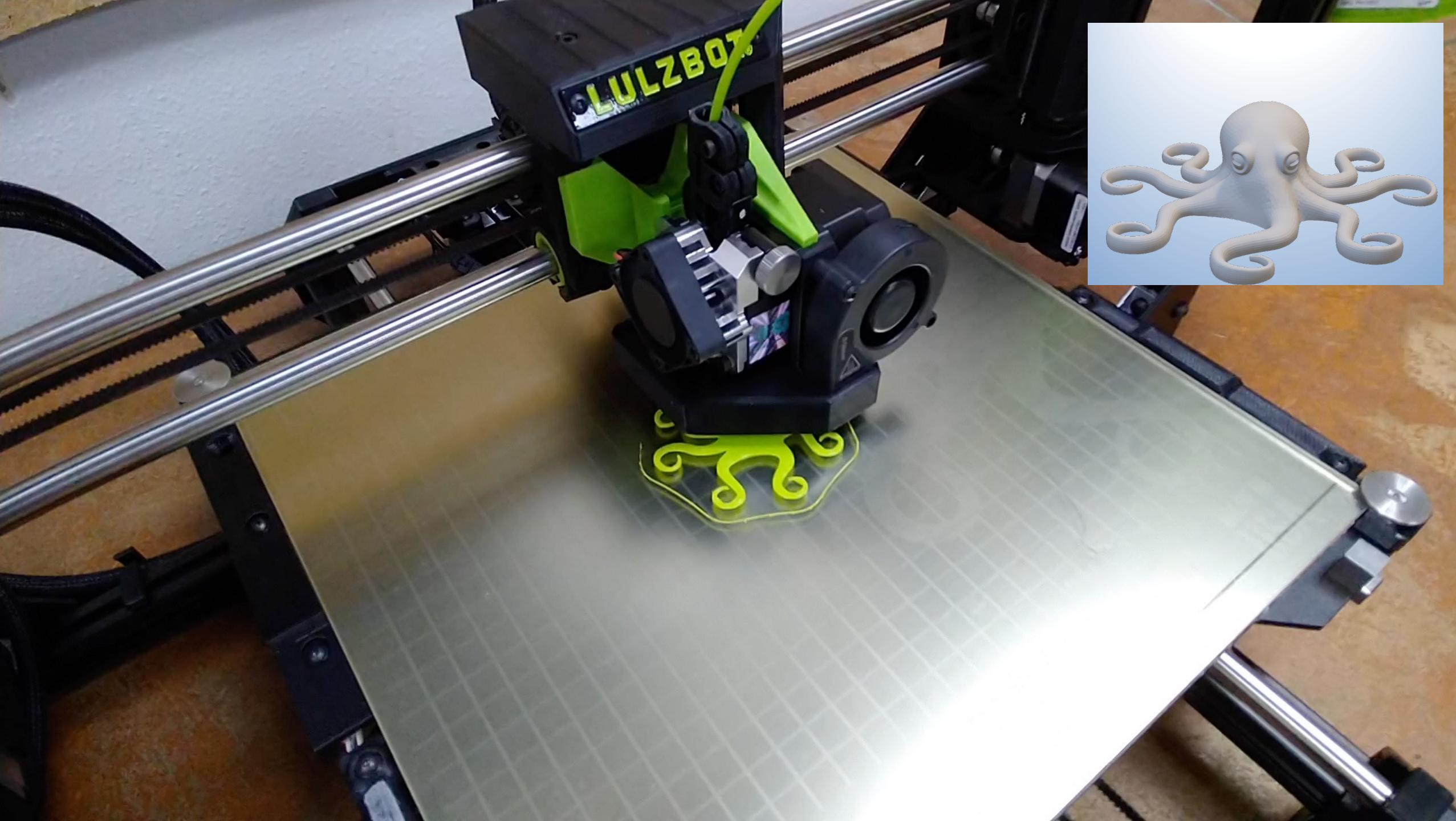


# Training Materials: Exploring Math through Programming and Visualization of Crystal Structures

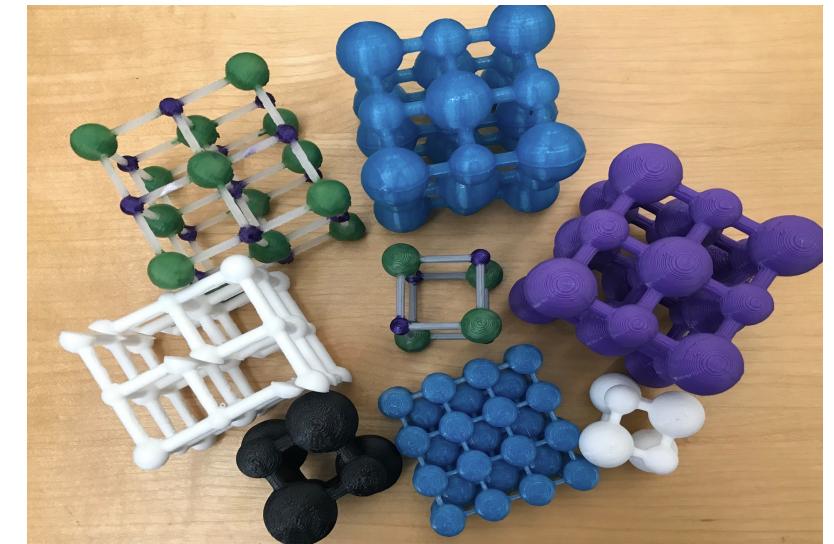
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Min Long, Andy Lau  
Department of Computer Science  
Boise State University  
<https://cs.boisestate.edu/~mlong/education.html>  
<https://minlong1.github.io/education.html>



# Objective

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



# Training Materials

- Lecture 1: Introduction to Online Toolkit and STEM Concepts
- Lecture 2: Introduction to 3D printing and operation of 3D printer
- Lecture 3: Printing Practice: print simple cubic and fcc materials
- Lecture 4: Design bcc and Perovskite materials
- Worksheet: Part 1 and Part 2

# Lecture 1: Online Tool, STEM Concepts

# Lecture 1

- Overview of STEM Concepts
  - Math Concepts
  - Materials Concepts
  - Computer Science Concepts
- Online Toolkit: Learning Math in STEM Context
- Design simple cubic and face-center cubic 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

