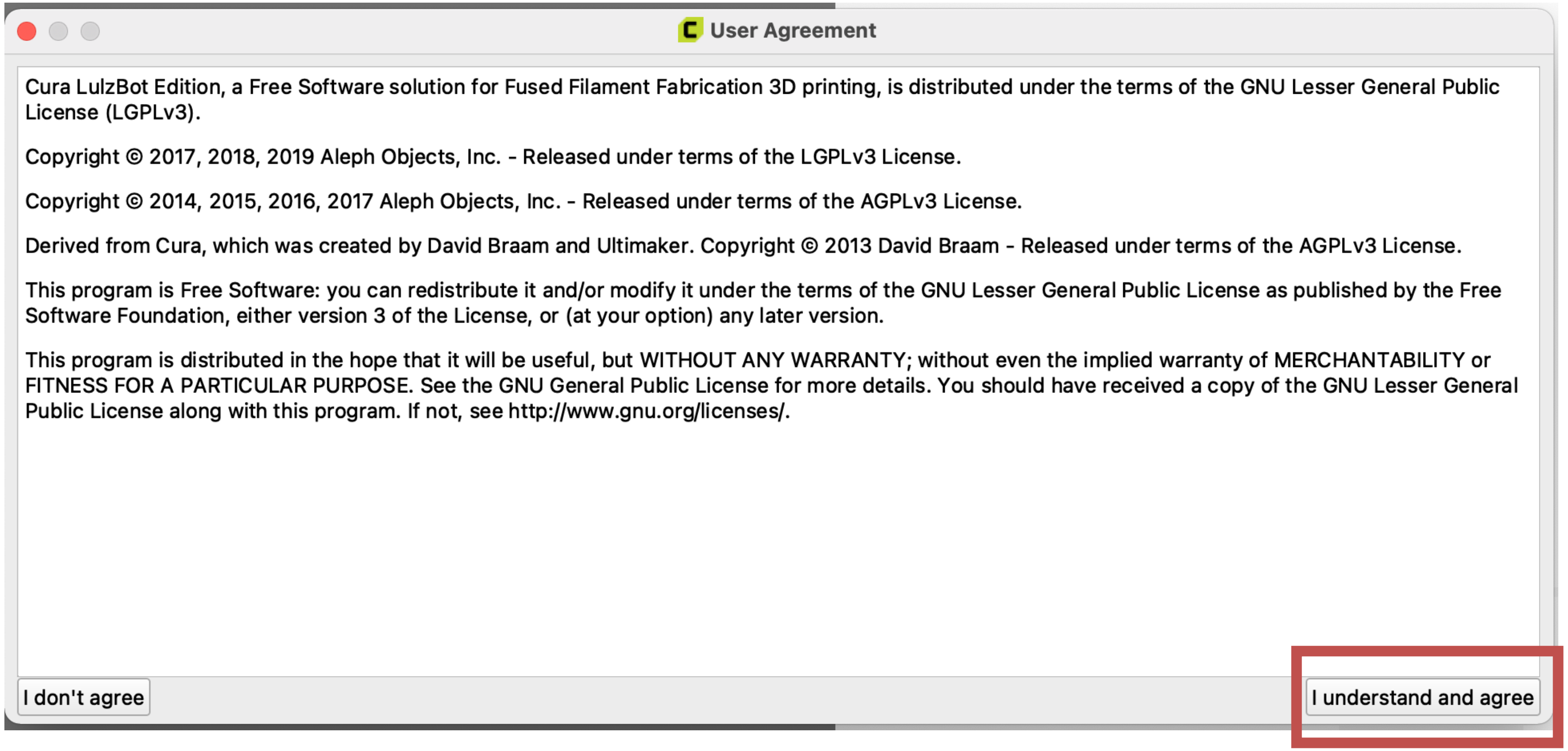
CURA LulzBot Edition DEBIAN

CURA LulzBot Edition FEDORA

CURA LulzBot Edition UBUNTU

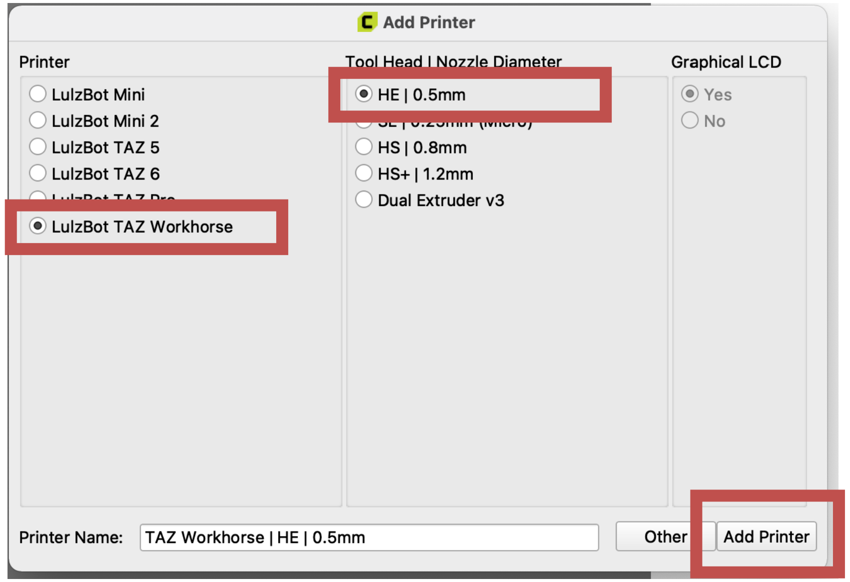
Step 2. Access Cura LulzBot: first time user

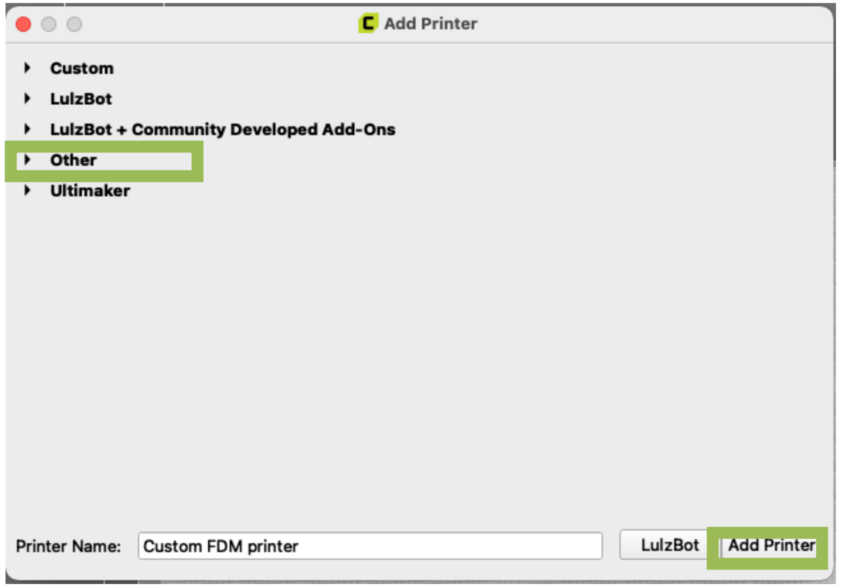
- User Agreement:
  - Select "I understand and agree"



Step 2. Access Cura LulzBot: first time user

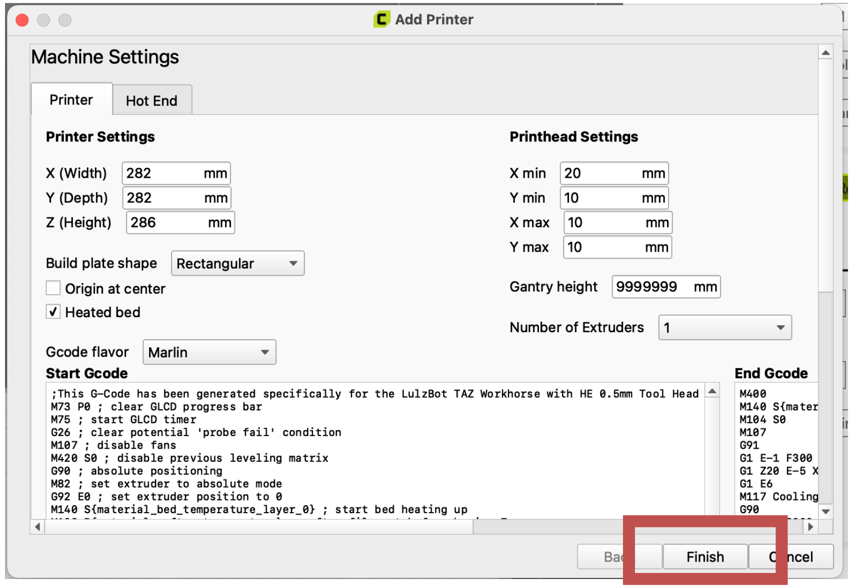
- Add a printer
  - For Lulzbot, select **Lulzbot TAZ Workhorse**
    - For Tool Head: select HE | 0.5 mm
    - Click the “Add Printer” button to confirm
  - For Prusa, select **Other** and select **Prusa i3 Mk2**



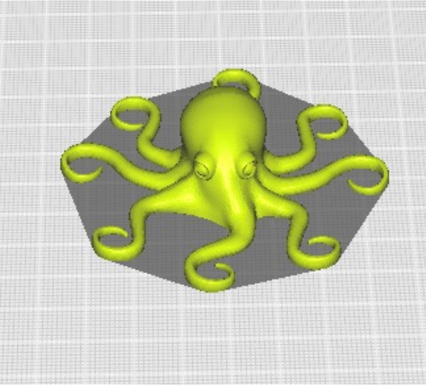


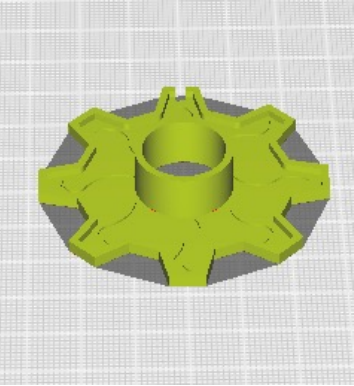
Step 2. Access Cura LulzBot: first time user

- A dialogue box with machine settings will appear. Don't change anything and select "Finish".



- A built-in **Octopus** or **Gear** will appear in the build area.

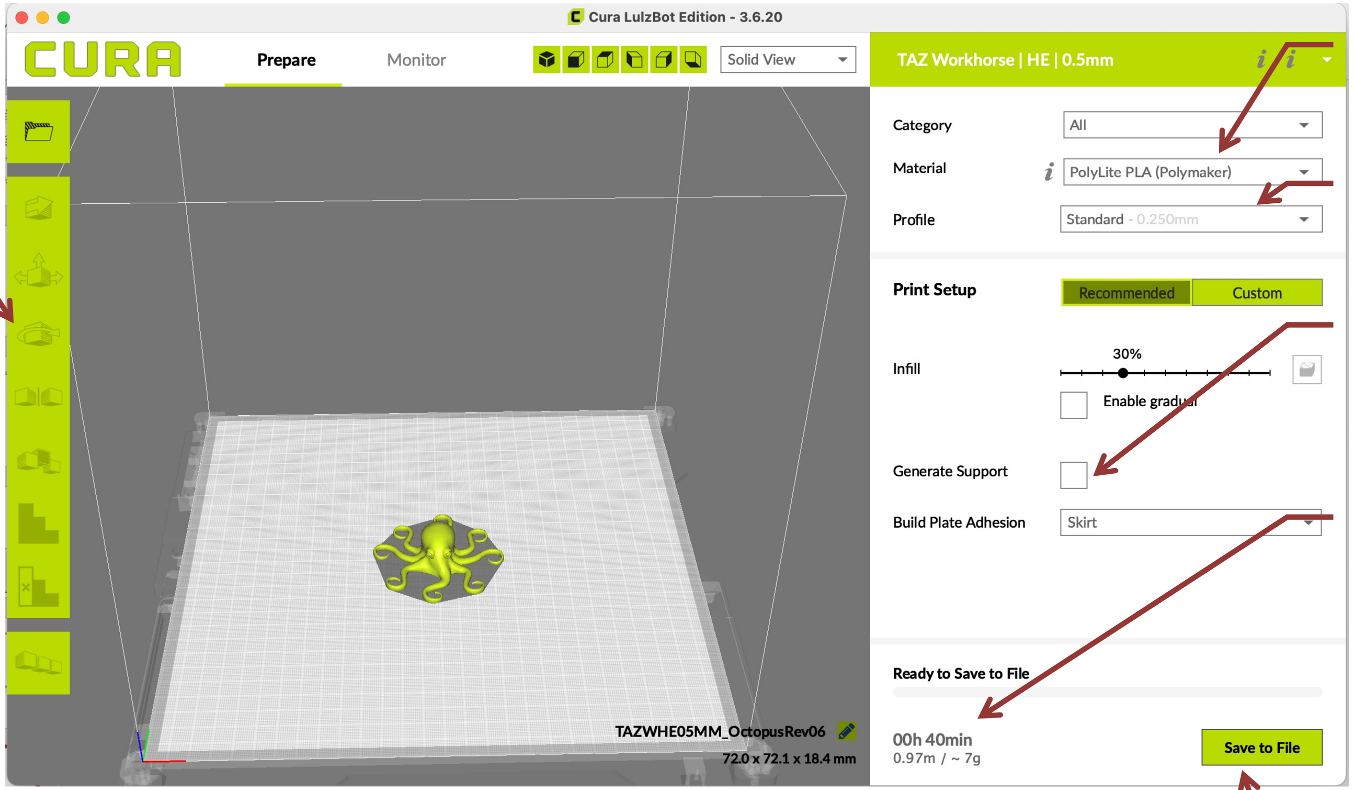




Step 3. Prepare for 3D Printing

- Select "octo_gear_v1.stl", you will see

Tool Bar for manipulating file



Material (PolyLite PLA)

Profile (0.25mm)

For better support between printed parts (usually not needed)

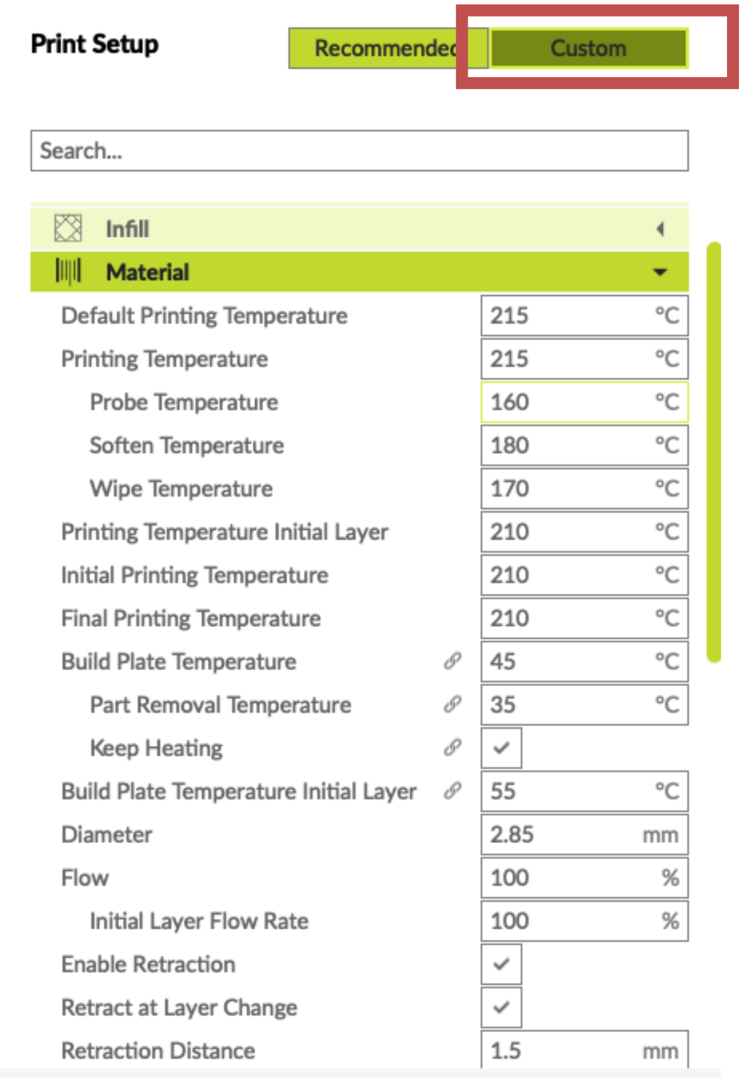
Approximate Time

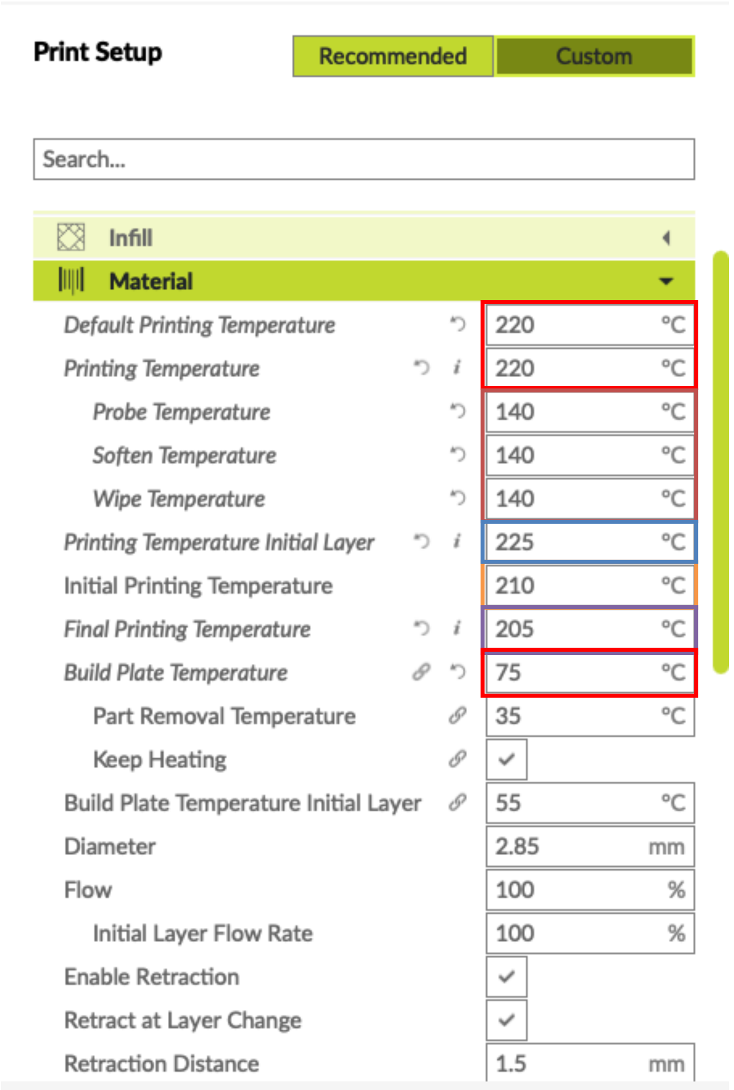
Save to File

Step 3. Prepare for 3D Printing (Lulzbot)

- Click "Custom" (optimize parameters to avoid printer jam)