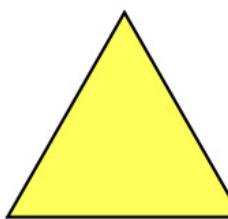
Materials

3D  
Printing

# Math Concepts

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

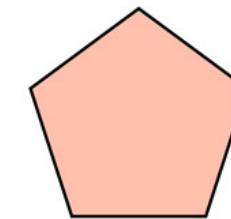
## Polygons



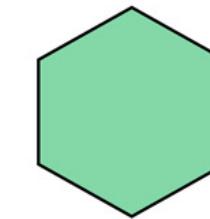
Triangle



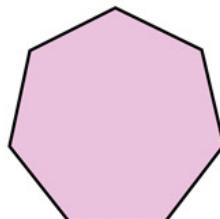
Quadrilateral



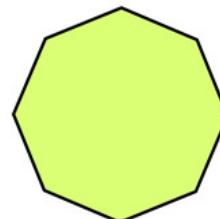
Pentagon



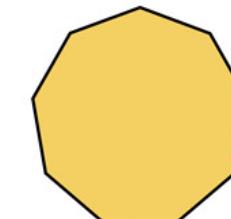
Hexagon



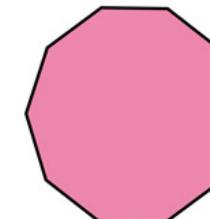
Heptagon



Octagon



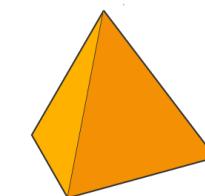
Nonagon



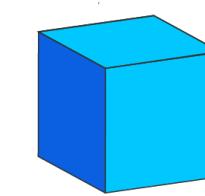
Decagon

MATH  
MONKS

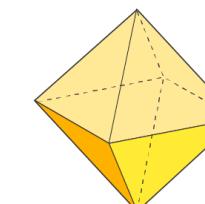
## Regular Polyhedrons



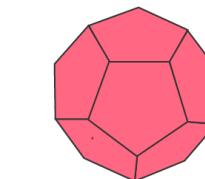
Tetrahedron



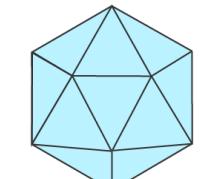
Cube



Octahedron



Dodecahedron



Icosahedron

 cuemath  
THE MATH EXPERT

# 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.



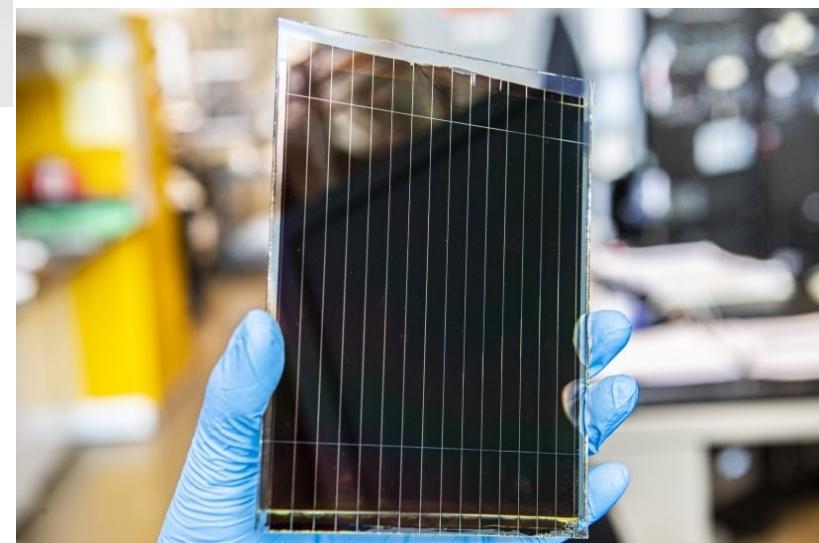
Salt Crystal



Hope diamond



Iron

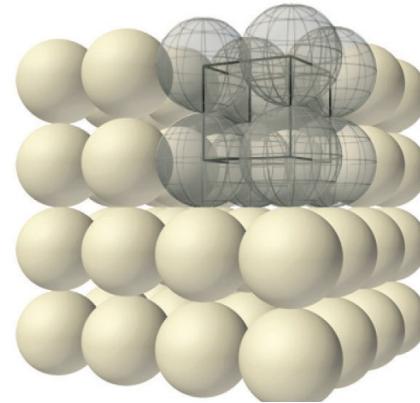
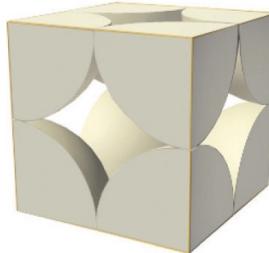
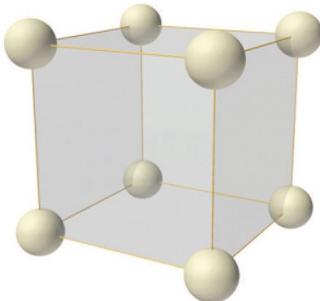


Perovskite Solar Cell

# Crystal Structures

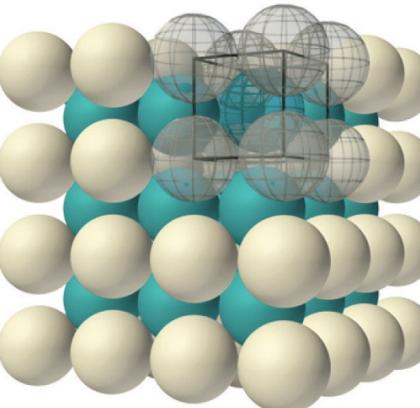
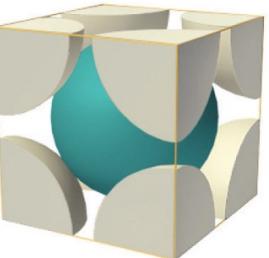
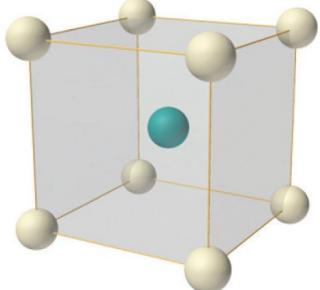
- Many...

Simple Cubic



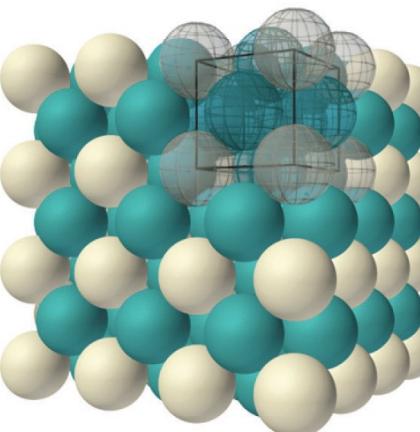
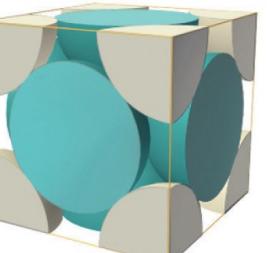
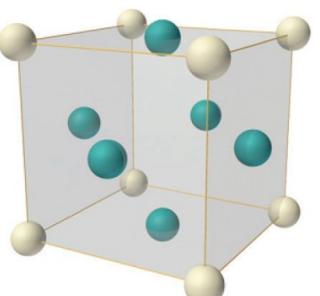
Polonium

Body-centered  
Cubic (bcc)



Iron

Face-centered  
Cubic (fcc)

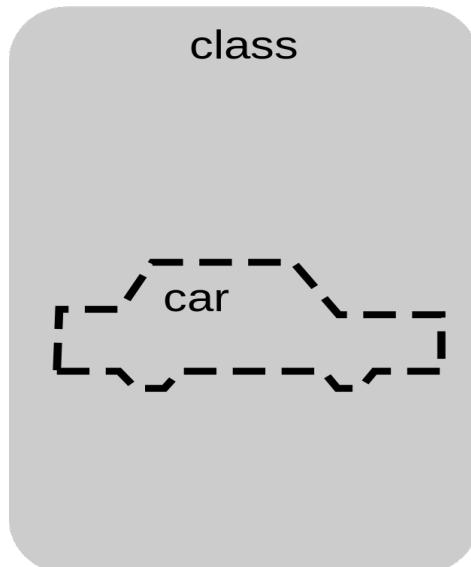


“Unit Cell”

# Computer Science: Programming

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

Car
<b>Attribute:</b>
Color
Brand
Model



“blueprint”