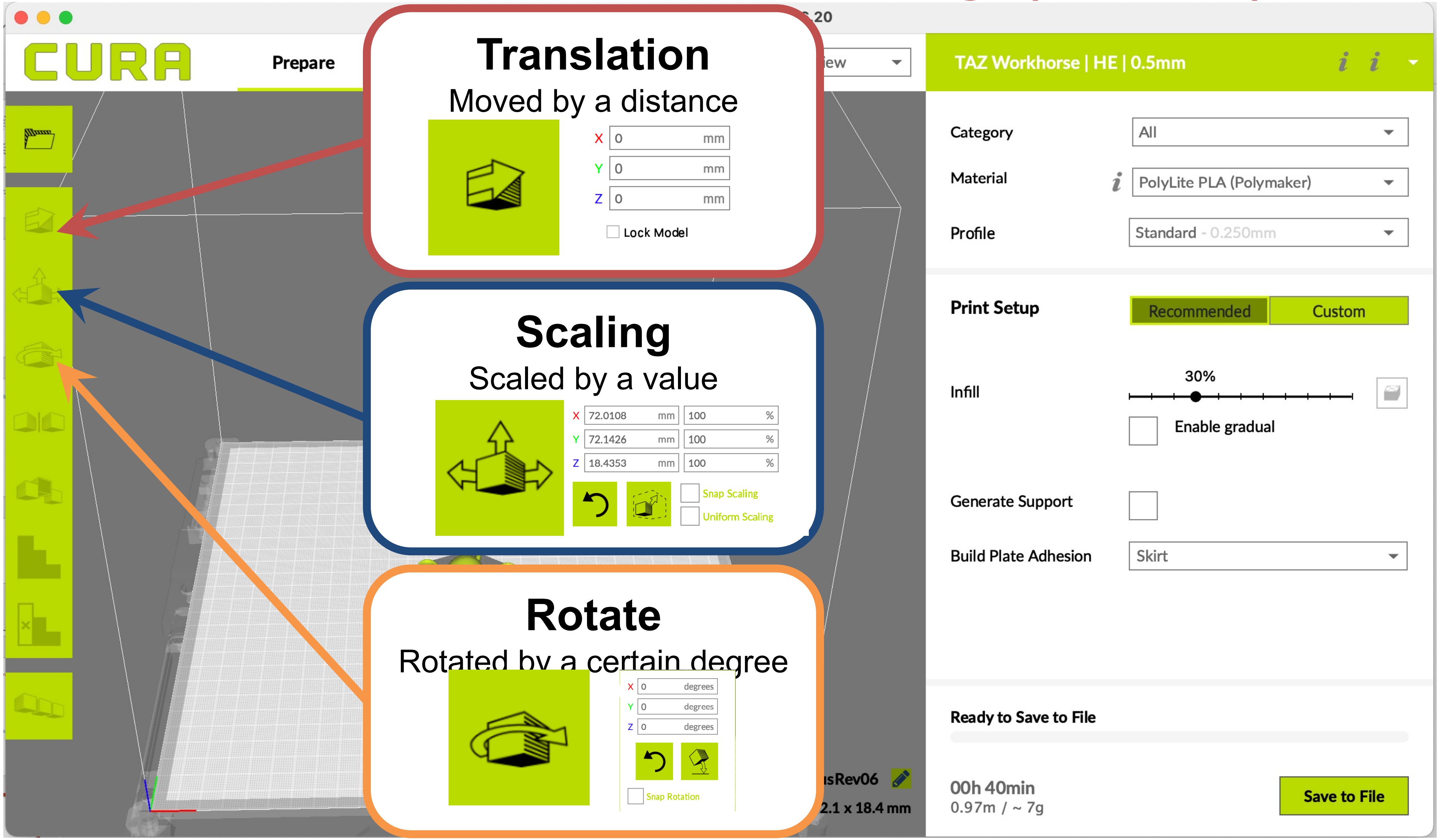
Before





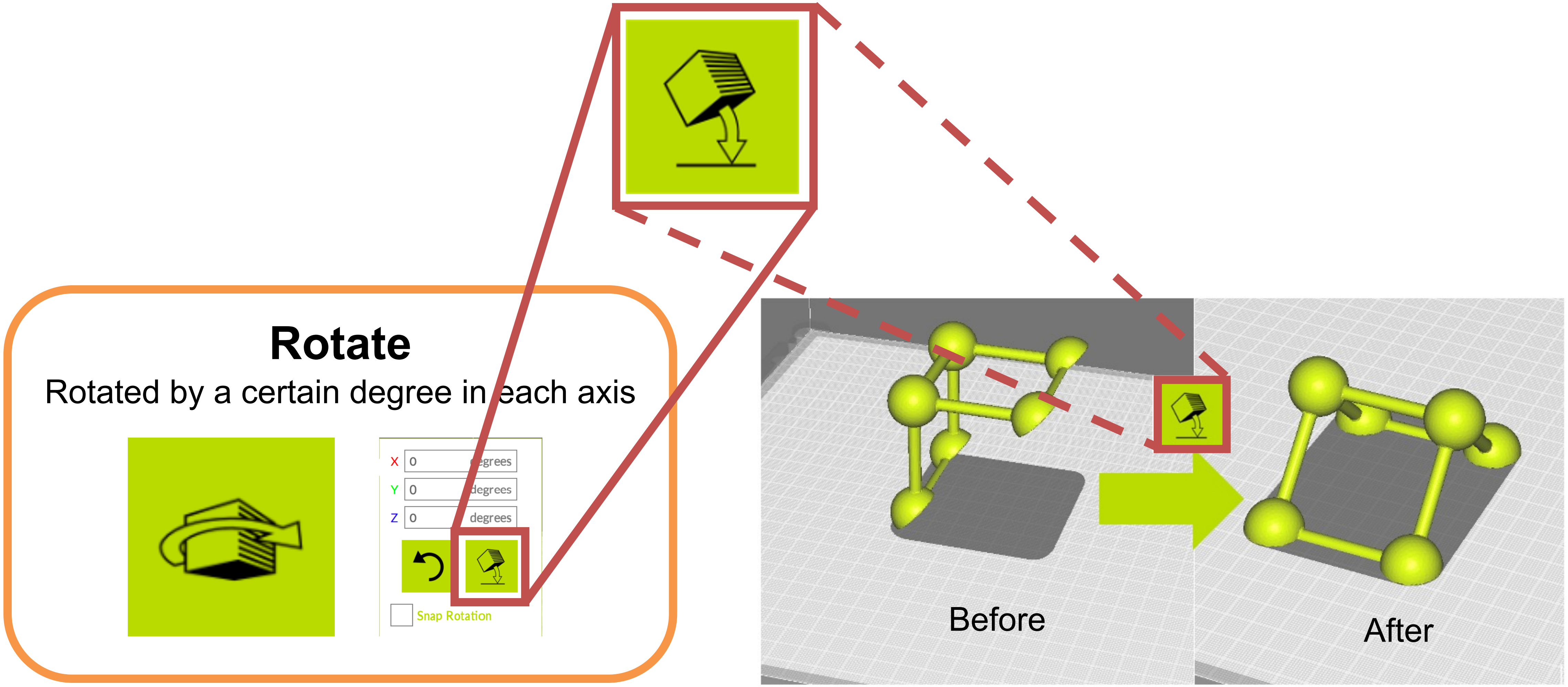
After

Step 3. Prepare for 3D Printing (cont'd)



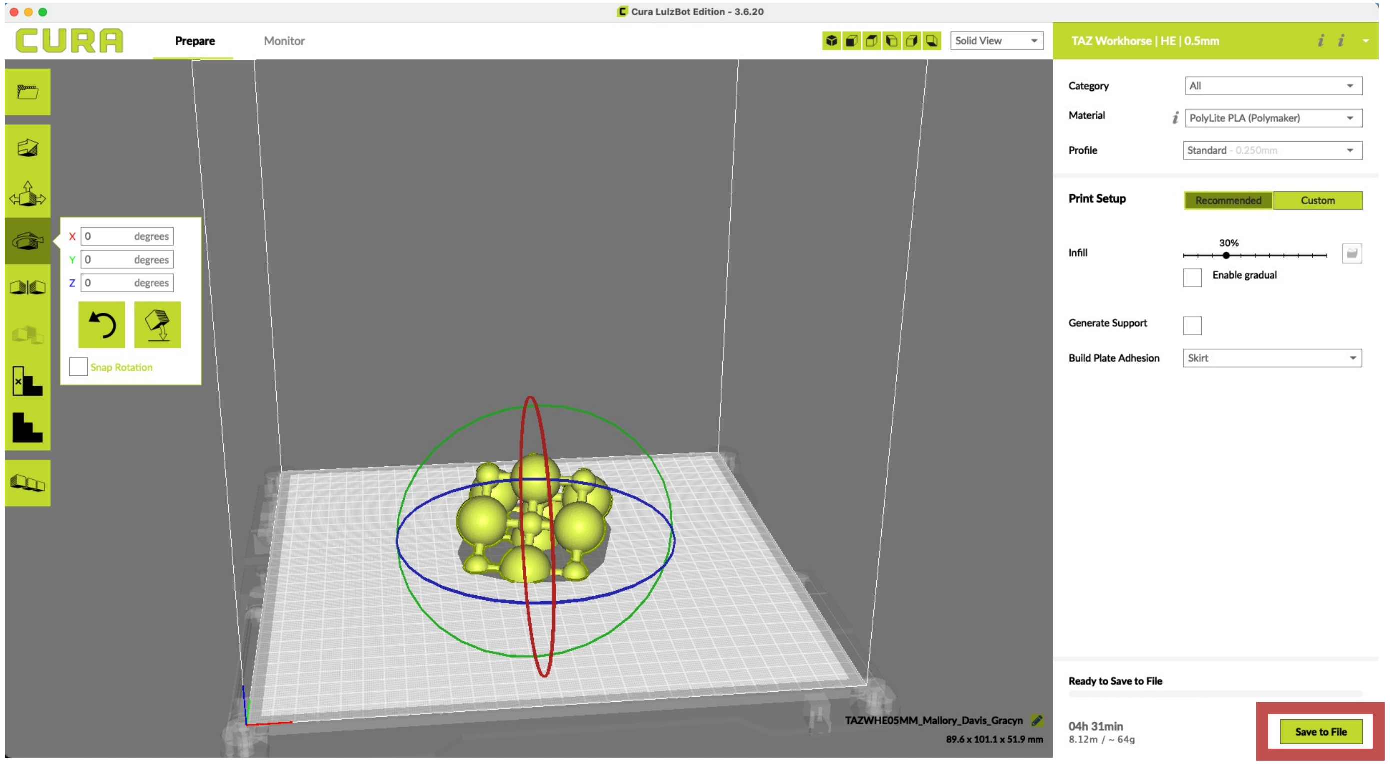
Step 3. Prepare for 3D Printing (cont'd)

- For the rotation, we **highly** recommend using the "Lay Flat" button.



Step 4. 3D Printing Time!

- Option 1: Print through SD card (Prusa/Lulzbot)
  - Click **Save to File** in Cura
    - Save the model in .Gcode format to a SD card
  - Use printer's control panel for printing



Controller

SD Card

USB

SD Card

Controller

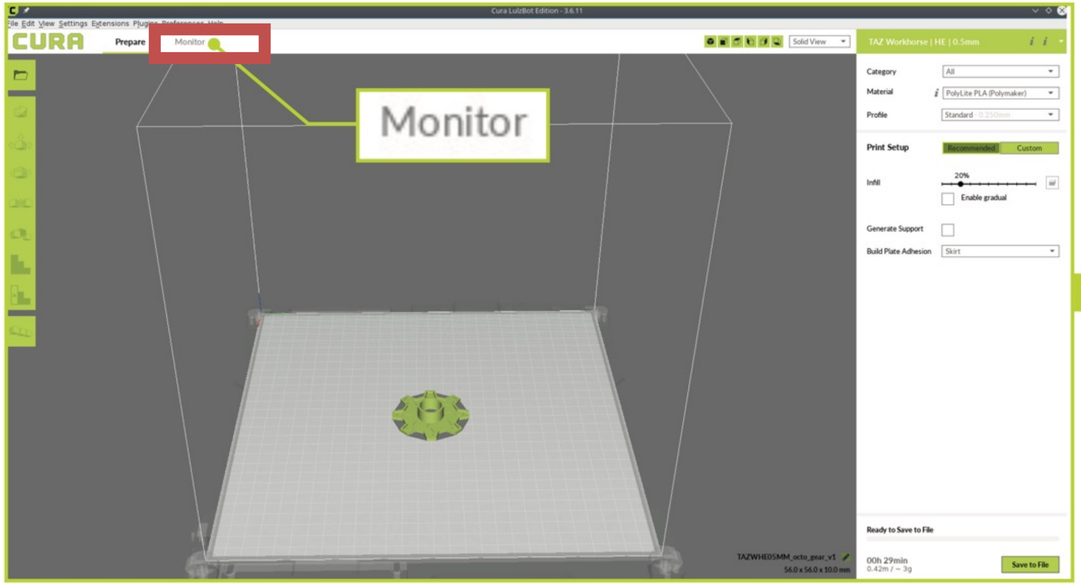
Step 4. 3D Printing Time!

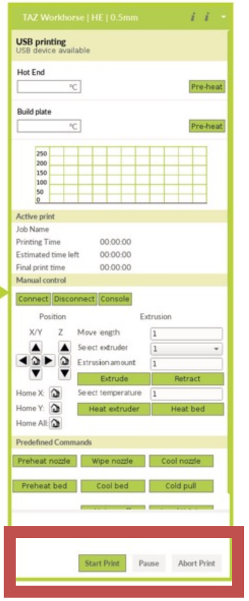
- Option 2: Print through Computer (Lulzbot only)
  - Click "Monitor" in Cura
  - Click "Start Print"

Controller

SD Card

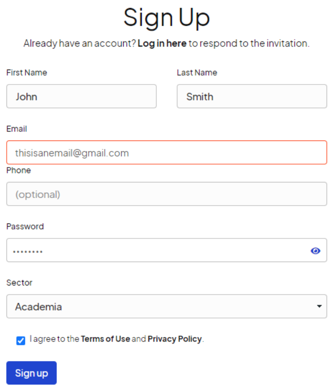
USB to Computer



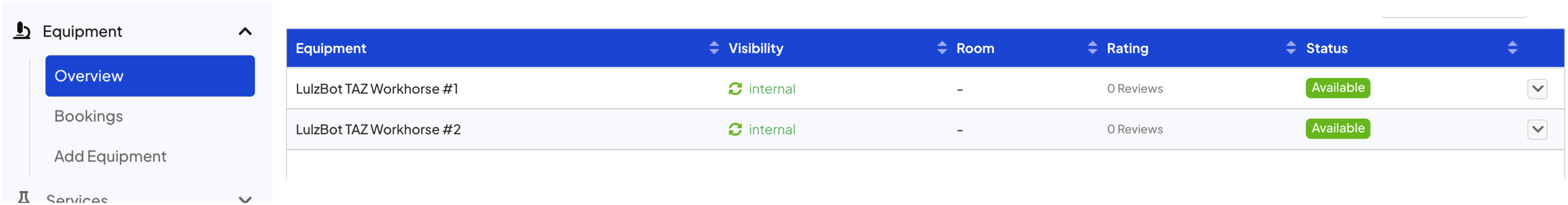


Step 5: Lab Scheduling Management (Optional)

- Lab Scheduling Management using ClusterMarket.com Platform
  - You should have gotten an email from clustermarket invite to join.
  - Select the link provided from the email.

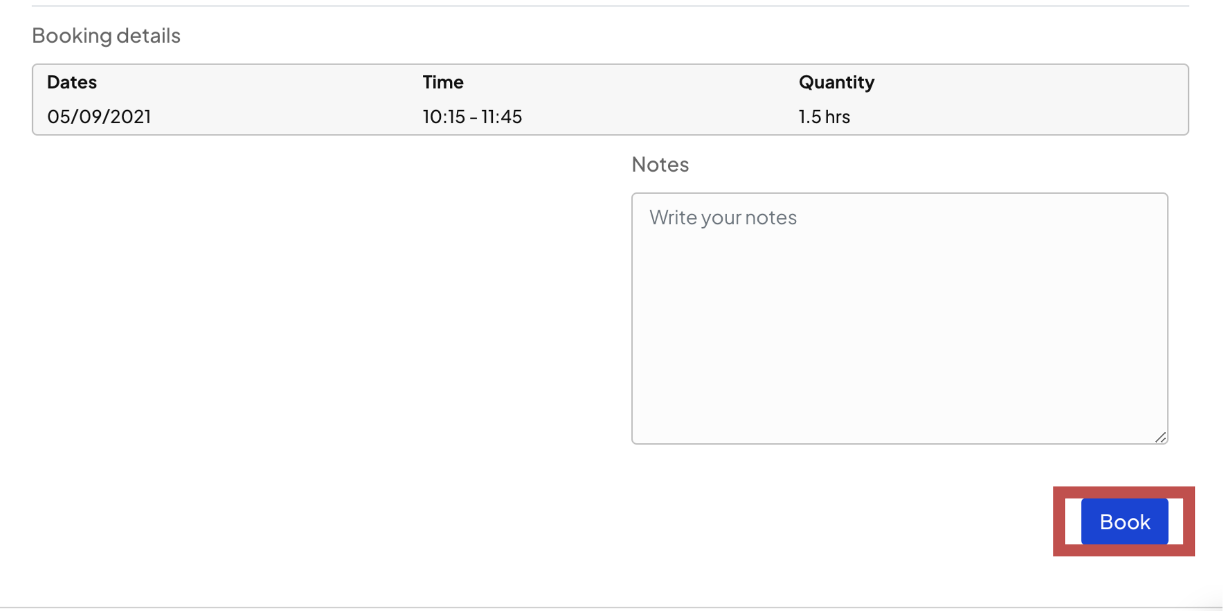


  - Afterwards, you will get the ability to schedule timeslots for 3D Printers. Select the **Equipment** tabs on the left and select one of the 3D Printers.



Step 5: Lab Scheduling Management (Optional)

- Select the approximate time period (from CURA)
  - For example, an Octupus takes about 40 min for printing.
  - Make sure to give yourself and others extra time.
- Select **Book** to confirm the booking



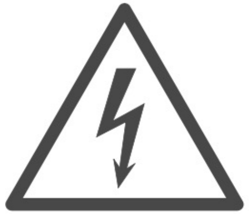
Stay Safe!

1. Burn Hazard
2. Electric Shock Hazard
3. Fire Hazard
4. Pinch Hazard

If you are not sure, ASK US in the lab

Burn Hazard

Never touch the extruder nozzle or heater block without first turning off the hot end and allowing it to completely cool down. The hot end can take up to 20 minutes to completely cool. Never touch recently extruded plastic. The plastic can stick to your skin and cause burns. The heated bed and stepper motors can reach high temperatures that are capable of causing burns.



Electric Shock Hazard

Always power down and unplug your 3D printer before connecting or disconnecting wiring harnesses or opening the electronics enclosure.
Never open the external power supply enclosure. The power supply can cause harm from electric shock even when powered down and unplugged.

Fire Hazard

Never place flammable materials or liquids on or near the 3D printer when it is powered on or operational.

Pinch Hazard

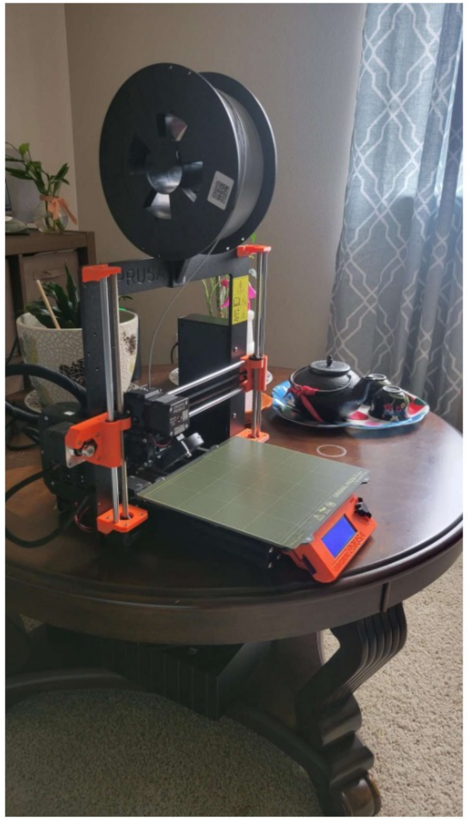
When the 3D printer is operational take care to never put your fingers in any moving parts including belts, pulleys, or gears. Tie back long hair or clothing that can get caught in the moving parts of the 3D printer.

Printer Maintenance

- Check User Manual https://cs.boisestate.edu/~mlong/education.html

3D Printer 1: Prusa 3 MK3S+

[Installation Guide]()



3D Printer 2: Lulzbot Workhorse (Use with caution. Hot end jam happens frequently)

[Quick Start Guide]()

[User Manual]()

[Test Printing]()

How to do Filament Change

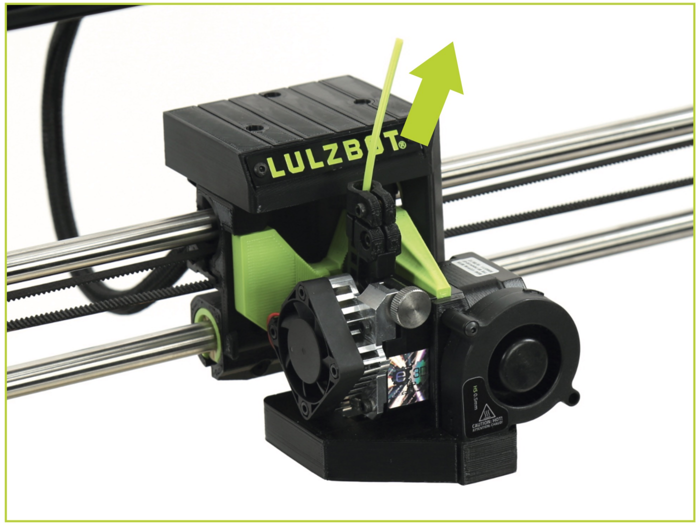
- Follow User’s Guide, Section 5
  - TAZ_Workhorse_QuickStartGuide_08-2019.pdf
  - Available at our website

5 Preparing Your LulzBot TAZ Workhorse to Print

Your LulzBot TAZ Workhorse was tested for quality assurance before being packaged. You will need to remove the remaining filament left in the tool head from this process before loading new filament for your next print. Follow the steps below to remove or change filament.