Objects
<b>Color:</b> Silver
<b>Brand:</b> Toyota
<b>Model:</b> Camry



Objects
<b>Color:</b>
<b>Brand:</b>
<b>Model:</b>

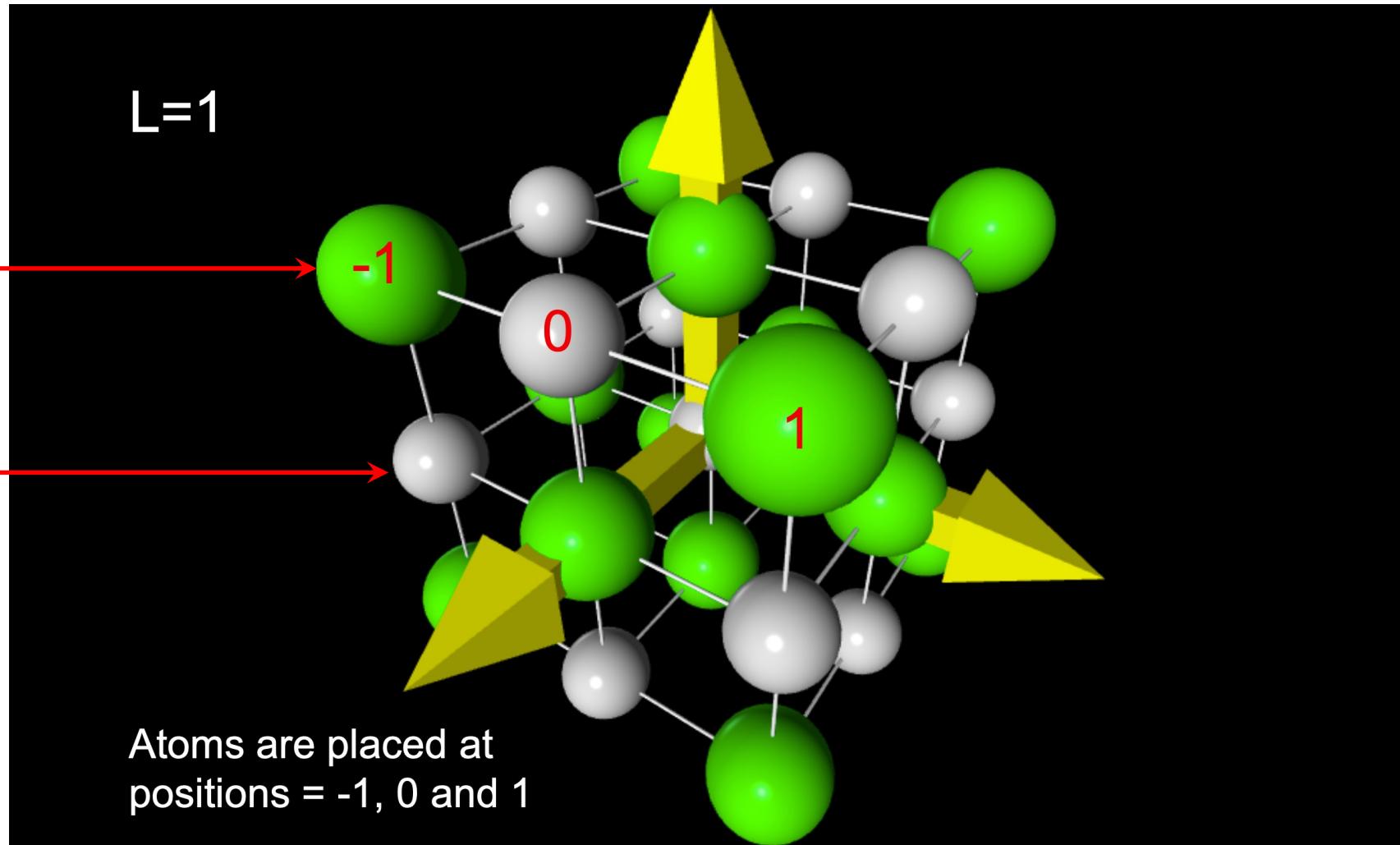
“realization”