5.1 Press in on the LCD Control Knob to access the main menu on the LCD Screen. Turn the LCD Control Knob clockwise to scroll down to **Change Filament** and press in to select. Select **Preheat Custom** and turn the LCD Control Knob clockwise to increase the target temperature 220°C, then press in on the LCD Control Knob to confirm the preheat temperature.

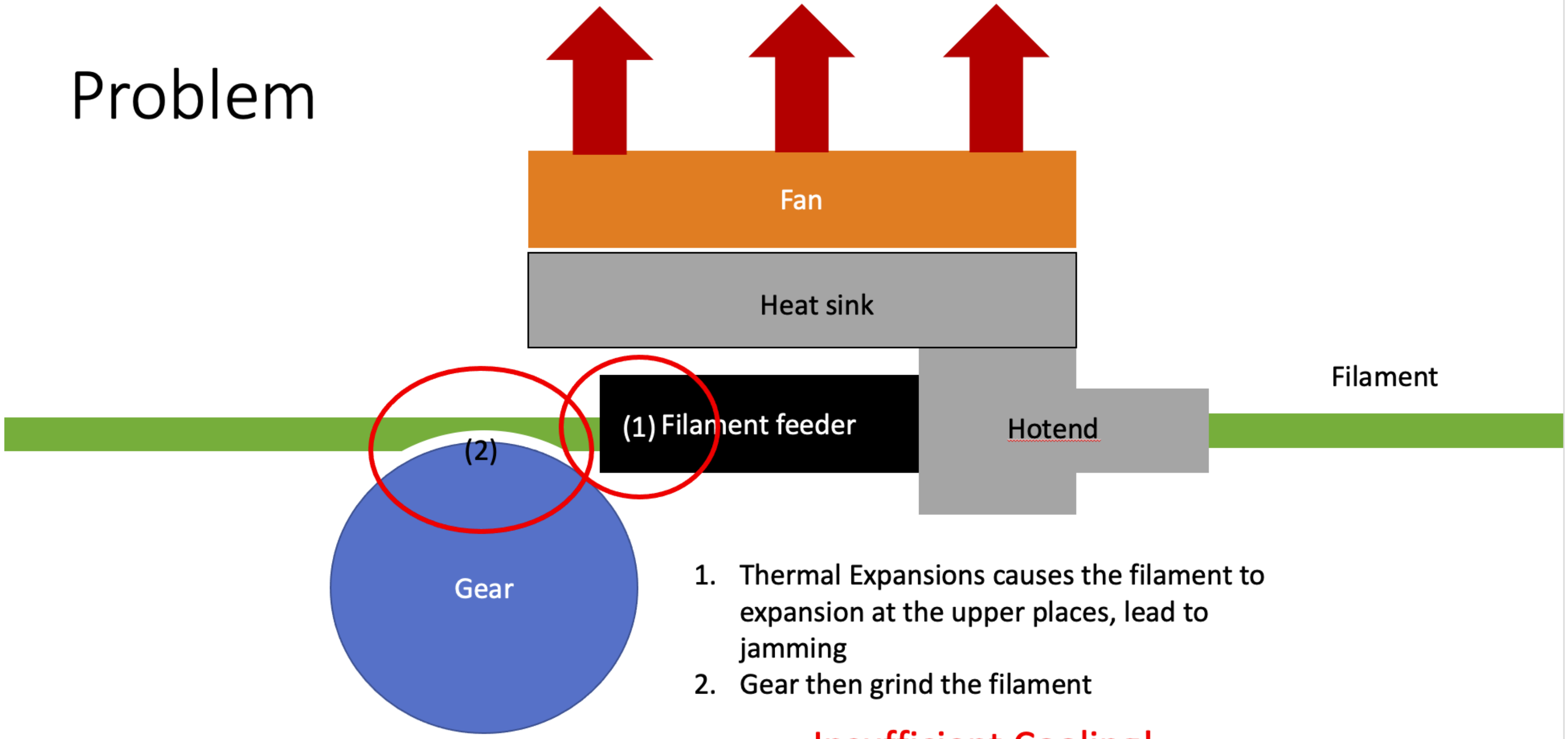
5.2 Once the hot end reaches the target filament removal temperature, the filament will automatically begin to retract. Once the filament stops moving, pull it out of the idler.



5 Preparing to Print

Potential "Hotend Jam" Issues in Lulzbot Printer

- An intrinsic design problem
- We are working on workarounds



1. Thermal Expansions causes the filament to expansion at the upper places, lead to jamming
2. Gear then grind the filament

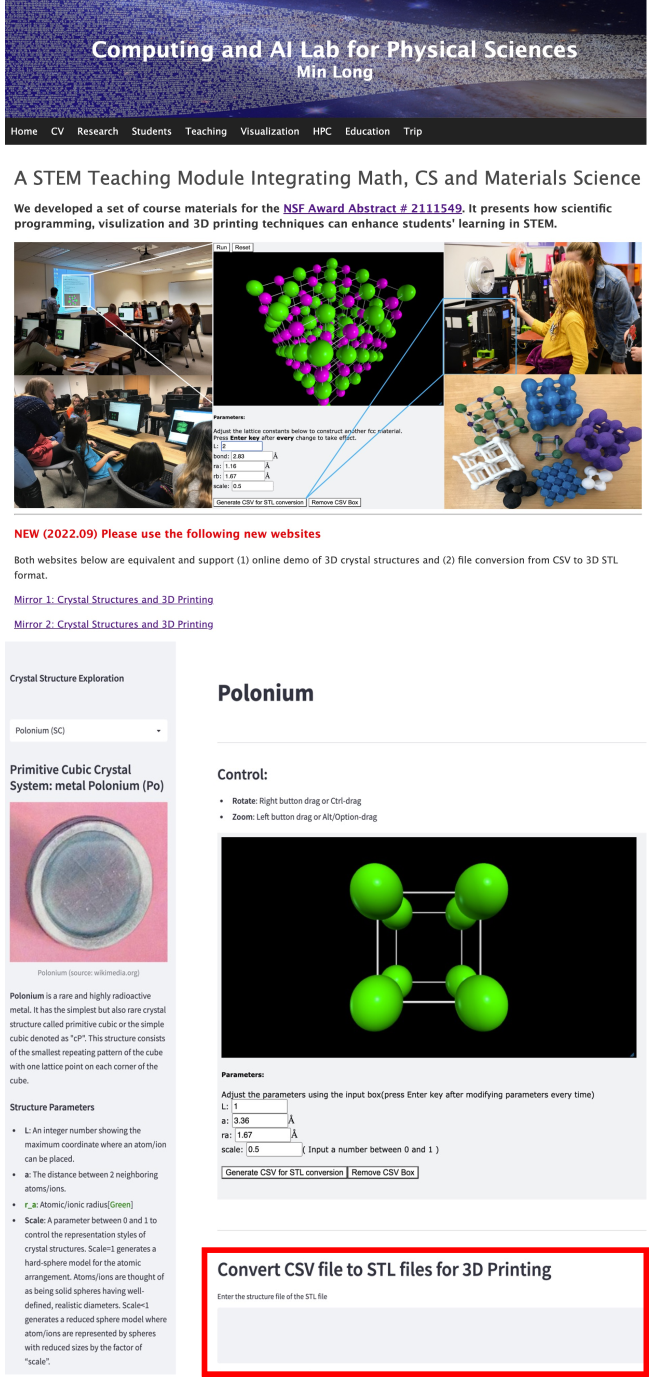
Insufficient Cooling!

Training Materials

- Overview and Objectives
- Lecture 1: Introduction to Online Toolkits and STEM Concepts (For instructors)
- Lecture 2: Introduction to 3D Printing
- Lecture 3: Design and Print SC and FCC Materials
- Lecture 4: Design BCC and Perovskite Materials

Websites for Resources

- Main Websites:
  - Toolkit, tables of data, 3D printer manuals...
  - https://cs.boisestate.edu/~mlong/education.html
  - https://minlong1.github.io/education.html
- Converting structure files (CSV) to 3D STL files:
  - Toolkit and converting tool
  - https://minlong1-csv2stl-streamlit-app-1nkv76.streamlitapp.com/
  - https://laumiulun-csv2stl-streamlit-app-lcc7hm.streamlitapp.com/

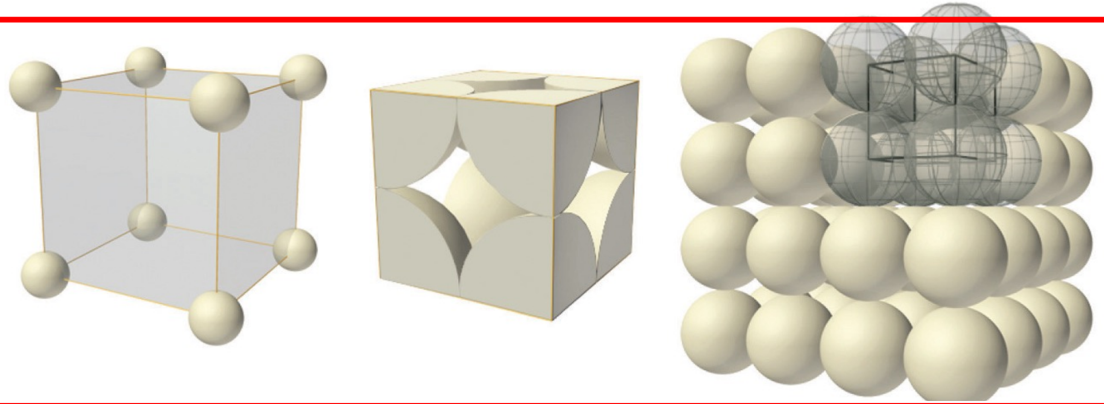


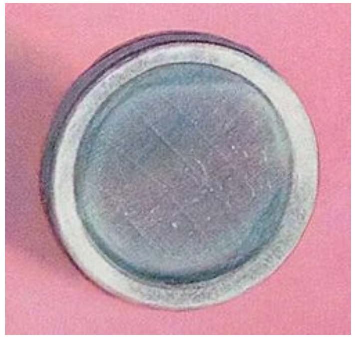
Outline

- All resources are available at Canvas
- Review Crystal Structures Learned in Class 1
- Access Online Toolkit
- Create your new fcc material
- Generate CSV files
- Upload CSV files
- We will convert CSV files to STL files for printing
- Bring the STL files to Lab

Crystal Structures – Let's print them

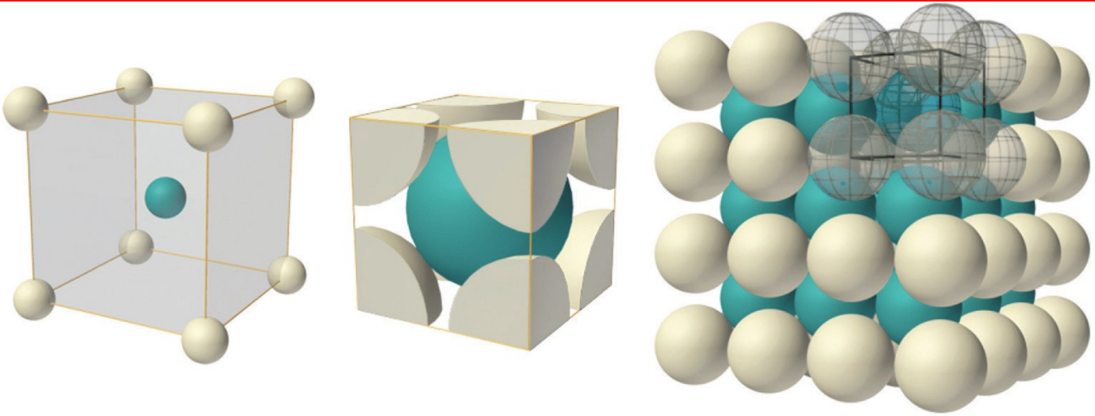
Simple Cubic





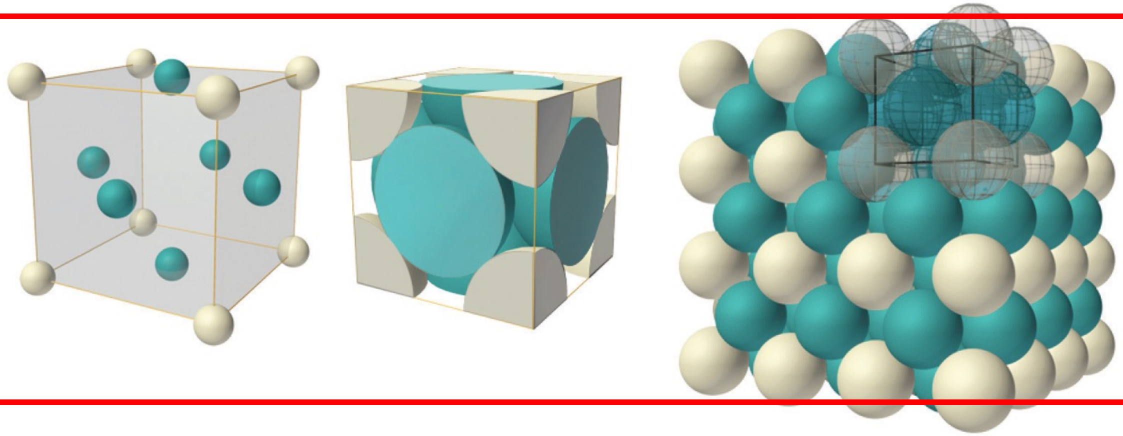
Polonium

Body-centered Cubic



Iron

Face-centered Cubic

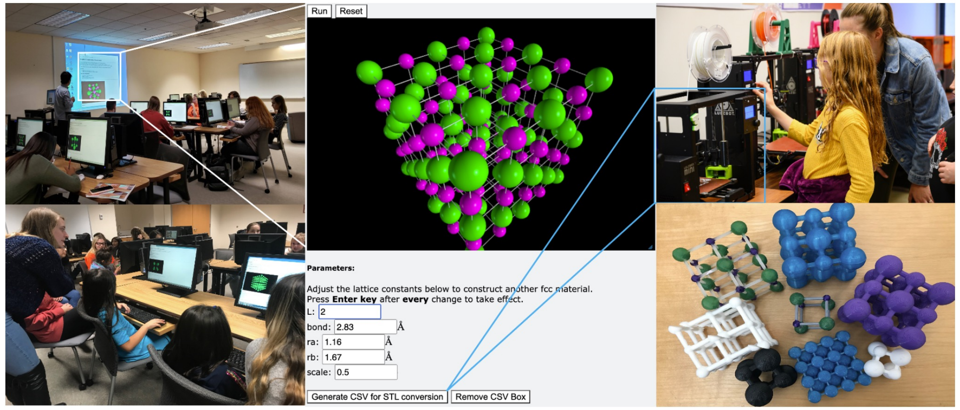


Access Online Toolkit

- Use online toolkit you have learned in lecture 1
  - http://cs.boisestate.edu/~mlong/education.html

A STEM Teaching Module Integrating Math, CS and Materials Science

We developed a set of course materials for the NSF Award Abstract # 2111549. It presents how scientific programming, visulization and 3D printing techniques can enhance students' learning in STEM.



Slides

Lecture Slides

Work Sheets

Part 1 Part 2

Primitive/Simple Cubic (cP) Lattice Structure

Polonium (metal)

It may take some time to load the page on your computer.

Face-Centered Cubic (fcc) Lattice Structure

Cu (Solid Copper)

NaCl (Salt)

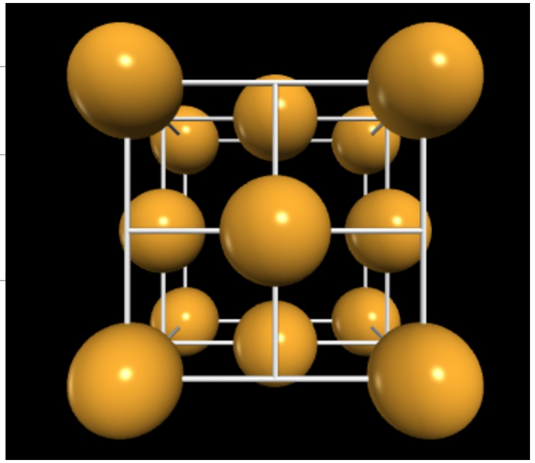
AgCl (Silver Chloride)

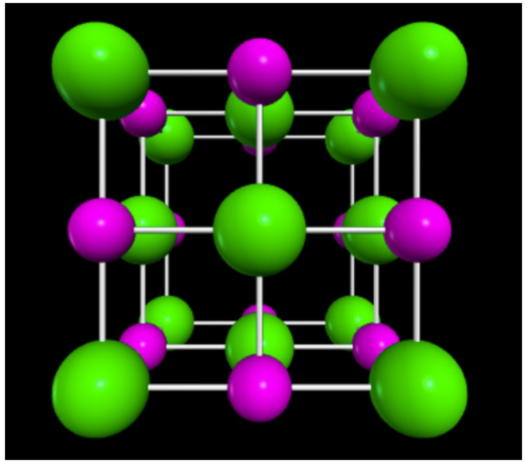
It may take some time to load the page on your computer.

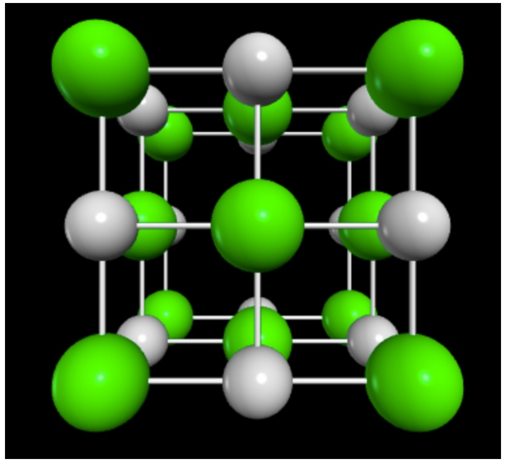
We provided 3 versions of Face-Centered Cubic (FCC) models, which represents two common materials: salt and silver chloride.

They have the same type of structure but different lattice parameters, atom size, and atom types.

You can choose anyone of them as the start point.



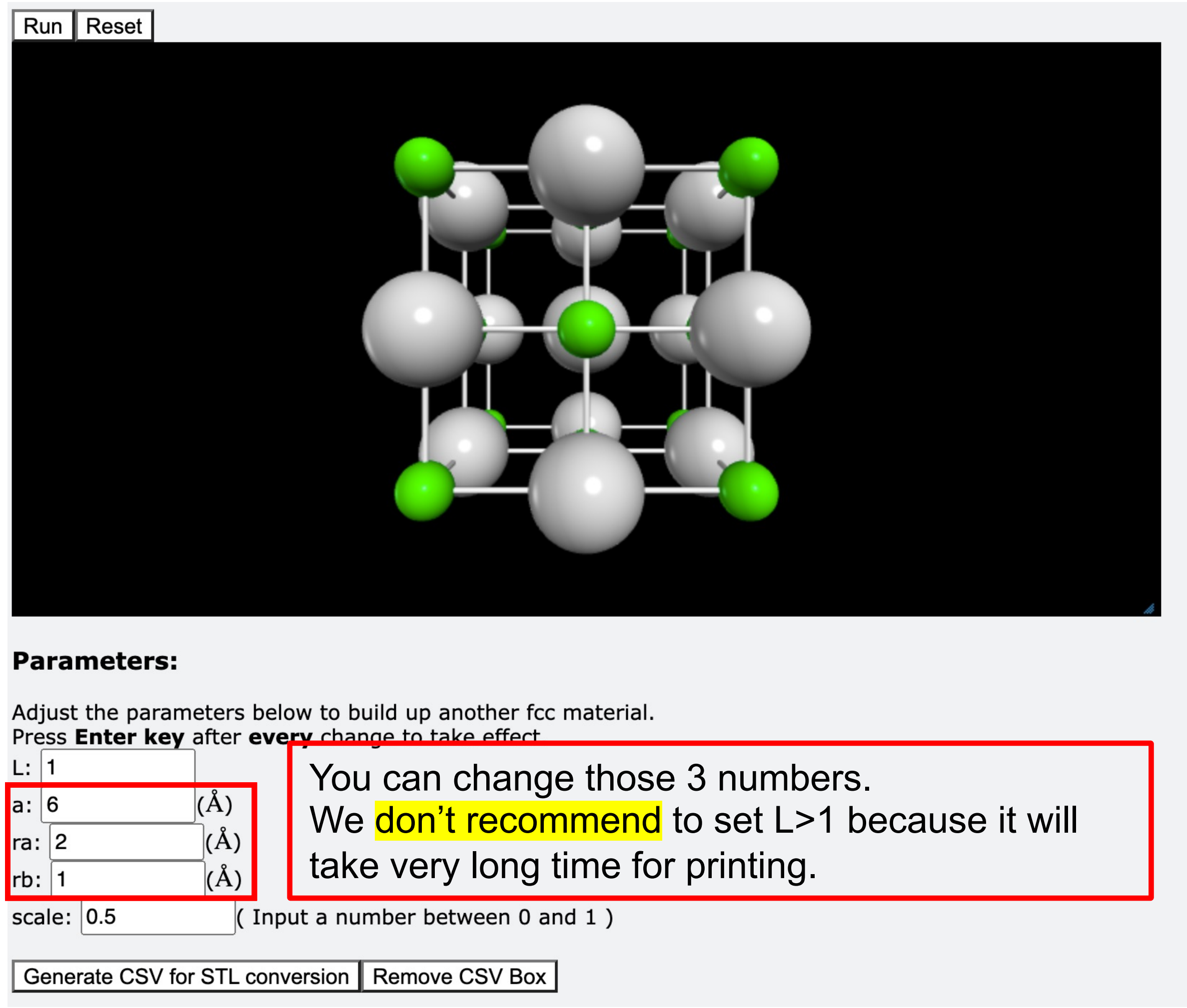




Optional: Create Your Own FCC Material

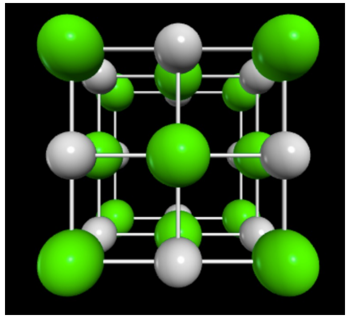
- You can create your own fcc material by changing parameters
  - L: An integer number showing the maximum coordinate where an atom/ion can be placed.
  - a: A standard lattice constant showing the distance between 2 neighboring Ag+ ions.
  - ra: Ionic radius of Silver [Silver] (Å)
  - rb: Ionic radius of Chloride [Green] (Å)
  - scale: A parameter between 0 and 1 to control the representation styles of crystal structures.

A toy “new” material



Create a CSV file

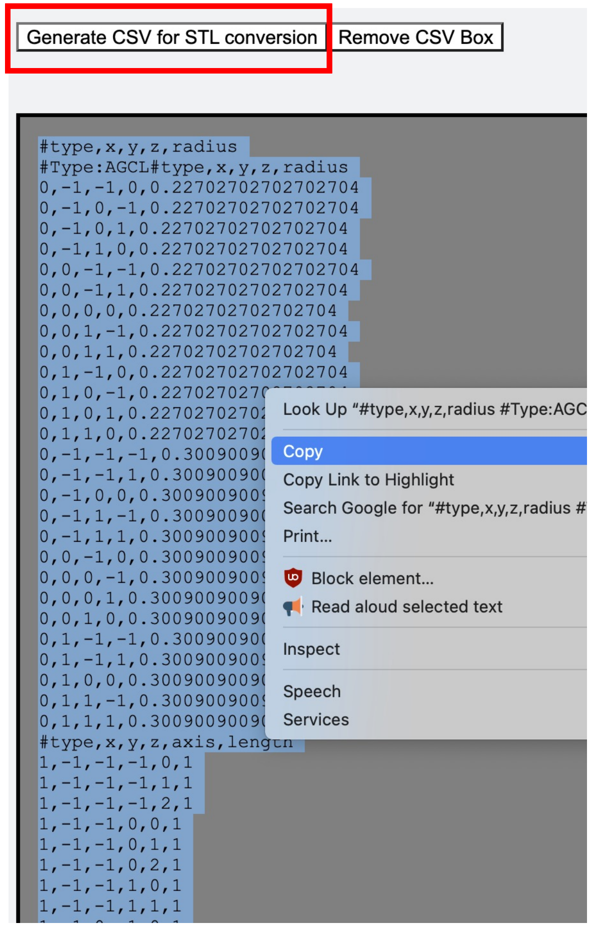
- CSV (comma-separated values) format
  - A simple text file in which information is separated by commas
  - It is used to save object information, such as spheres, bonds.



1. Click this button

2. Select all lines in the box

3. Right click and choose copy

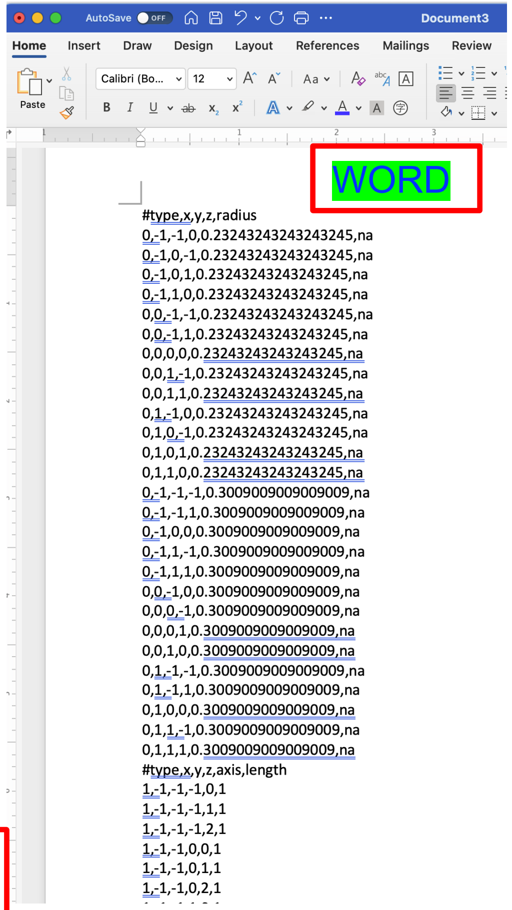


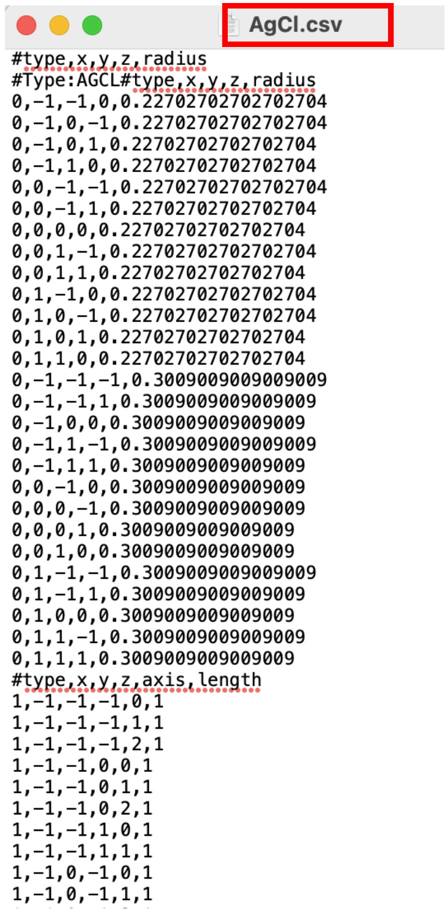
4. Open a text editor such as WORD or notepad in windows or TextEditor in Mac

5. Paste the content

6. Save it: AgCl.docx or AgCl.csv

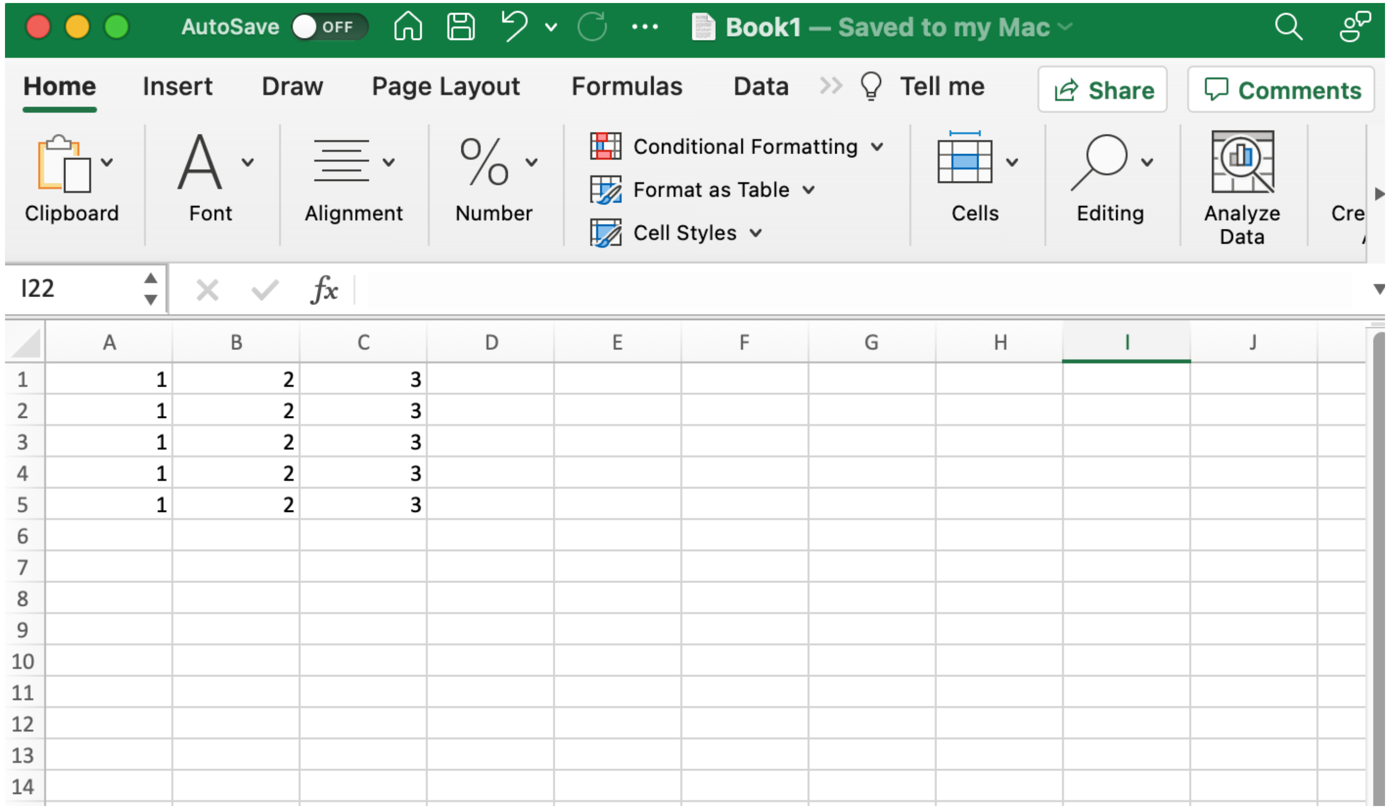
1 structure 1 file !





A sample CSV file

- You’ve used CSV files before, indeed

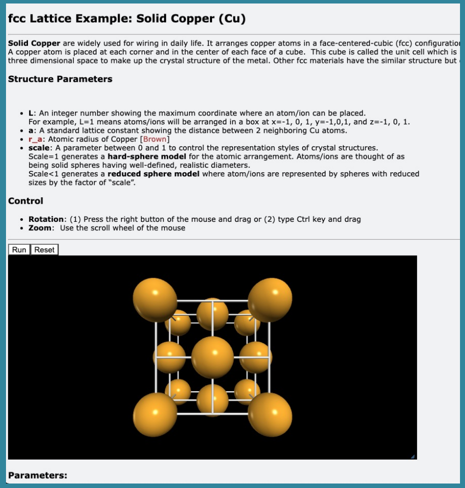


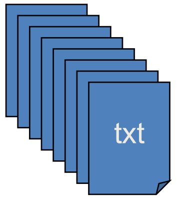
What’s Next?

- A Complete Pipeline to Prepare a Pintable 3D STL file for Printing

GUI Website

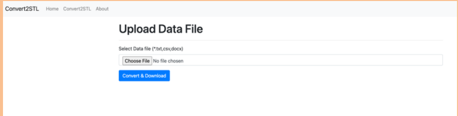
Create a Desired CSV file

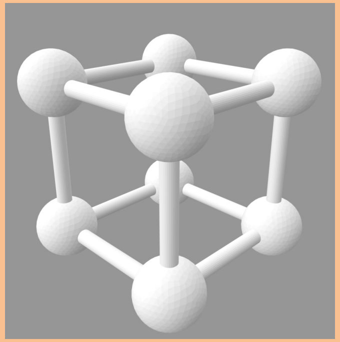


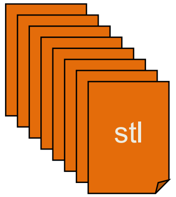


CSV2STL

Convert STL from CSV, TXT, or DOCX



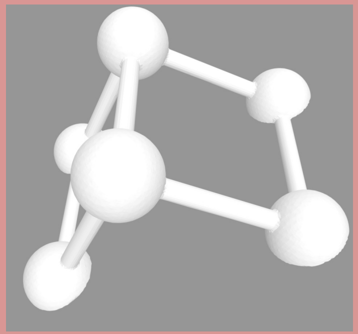




Mesh mixer

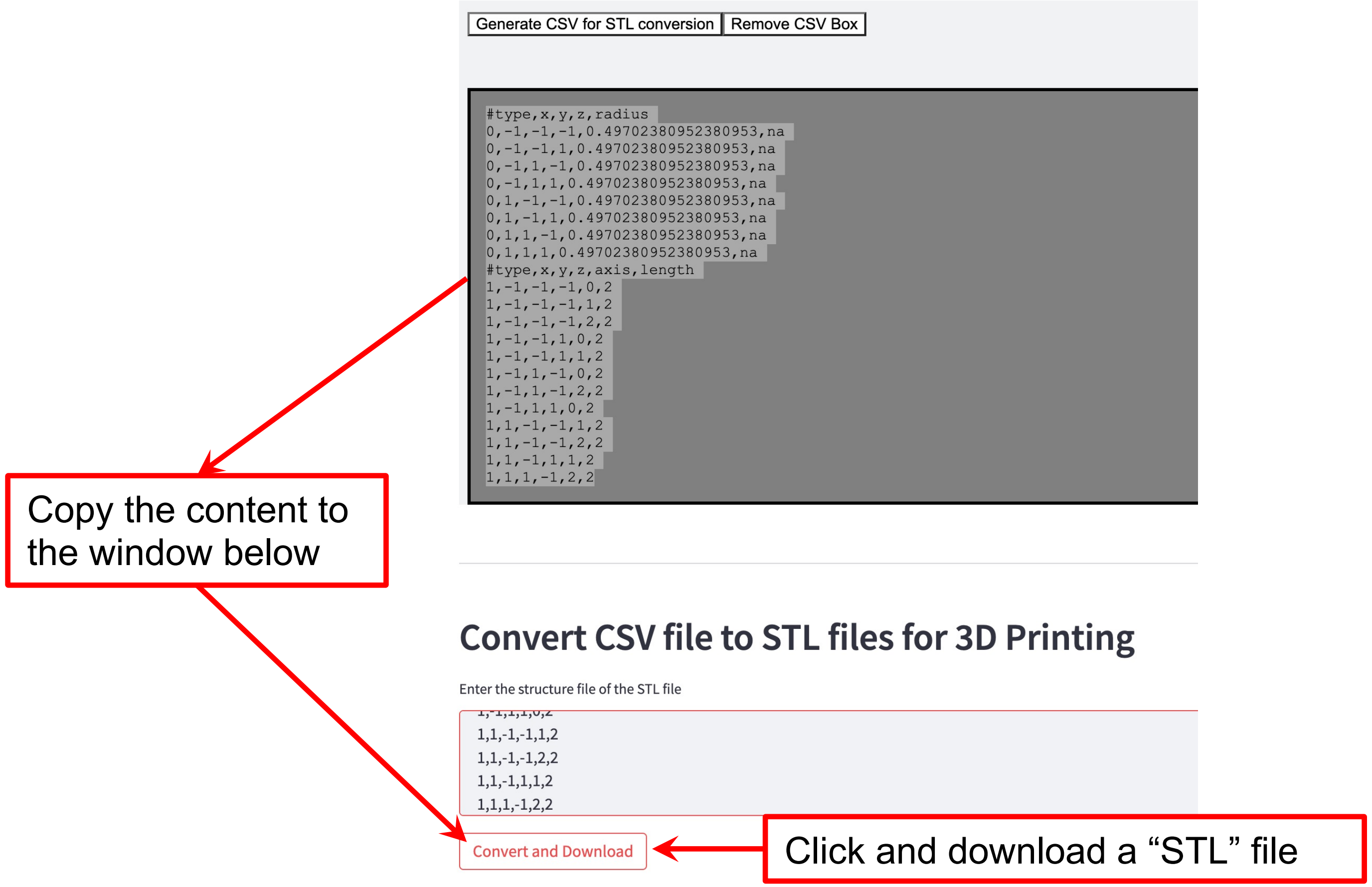
Split in half using meshmixer

AUTODESK® MESHMIXER®



Convert the CSV file to a STL file for Printing

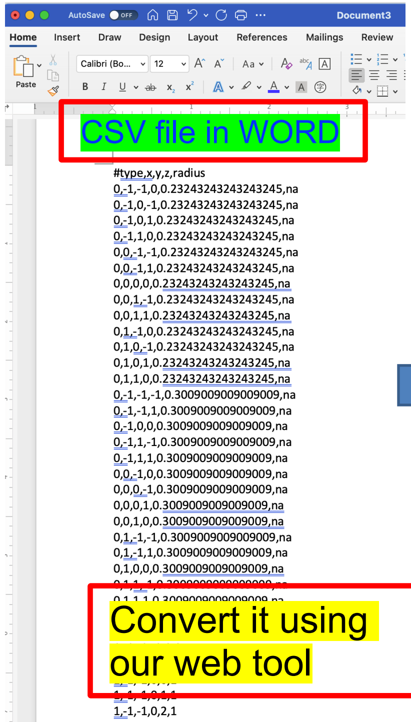
- Utility Websites
  - https://minlong1-csv2stl-streamlit-app-1nkv76.streamlitapp.com/
  - https://laumiulun-csv2stl-streamlit-app-lcc7hm.streamlitapp.com/



What's a STL file?

- STL format
  - A file format native to the STereoLithography CAD software for 3D Systems
  - Referred to as "Standard Tessellation Language" or "Standard Triangle Language."
  - Describe the surface geometry of a 3D object

CSV file in WORD


```
#type,x,y,z,radius
0,-1,-1,0,0.23243243243243245,na
0,-1,0,-1,0.23243243243243245,na
0,-1,0,1,0.23243243243243245,na
0,-1,1,0,0.23243243243243245,na
0,0,-1,-1,0.23243243243243245,na
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0,-1,-1,1,0.3009009009009009,na
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0,0,0,1,0.3009009009009009,na
0,0,1,0,0.3009009009009009,na
0,1,-1,-1,0.3009009009009009,na
0,1,-1,1,0.3009009009009009,na
0,1,0,0,0.3009009009009009,na
1,-1,-1,0,2,1
```

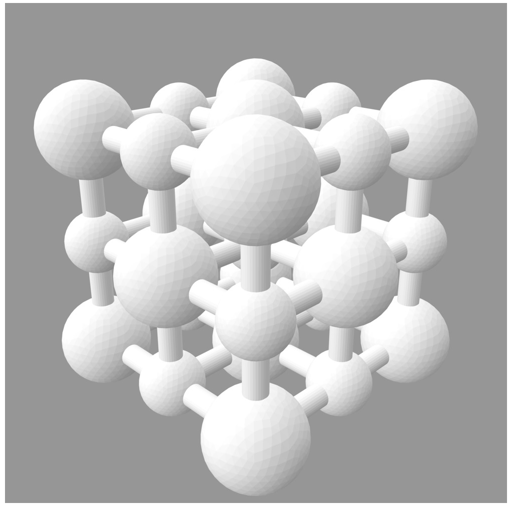
Convert it using our web tool

A STL file

```
solid Group_1_AgCl.stl
facet normal 1.948915 -1.754676 -0.673725
  outer loop
    vertex -18.610298 -33.247864 -30.277264
    vertex -18.238762 -33.499619 -28.546825
    vertex -19.497400 -34.460110 -29.686203
  endloop
endfacet
facet normal 1.927930 -1.885348 -0.540389
  outer loop
    vertex -18.238762 -33.499619 -28.546825
    vertex -19.198681 -34.661495 -27.917862
    vertex -19.497400 -34.460110 -29.686203
  endloop
endfacet
…
```

This is what you will get

Now, you can Open it using Preview in Mac to view the 3D model.

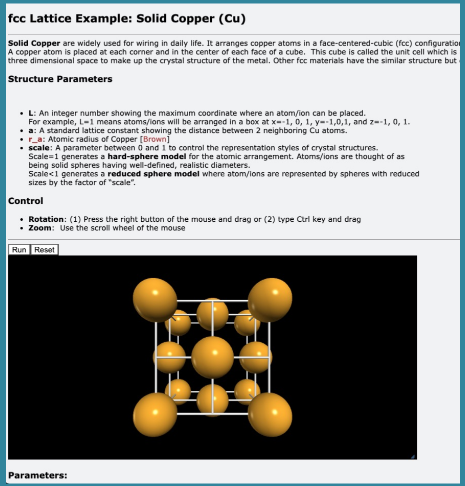


Last Step: Split STL in Half for Stable Printing

- A Complete Pipeline to Prepare a Pintable 3D STL file for Printing

GUI Website

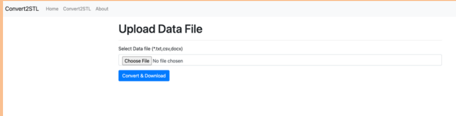
Create a Desired CSV file

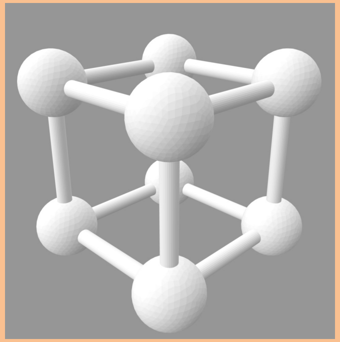


txt

CSV2STL

Convert STL from CSV, TXT, or DOCX



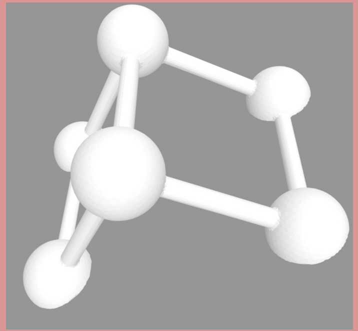


stl

Mesh mixer

Split in half using meshmixer

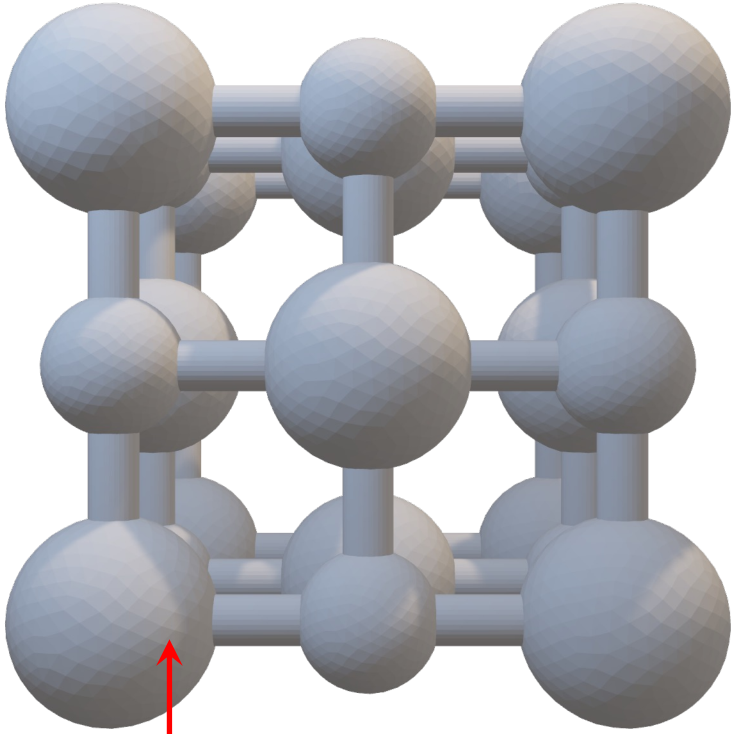
AUTODESK® MESHMIXER®



✓ ✓ ?

Split STL file in Half for Stable Printing

- For example, you will get a file ("half-cube.stl") showing a half cube

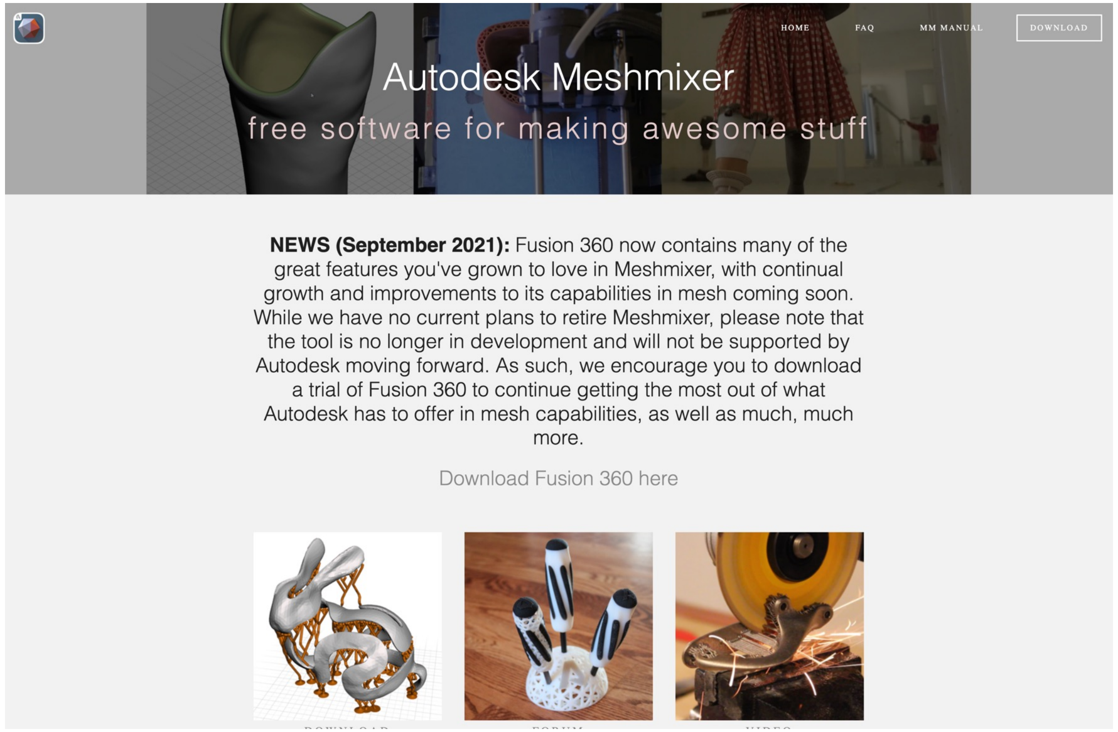


Unstable for printing: Melt plastics in bottom layers may not be strong enough to support top layers.

Stable for printing: Sufficient support from bottom layers.

How to Split?

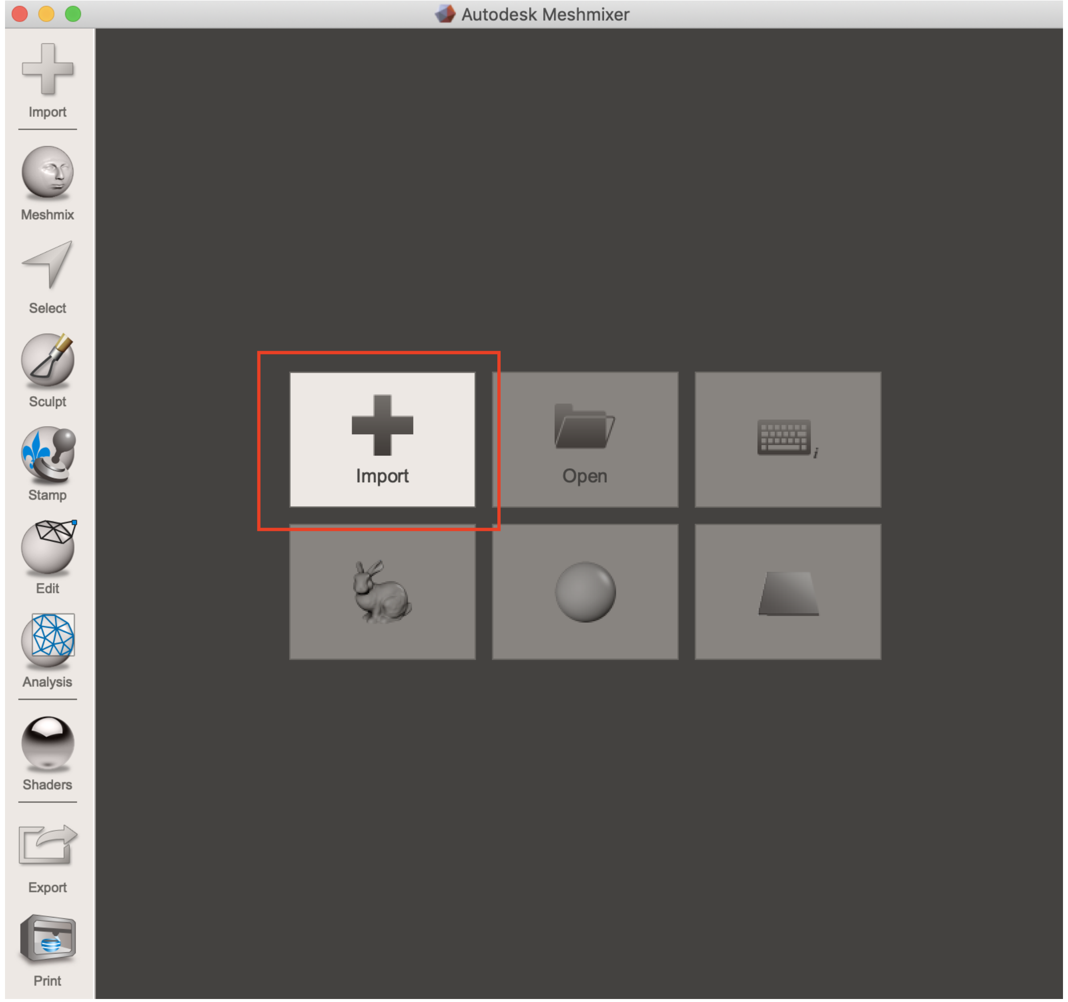
- 1. Do by yourself
  - Download Autodesk Meshmixer from meshmixer.com
  - It should be already installed in lab PC at Boise State



- 2. Upload your STL files and we can help split them

Method 1: Use MeshMixer by yourself

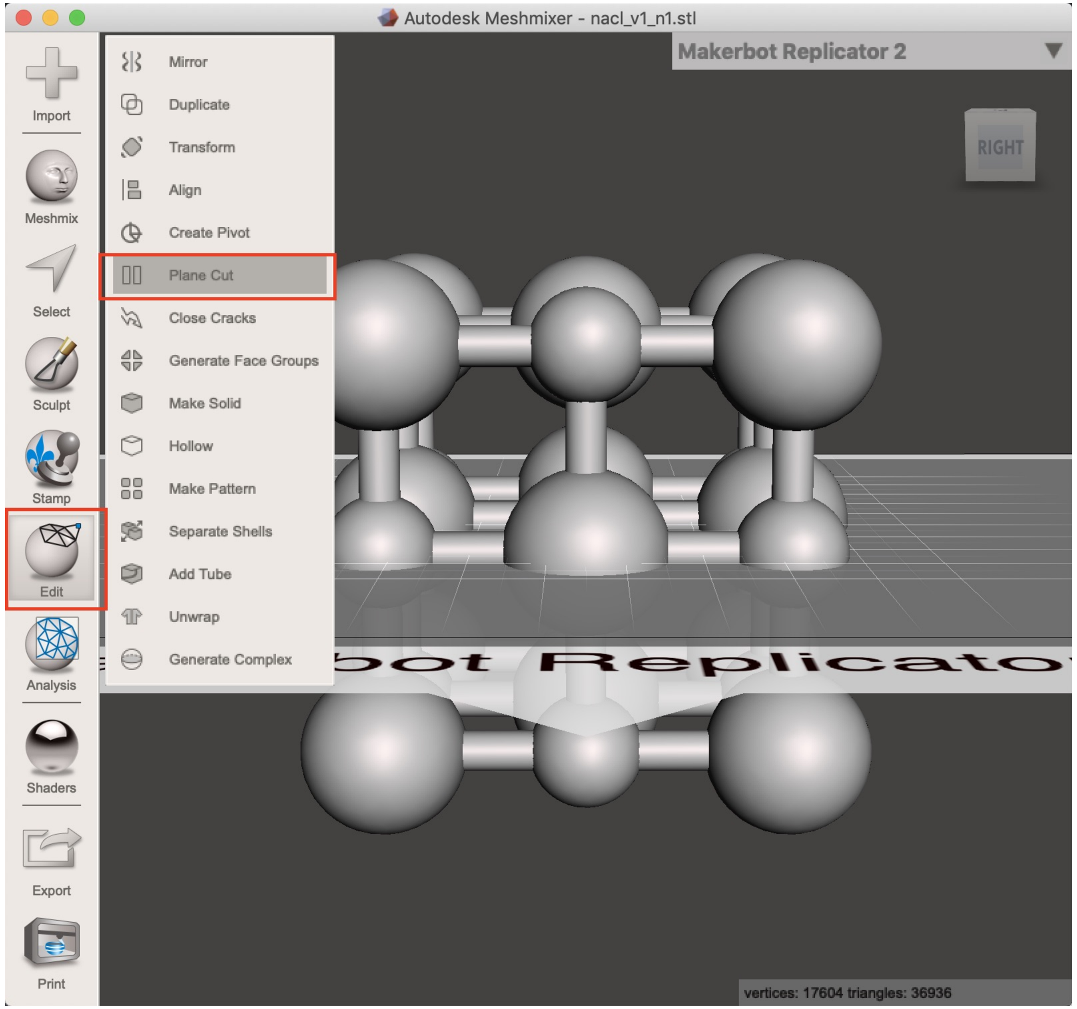
- Step 1: Open Mesh Mixer in the File Browser. Once *MeshMixer* is open, select **Import** and navigate it to the desired STL file

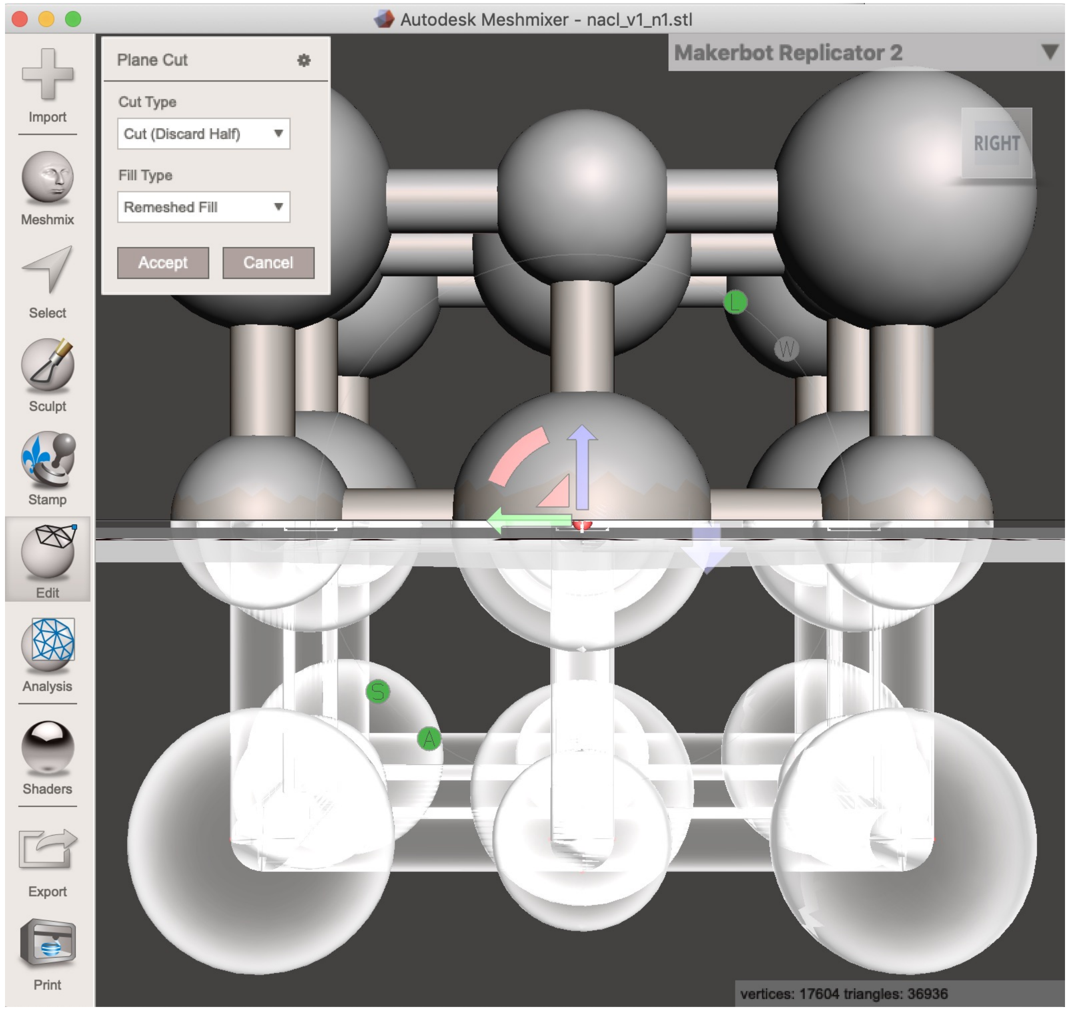


Method 1: Use MeshMixer by yourself

- Step 2: Select **Edit** on the left side panel, then select **Plane Cut** for diagonal cutting.

The **plane cut** tools provide rotation capability in each axis





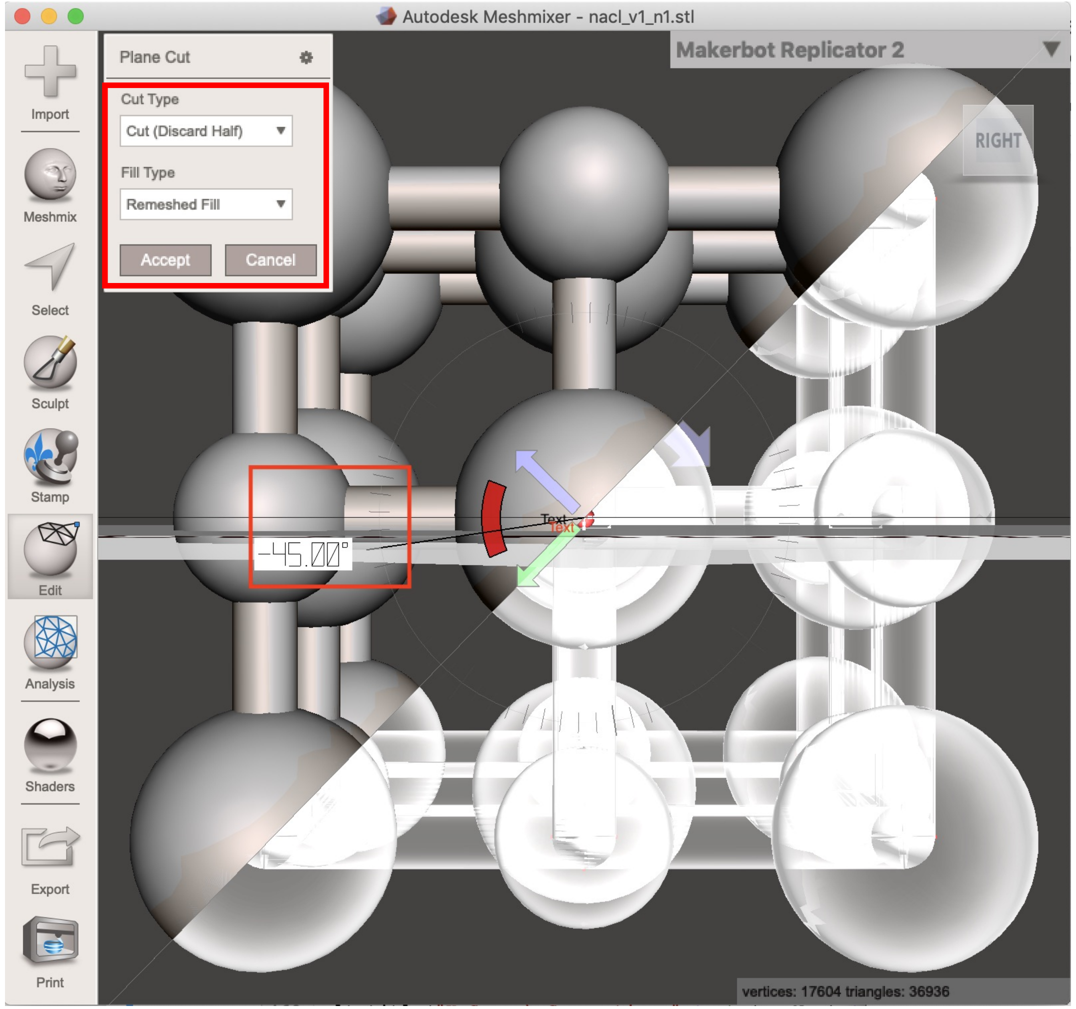
Method 1: Use MeshMixer by yourself

- Step 3: Rotate/extend the cursor till it aligns with black lines of predefined cut measurement (i.e. 45 degrees).

Enable those options:

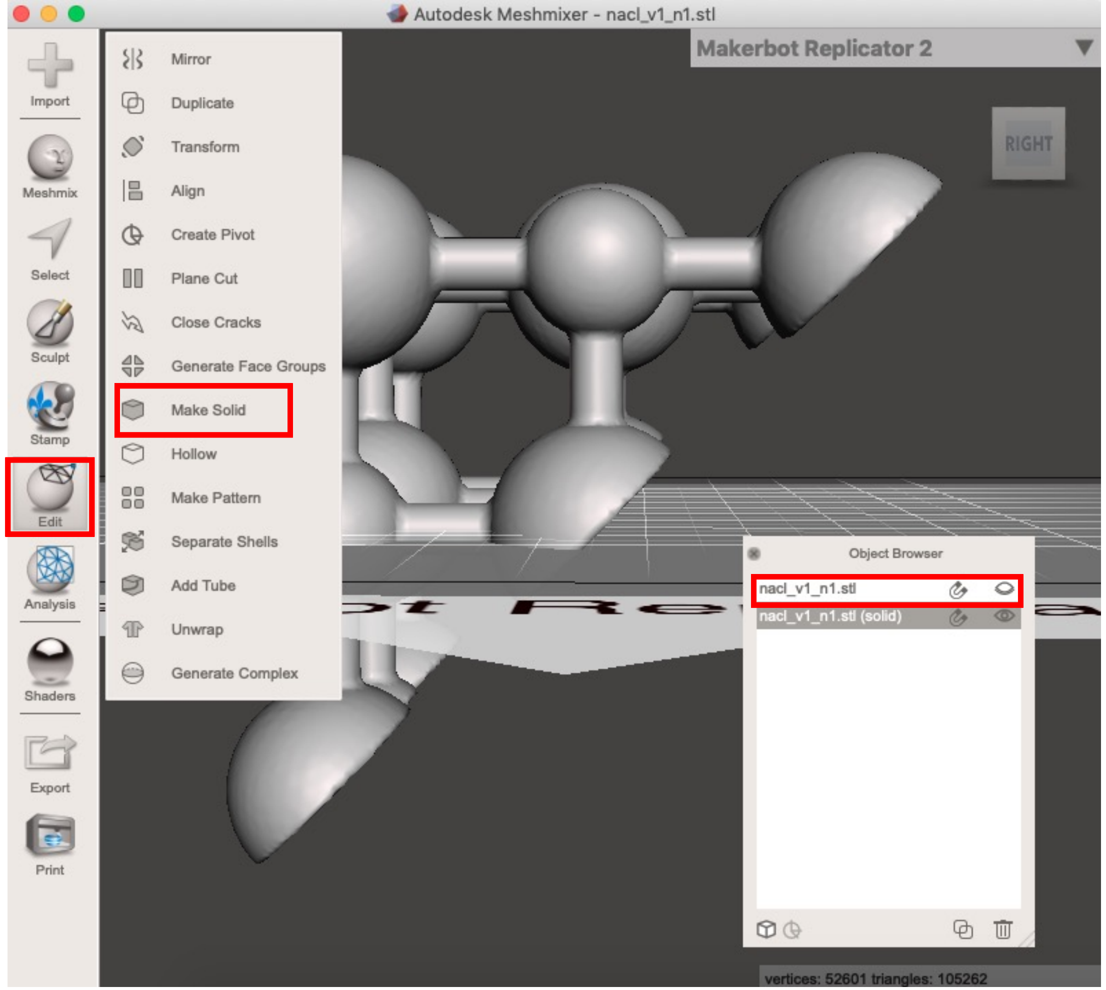
Cut type: **Cut (Discard Half)**
Fill type is **Remeshed Fill**

Then click **Accept.**



Method 1: Use MeshMixer by yourself

- Step 4: Solidify the body. Select **Edit -> Make Solid ->** Click **Accept**

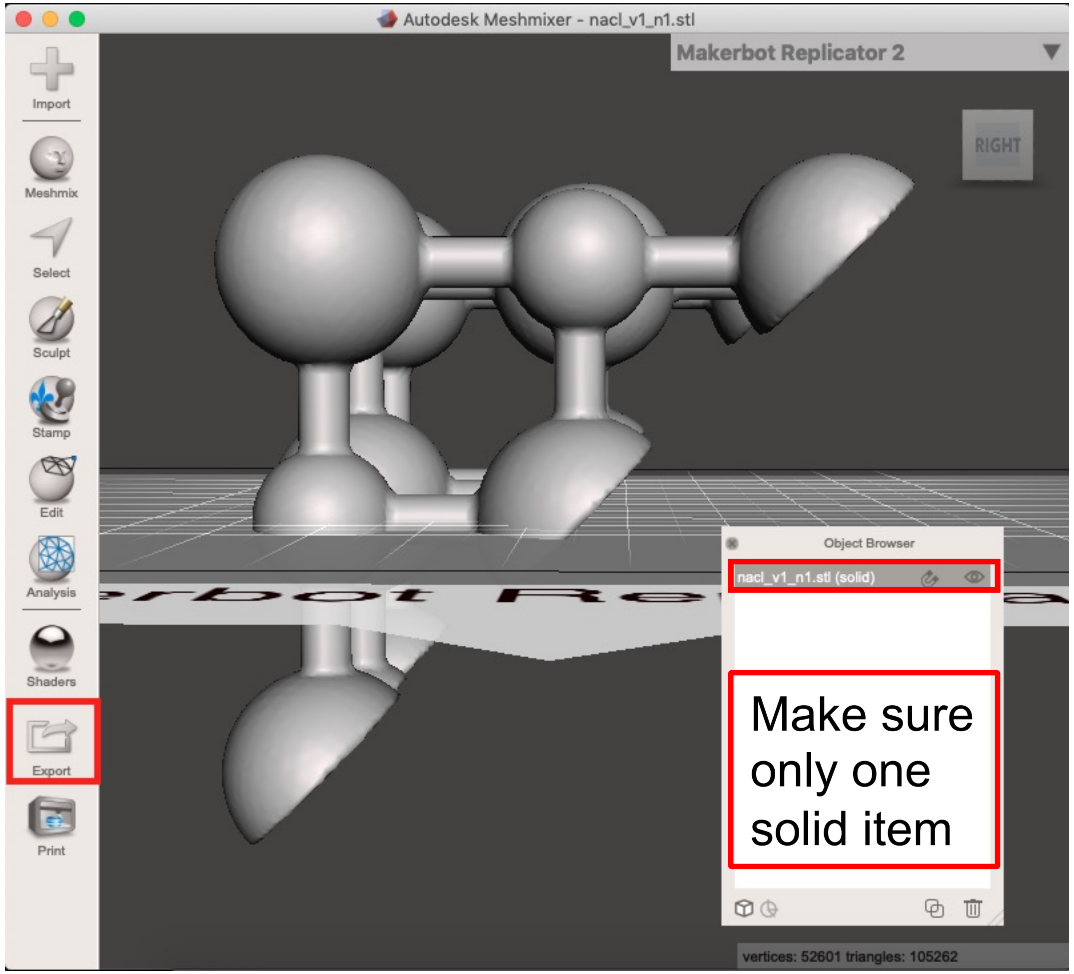


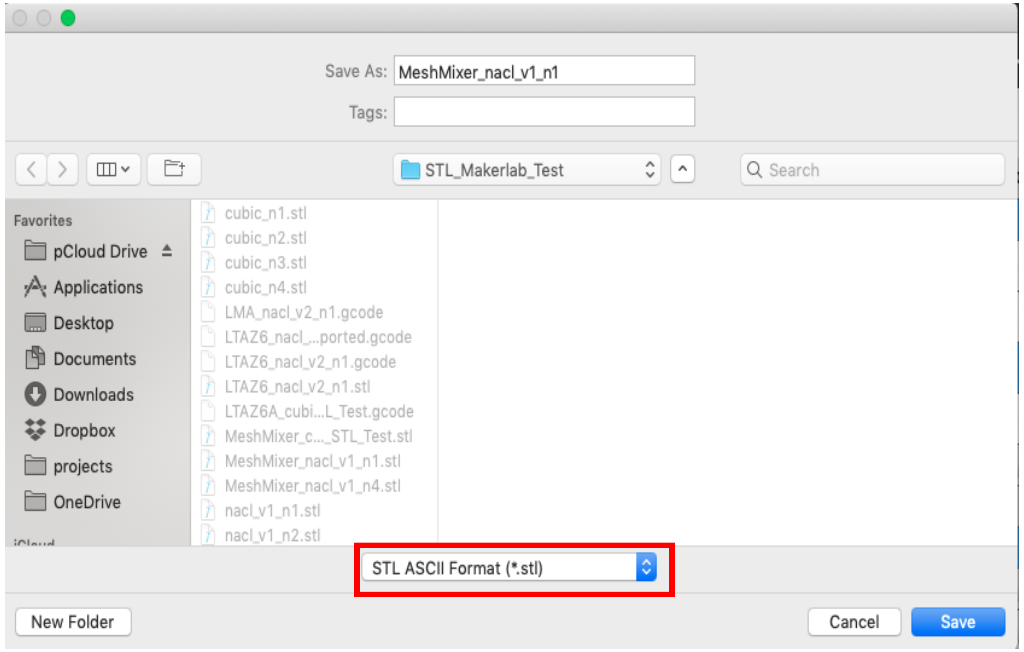
After you make the object solid, there should be a new menu **Object Browser**.

Select the one **WITHOUT (solid)** and click the **Trashcan** button below to delete it.

Method 1: Use MeshMixer by yourself

- Step 4: Export the file & Save it as a STL file.





Method 2: Upload STL files to Google Drive (Boise State)

- Section 1
  - https://drive.google.com/drive/folders/1fH6CuWyXZ0aIDGhqT0HjvHOAyyoVRHqn?usp=sharing

- Section 2
  - https://drive.google.com/drive/folders/1GuHV2k84seBOZ--wLyJE7zkPJXz1DA68

- Links will also be posted on Canvas

- One group sends 2 stl file (Or talk to Dr. Wang if want to print more)
  - Group_1_AgCl_original.stl
  - Group_1_fcc_new_material.stl

Method 2: Upload STL files to Google Drive (Partner Universities)

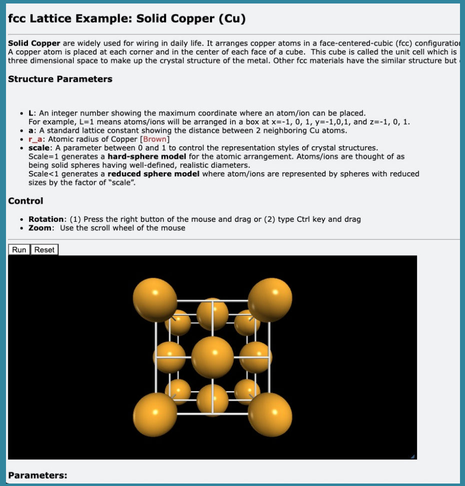
- Co-PIs and instructors from partner universities, please
  - Prepare all CSV files using good naming schemes (e.g., Group_1_NaCl.csv)
  - Upload them to the following Google Drive folders
  - Notify us through email (e.g. "All files are ready. We need them by Friday…")
- KPCC (Hawaii)
  - https://drive.google.com/drive/folders/1LozcoP6GN8mLxdYmBid264rZIn3K4AJt
  - Shared with herve@hawaii.edu, jdf8043@hawaii.edu, and marye@hawaii.edu
- UTSA
  - https://drive.google.com/drive/folders/1S5YBsR_cxMabeF19HmHUU6I4PS6loruY
  - Shared with Prof. Su and jessica.gehrtz@utsa.edu
- Augusta
  - https://drive.google.com/drive/folders/1eQApYHBqBMGETVaXeTSRsr3luCQuhDL6
  - Shared with Prof. He and mfreitag@augusta.edu

Ready for Print

- A Complete Pipeline to Prepare a Pintable 3D STL file for Printing

GUI Website

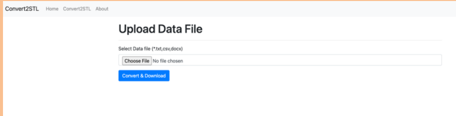
Create a Desired CSV file

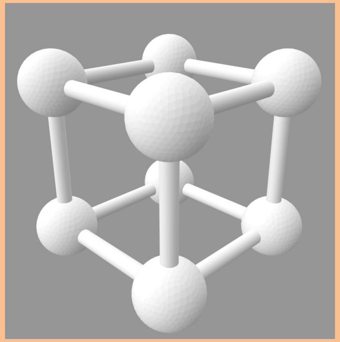


txt

CSV2STL

Convert STL from CSV, TXT, or DOCX



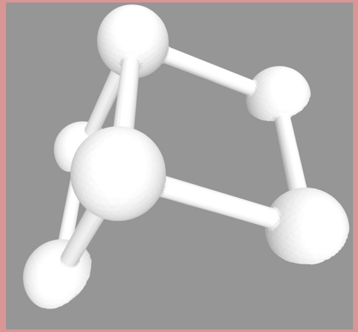


stl

Mesh mixer

Split in half using meshmixer

AUTODESK MESHMIXER



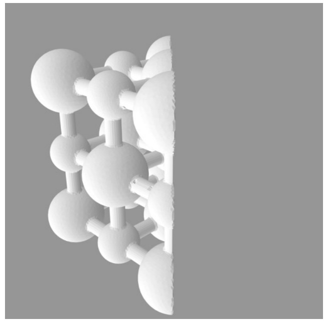
✓ ✓ ✓

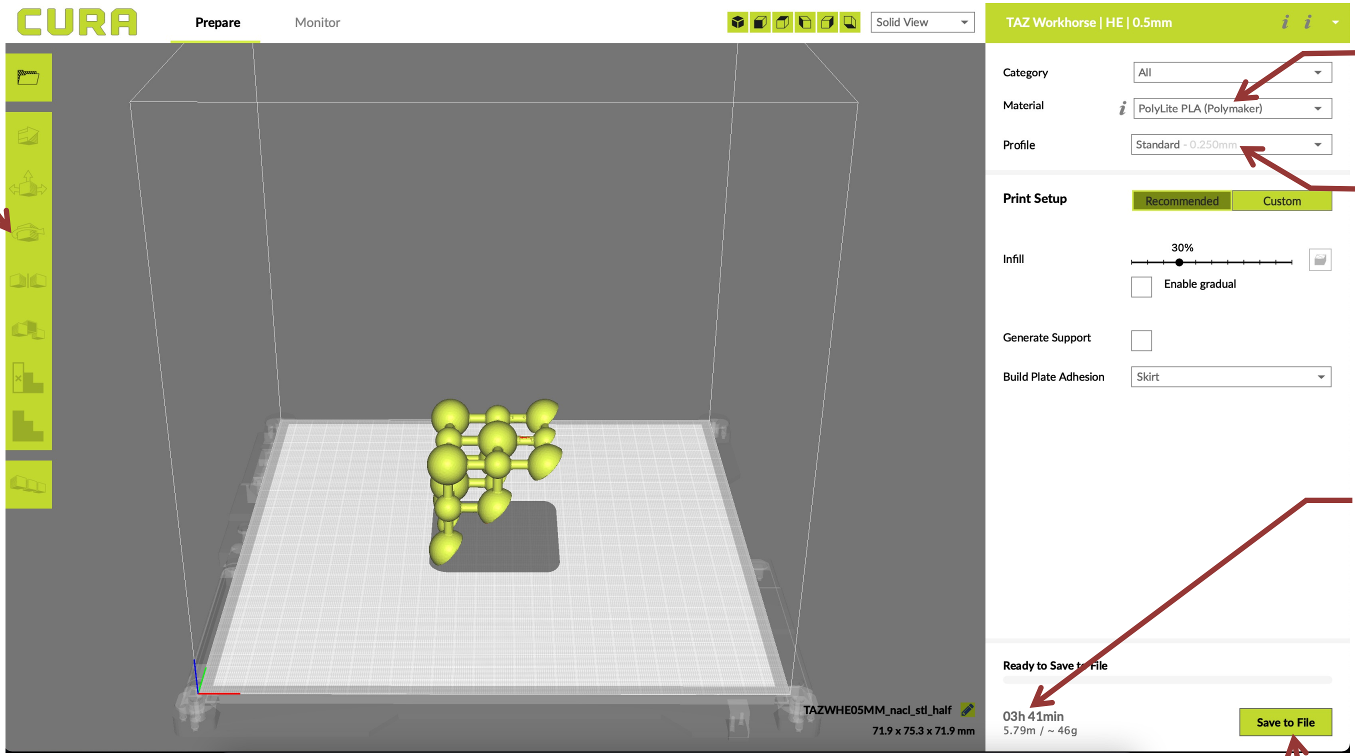
Go to Lab for Printing

- Bring the “Group_1_AgCl.stl” to Lab
- Load it in Cura

Tool Bar for manipulating file

half cube





Material (PolyLite PLA)

Profile (0.25mm)

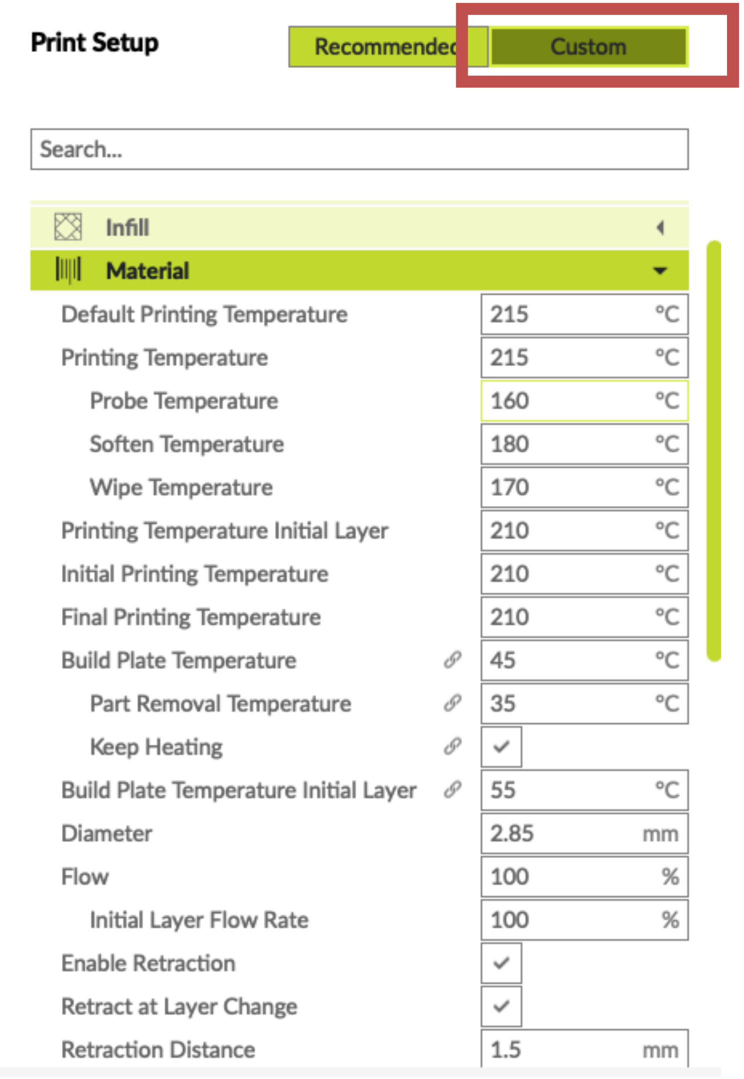
Approximate Time

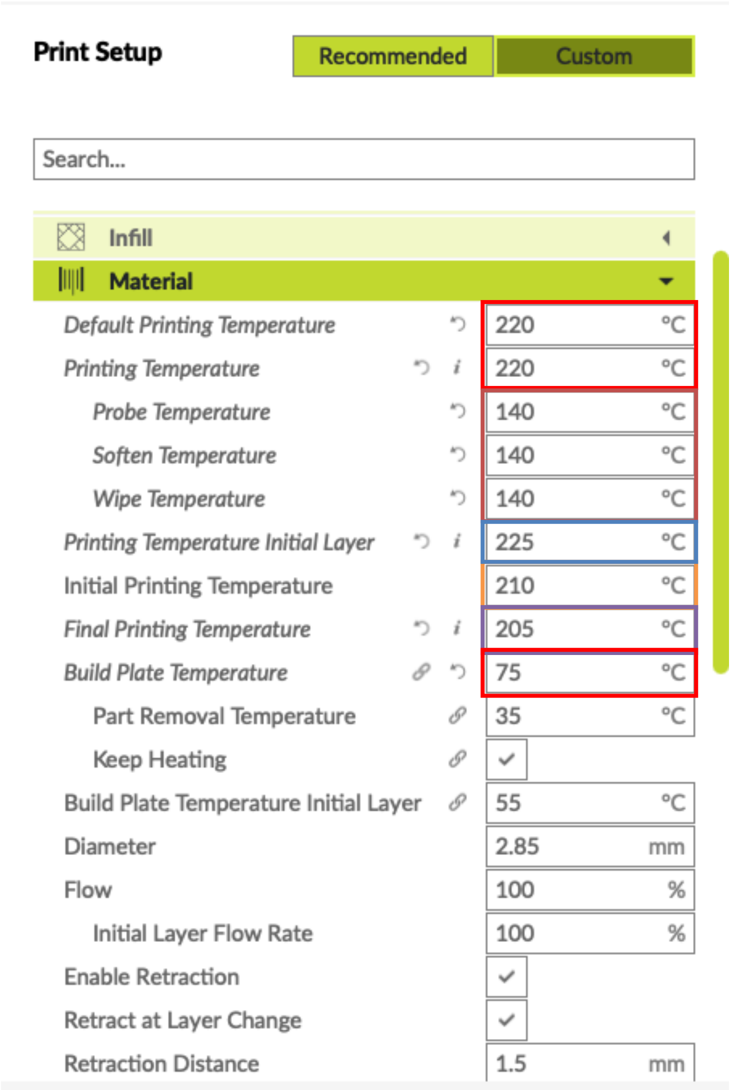
Save to File

Adjust Parameters (for Lulzbot only)

- Click “Custom” (optimize parameters to avoid printer jam)

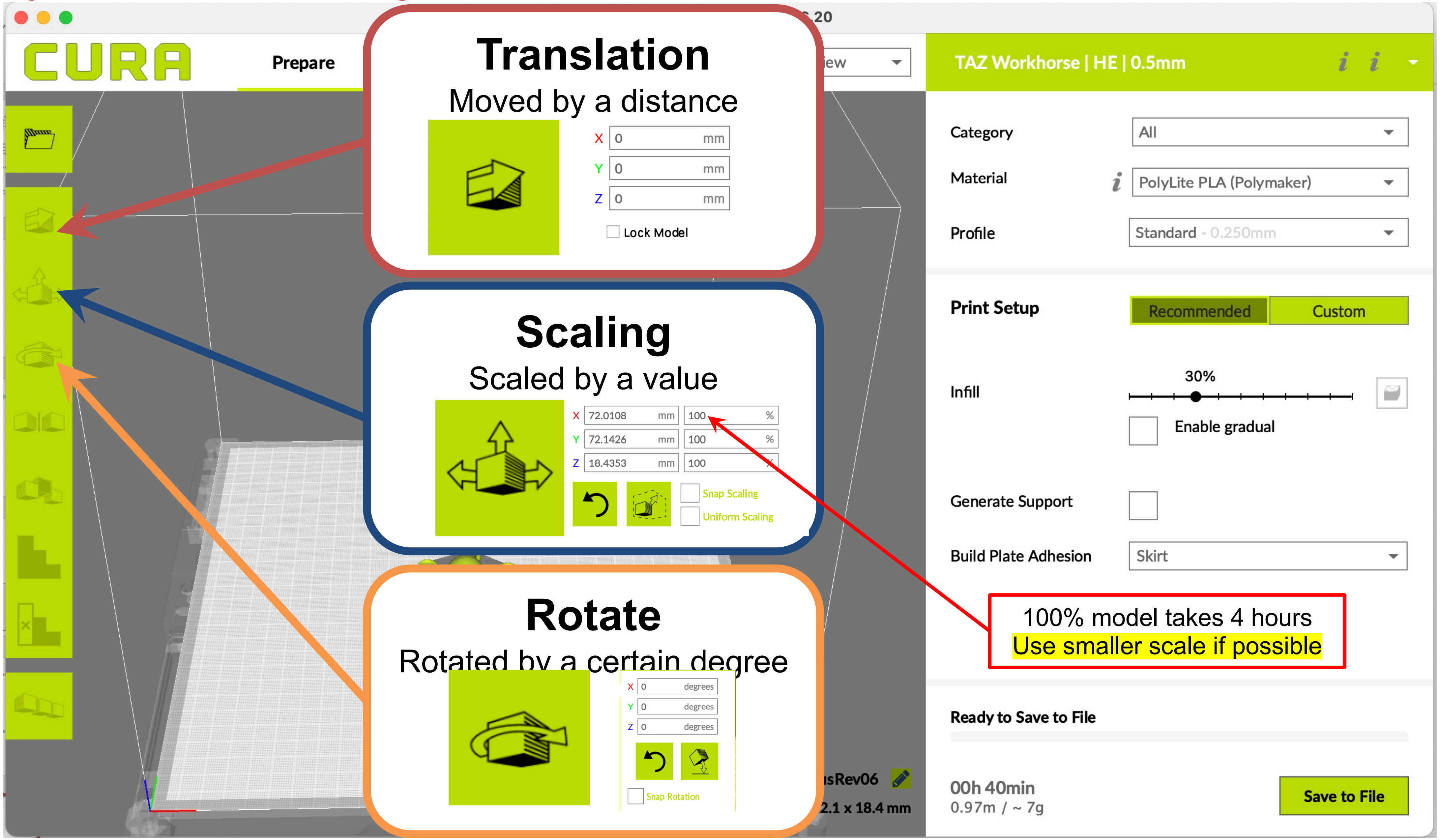
Before





After

Adjust Scaling and Rotate



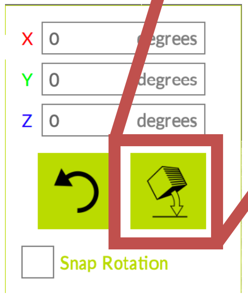
Important: Use "Lay Flat"

- To give the 3D object enough support during printing

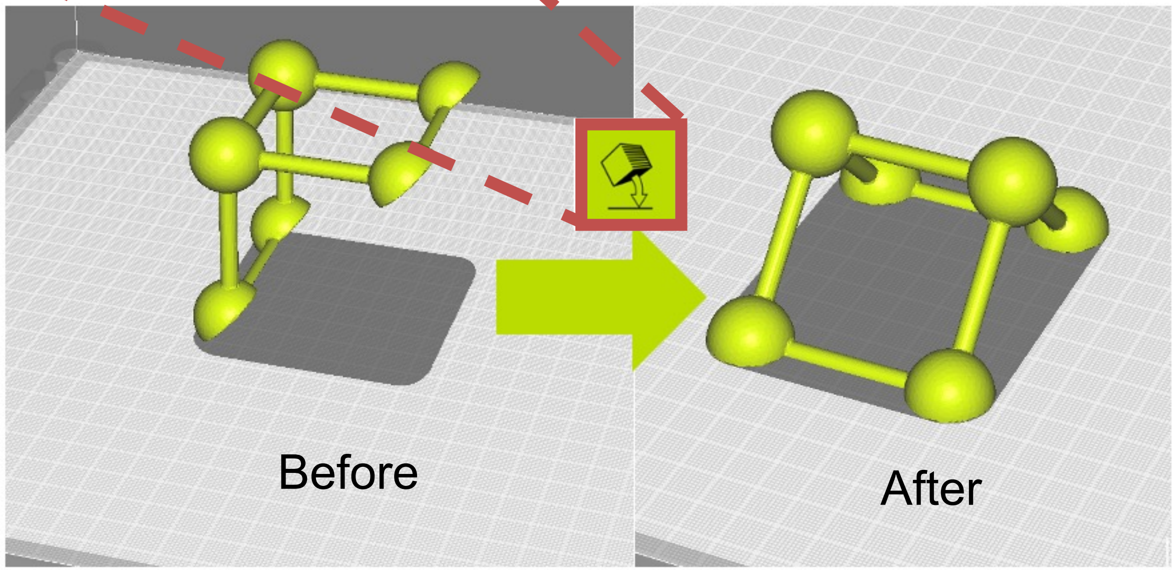
You can use 'Lay flat' multiple times

Rotate

Rotated by a certain degree in each axis

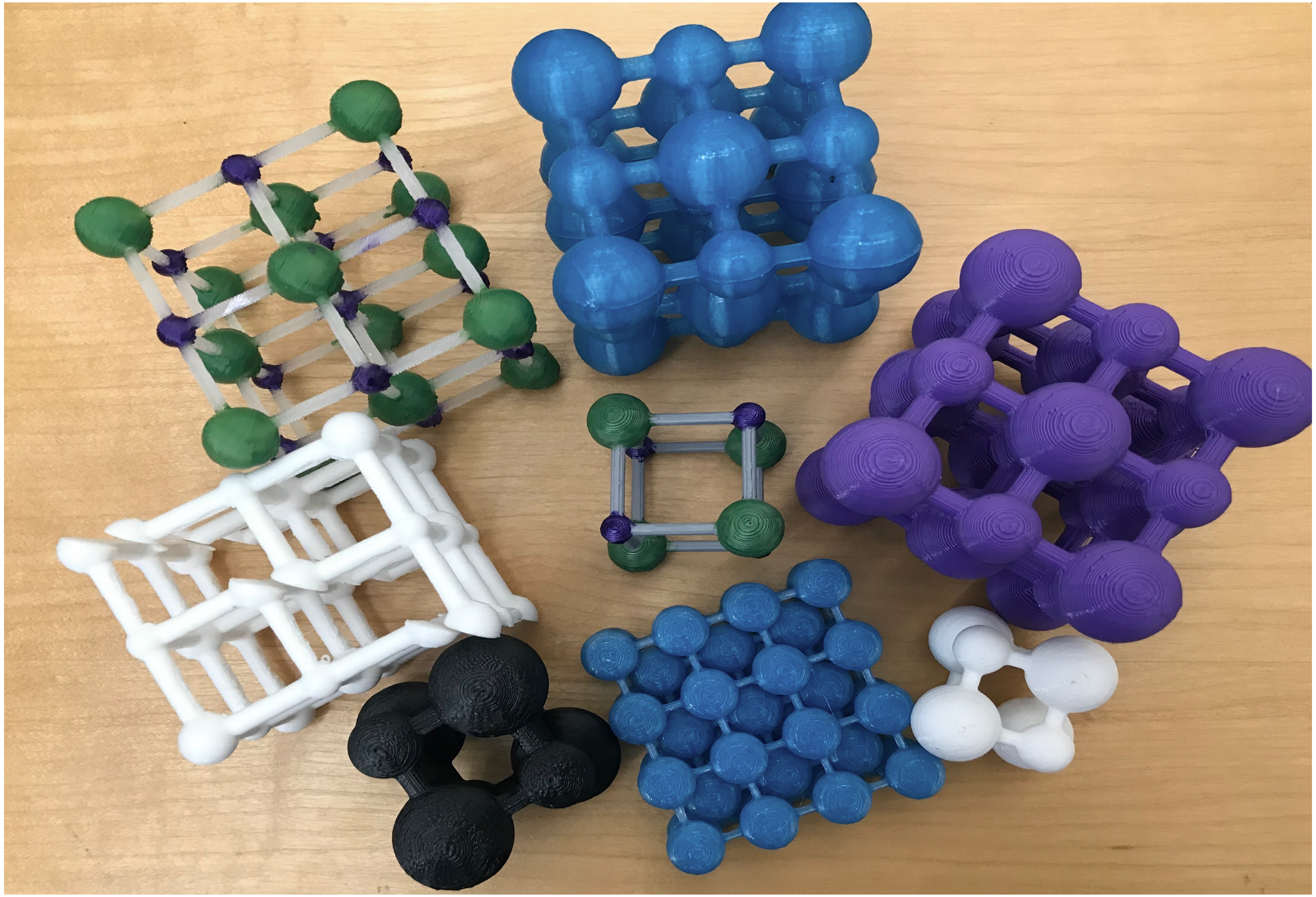


Print it twice and join the printed pieces together using SuperGlue (provided in the lab)



Enjoy printing your own materials!

- Examples

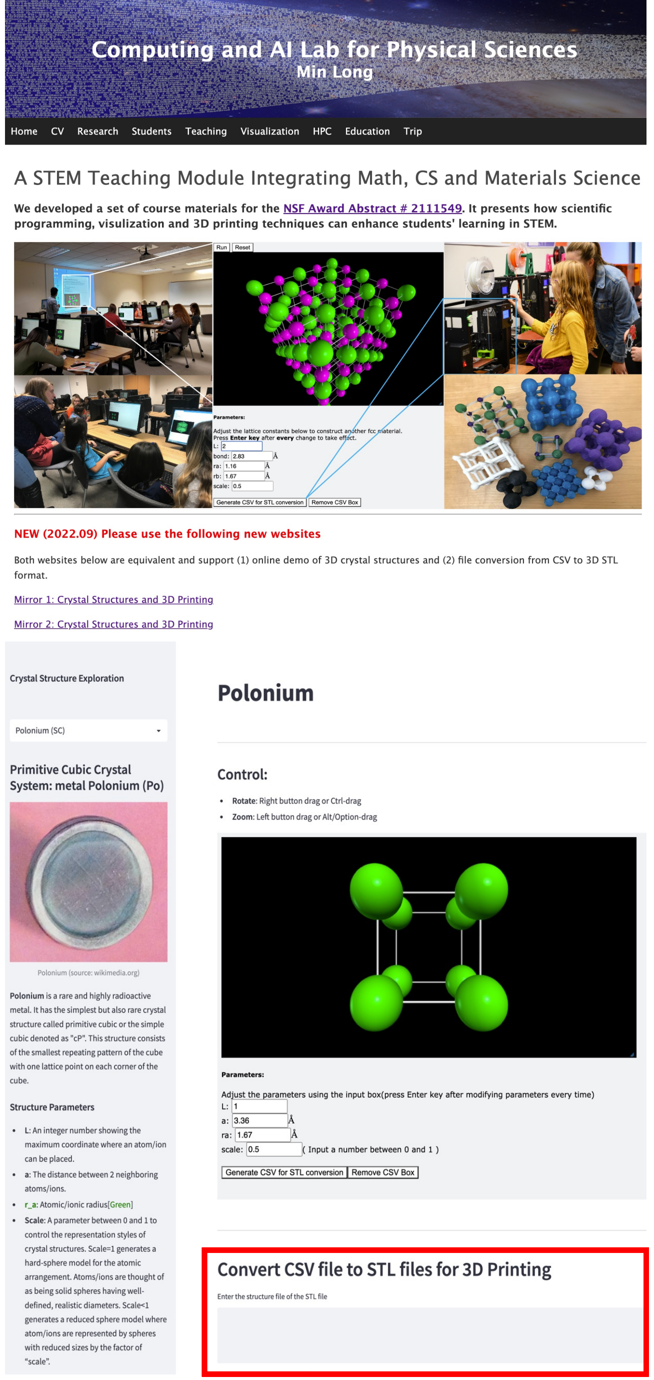


Training Materials

- Overview and Objectives
- Lecture 1: Introduction to Online Toolkits and STEM Concepts (For instructors)
- Lecture 2: Introduction to 3D Printing
- Lecture 3: Design and Print SC and FCC Materials
- Lecture 4: Design BCC and Perovskite Materials

Websites for Resources

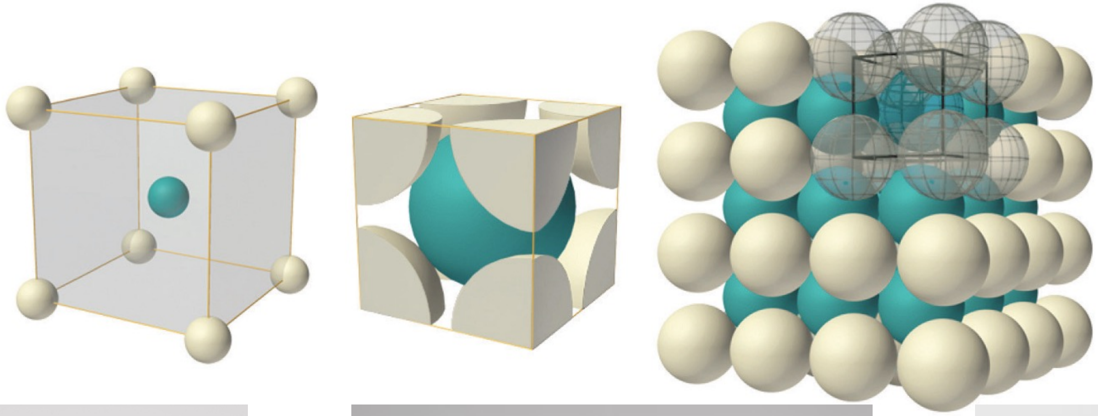
- Main Websites:
  - Toolkit, tables of data, 3D printer manuals...
  - https://cs.boisestate.edu/~mlong/education.html
  - https://minlong1.github.io/education.html
- Converting structure files (CSV) to 3D STL files:
  - Toolkit and converting tool
  - https://minlong1-csv2stl-streamlit-app-1nkv76.streamlitapp.com/
  - https://laumiulun-csv2stl-streamlit-app-lcc7hm.streamlitapp.com/



Outline

- Body-Centered Cubic: Structure and Materials
- Perovskite Structure

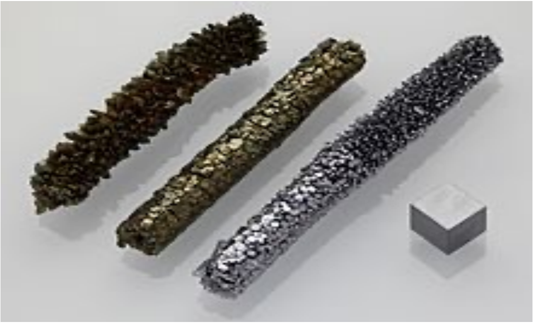
Body-Centered Cubic



Iron (Fe)

Molybdenum (Mo)

Tungsten (W)



Vanadium (V)

Niobium (Nb)

Tantalum (Ta)

Lattice Constants at 300K

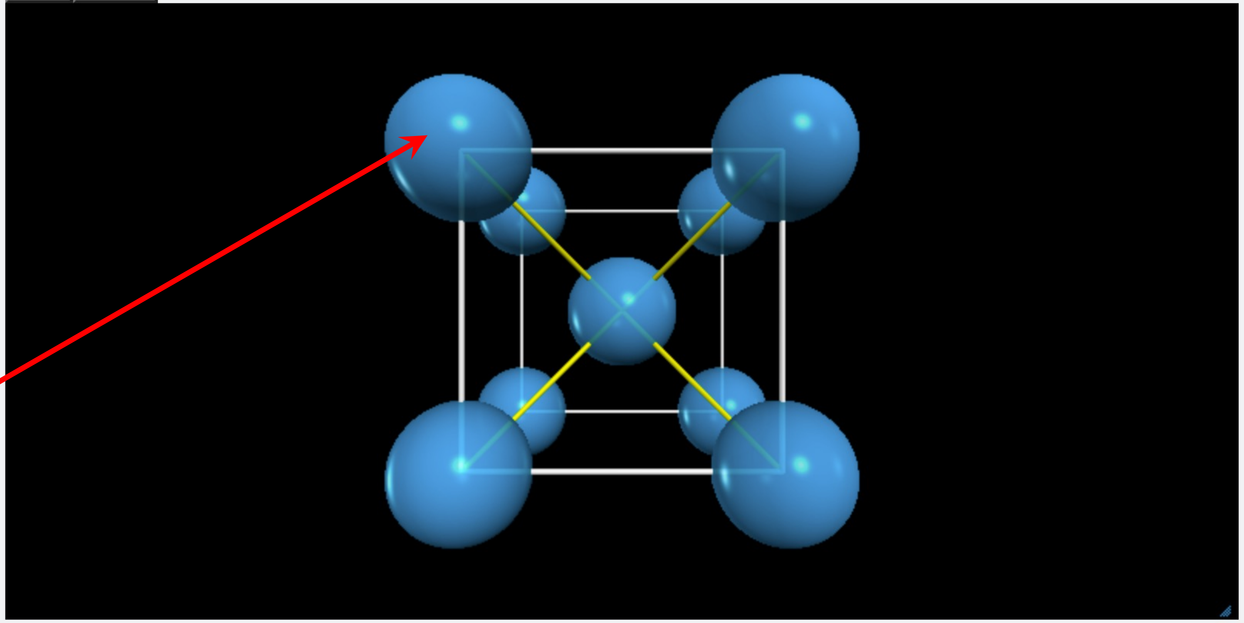
- BCC Materials

Material	a (Å)	radius (Å)
Iron (^{26}Fe)	2.856	1.26
Molybdenum (^{42}Mo)	3.142	1.39
Tungsten (^{74}W)	3.155	1.39
Vanadium (^{23}V)	3.0399	1.34
Niobium (^{41}Nb)	3.3008	1.46
Tantalum (^{73}Ta)	3.3058	1.46

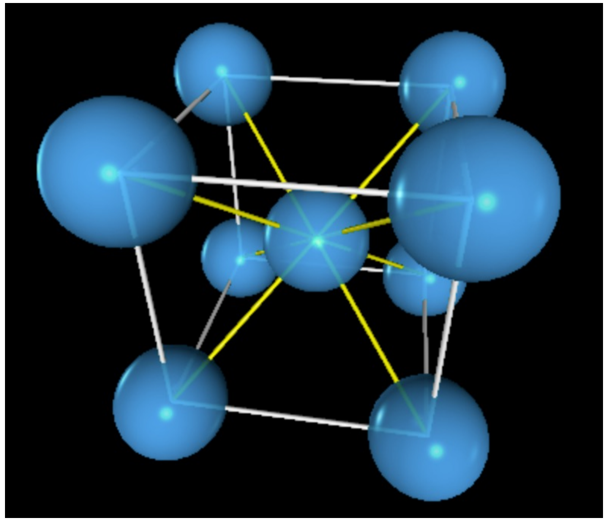
Visualization

- https://cs.boisestate.edu/~mlong/GUI/crystal_html/fe_obs.html

Run Reset



A different view



opacity: A parameter controlling the opacity of atom/ion spheres.

Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

Parameters:

Adjust the parameters using the input box(press Enter key after modifying parameters every time)

U: 1

a: 2.856 Å

ra: 1.26 Å

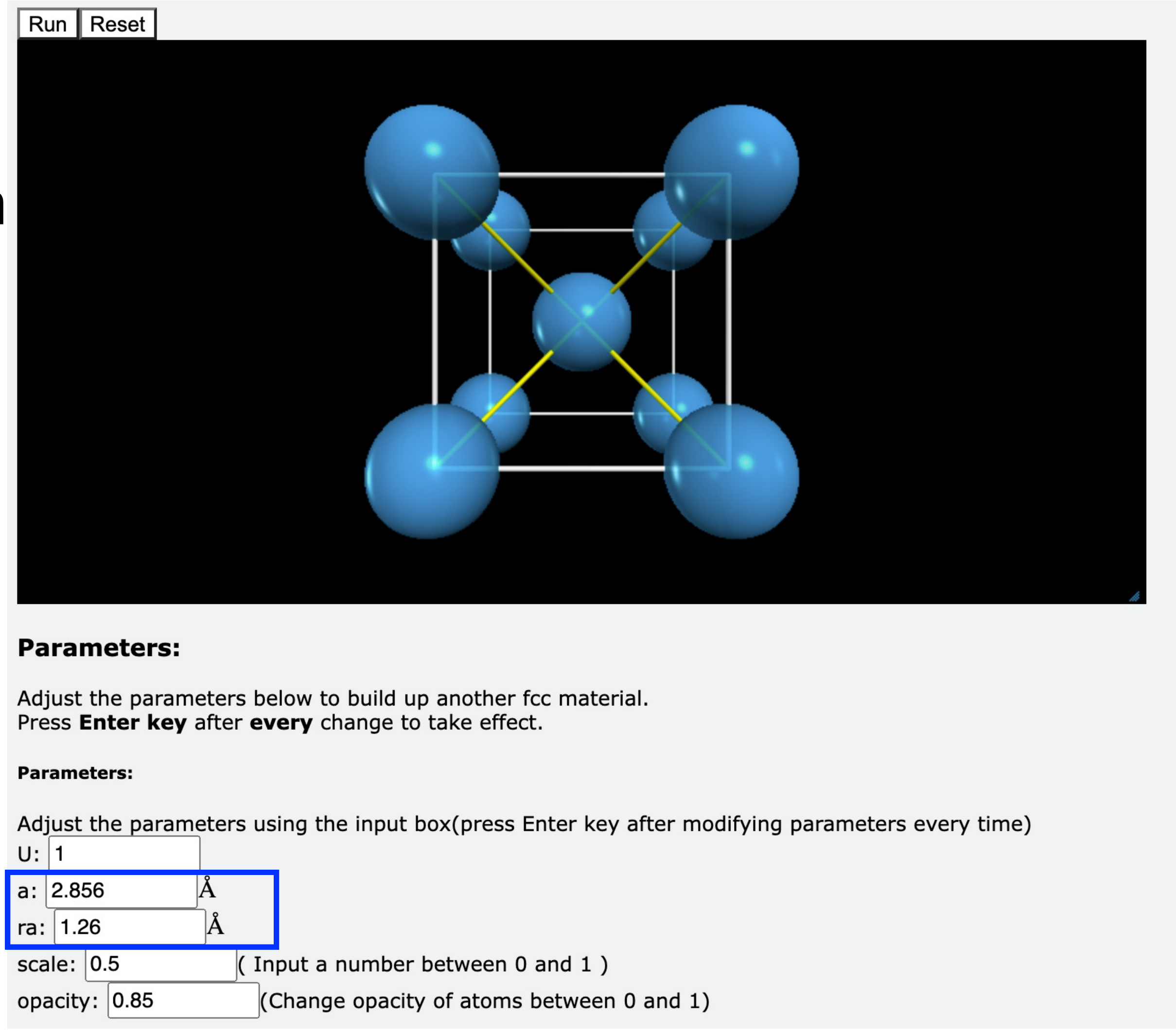
Iron at room temperature

scale: 0.5 (Input a number between 0 and 1)

opacity: 0.85 (Change opacity of atoms between 0 and 1)

Create another BCC Material

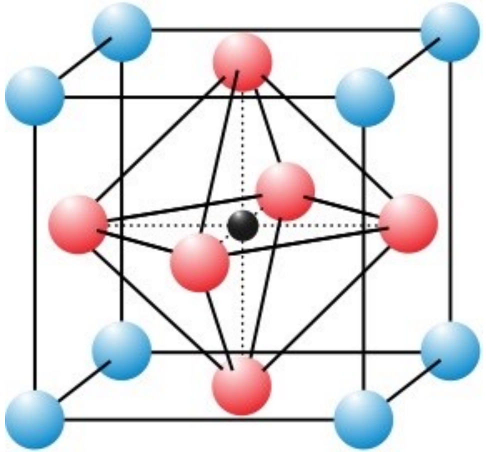
- Changing Parameters
  - L: An integer number showing the maximum coordinate where an atom/ion can be placed.
  - a: A standard lattice constant showing the distance between 2 neighboring atoms/ions.
  - ra: Atomic/ionic radius
  - scale: A parameter between 0 and 1 to control the representation styles of crystal structures.



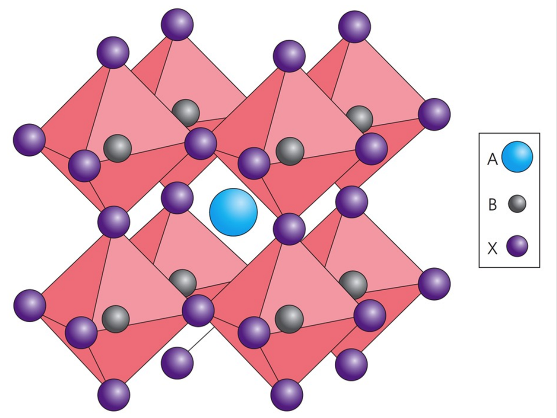
- Printing is not supported.

Ideal Perovskite Structure

- Perovskites are referred to a family of materials
  - A Perovskite was first referred to a colorless mineral of Calcium Titanate with the chemical formula $CaTiO_3$.
  - who named it after a Russian mineralogist Lev Alexeievitch Perovskite.
- The general chemical formula is ABX_3 ,
  - A is a metal cation (positively charged ion),
  - B is a cation and X is an anion (negatively charged ion).
  - A subgroup: ABO_3

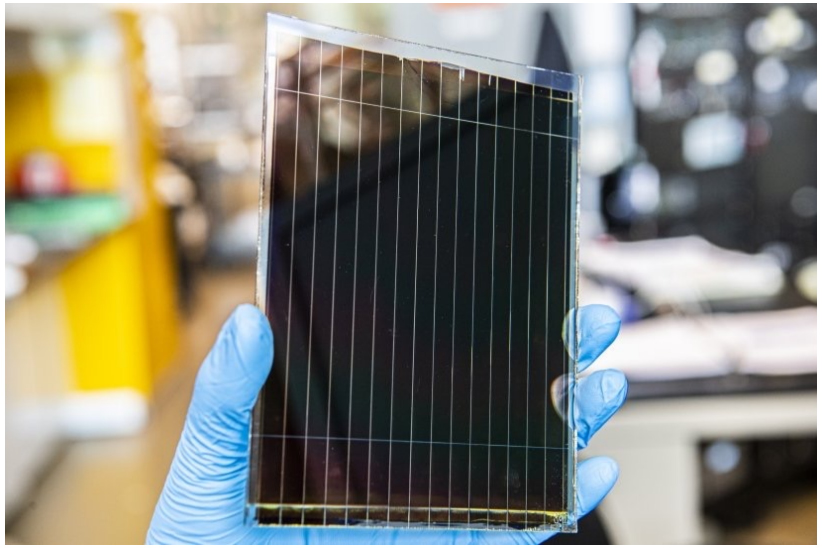


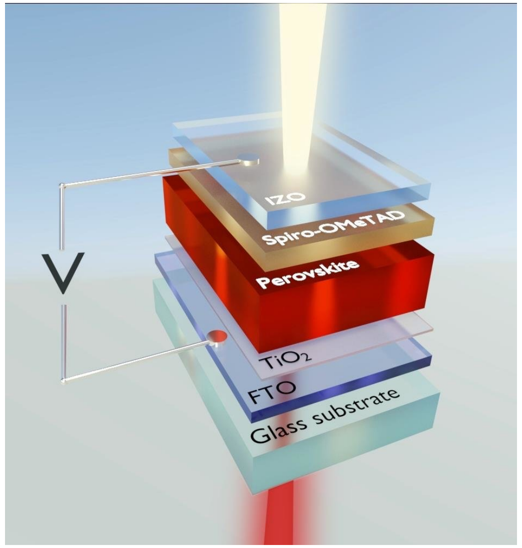
- Strontium Titanate is an ideal perovskite structure
  - $SrTiO_3$
  - No distortion
  - A diamond simulant



Solar Cells with Perovskite Structures

- High Energy Conversion Efficiency at Low Cost
  - Perovskite solar cells convert more than 20% of the incident light directly into usable current
    - Reports of about 3% in 2006 to over 25% in 2021
      - A peak efficiency of 25.6%: https://doi.org/10.1038/s41586-021-03406-5
    - Are thought to be a frontier energy solution.
  - Department of Energy (DoE) is of great interest in research to increase the efficiency and lifetime of hybrid organic-inorganic perovskite solar cells.
    - Targeted materials include methylammonium lead halide, i.e., $CH_3NH_3PbX_3$, where X = I, Br or Cl.

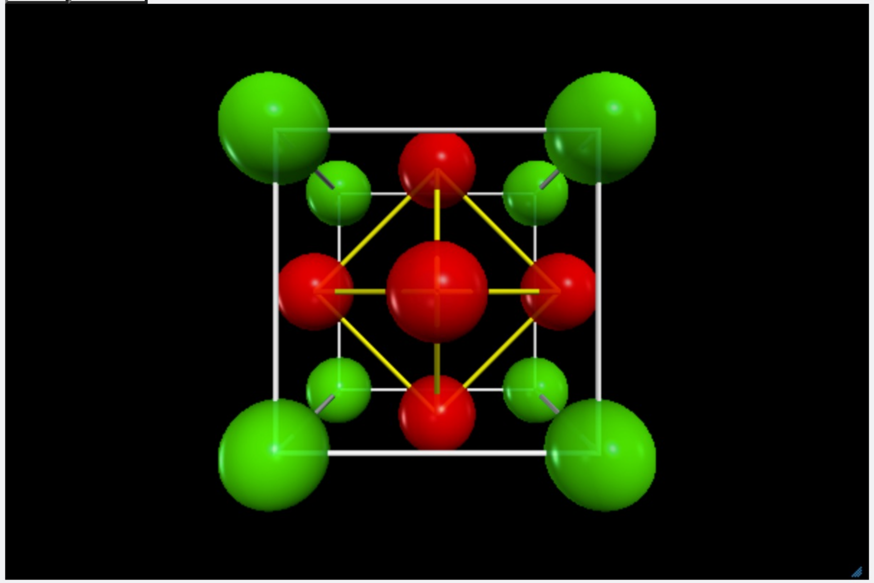




Visualization of Ideal Perovskite: $SrTiO_3$

- https://cs.boisestate.edu/~mlong/GUI/crystal_html/srtio3_obs.html

Run Reset



Parameters:

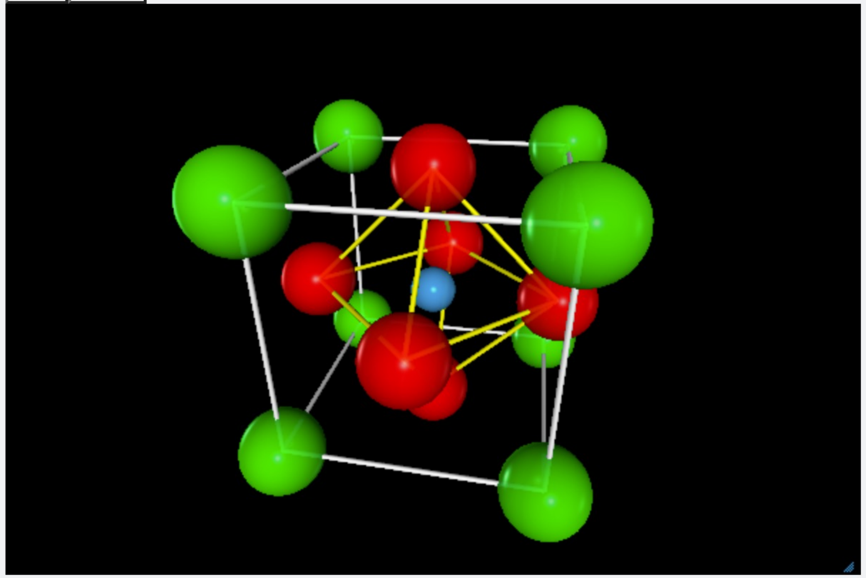
Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

Parameters:

Adjust the parameters using the input box(press Enter key after modifying parameters every time)

U: 1
a: 3.988 Å
ra: 1.32 Å
rb: 0.745 Å
ro: 1.26 Å
scale: 0.5 (Input a number between 0 and 1)
opacity: 0.85 (Change opacity of atoms between 0 and 1)

Run Reset



Parameters:

Adjust the parameters below to build up another fcc material.
Press **Enter key** after **every** change to take effect.

Parameters:

Adjust the parameters using the input box(press Enter key after modifying parameters every time)

U: 1
a: 3.988 Å
ra: 1.32 Å
rb: 0.745 Å
ro: 1.26 Å
scale: 0.5 (Input a number between 0 and 1)
opacity: 0.85 (Change opacity of atoms between 0 and 1)

Tetrahedron

Hexahedron

Lattice Constants at 300K

- Ideal Perovskite Materials

Material	a (A)	Radius of Ionic A^{2+} (A)	Radius of Ionic B^{4+} (A)	Radius of Ionic O^{2-} (A)
$SrTiO_3$	3.98805	1.32	0.745	1.26
$KTaO_3$	3.9885	1.52	0.82	1.26
$EuTiO_3$	7.810	1.31	0.745	1.26
$SrVO_3$	3.838	1.32	0.72	1.26
$CaVO_3$	3.767	1.14	0.72	1.26

- https://en.wikipedia.org/wiki/Ionic_radius
  - "Crystal ionic radii"

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Summary: Learning Math in STEM Context

Summary of STEM Concepts

- Math
  - Polygon (2D)
  - Polyhedron and Platonic solids (3D) • Measurement
  - Coordinates
  - Symmetry
  - Ratio
  - Similarity
- Materials
  - Atoms
  - Crystal Structures
  - Crystalline
- Programming
  - Class
  - Object
  - Attribute

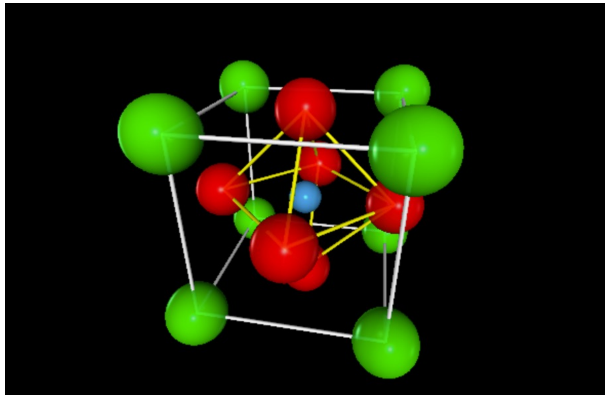
After the class: Review these concepts

Summary: Geometrical Concepts

- Polygon (2D)
  - A plane shape consisting of a finite number of line segments.
- Polyhedron and Platonic solids (3D)
  - (Regular) Tetrahedron has 4 triangular faces, with 3 meeting at each vertex, 6 straight edges, and 4 vertices.
  - Cube has 6 squares, with 3 meeting at each vertex, 12 straight edges and 8 vertices.
  - (Regular) Octahedron has 8 equilateral triangles, with 4 meeting at each vertex, 12 edges, and 6 vertices.
- Measurement
  - A comparison with a fixed reference amount of a quantity. The reference amount is called unit.
- Coordinates
  - A system using numbers (e.g., x, y, z) to determine positions of geometrical elements
- Symmetry
  - Translation: A shape or design if there is a translation of the plane such that the design or pattern as a whole occupies the same place in the plan both before and after translation.
  - Rotation: A shape or a design in a plan, if there is a rotation of the plane of more than 0 degrees but less than 360 degrees, such that the shape or design as a whole occupies the same points in the plan both before and after rotation.
  - Reflection: A shape or a design in a plan, if there is a line in the plane such that there are matching parts when the shape or design is folded along the line. Coordinates
- Ratio
  - Two quantities are in ratio A to B if there are N x A units of the first quantity, N x B units of the second quantity.
- Similarity
  - Two objects are similar if every point on one object corresponds to a point on the other object and there is a positive K, such that the distance between any two points on the second object is K times as long as the distance between the corresponding points on the first object.

Summary: Materials Concepts

- Atom
  - An atom is the smallest unit of ordinary matter that forms a chemical element.
- Crystal Structure
  - A description of the ordered arrangement of atoms, ions or molecules in a crystalline material
- Crystalline
  - A material in which the atoms are situated in a repeating or parodic array

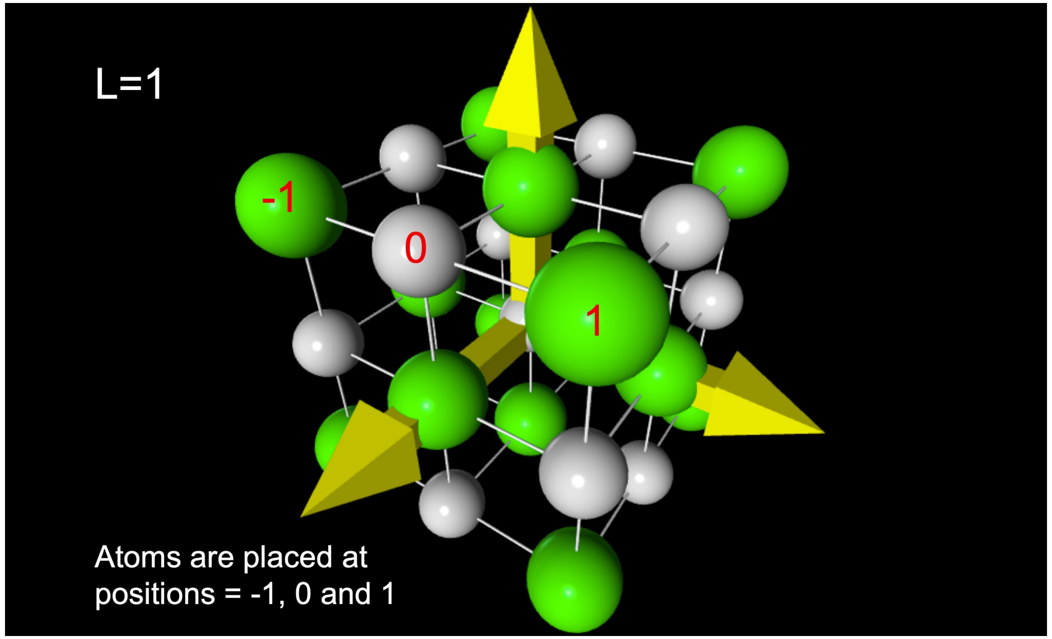


Summary: Computer Science Concepts

- Class
  - A user-defined type specifying attributes
- Object
  - An instance or run-time entity of a class
- Attribute
  - Properties of a class of objects

Make it is possible to program complex problems.

Class:
Sodium atom
Object:
Many Spheres
Attributes:
Color: Green
Size: 1.67
Position: X, Y, Z



Let’s discover Math in a STEM context

Questions?