# 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

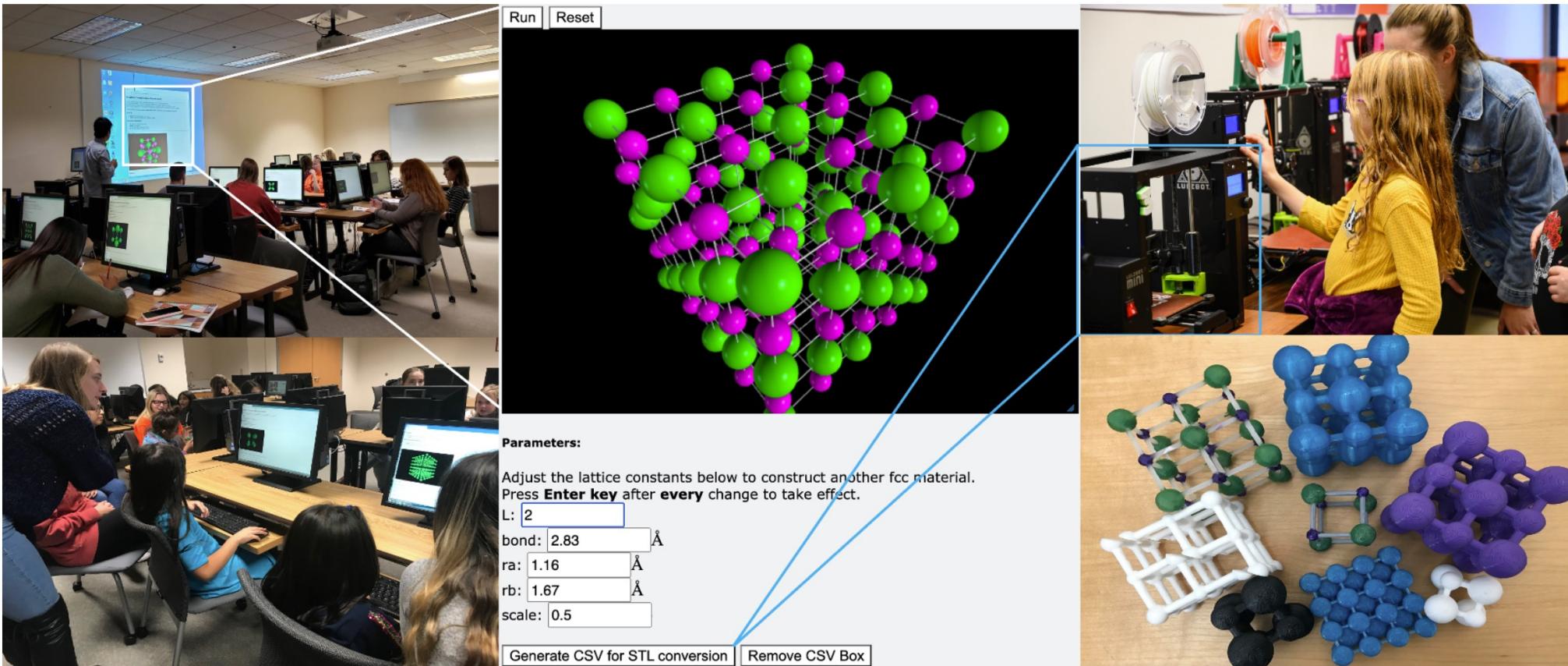


# Online Toolkit: Learning Math in STEM

- <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, visualization and 3D printing techniques can enhance students' learning in STEM.



# Summary of STEM Concepts

- Math

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

- Materials

- Atoms
- Crystal Structures
- Crystalline

- Programming

- Class
- Object
- Attribute

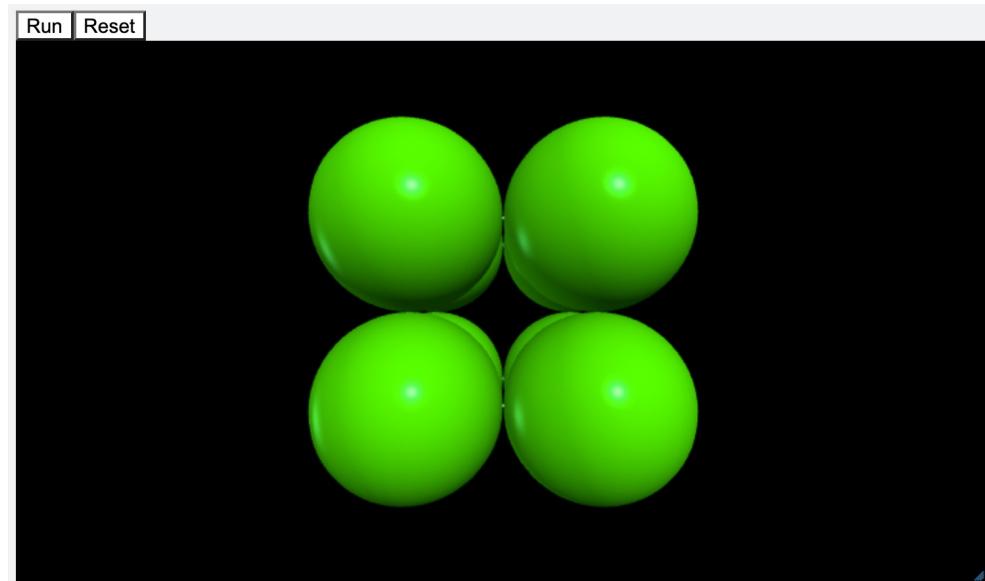
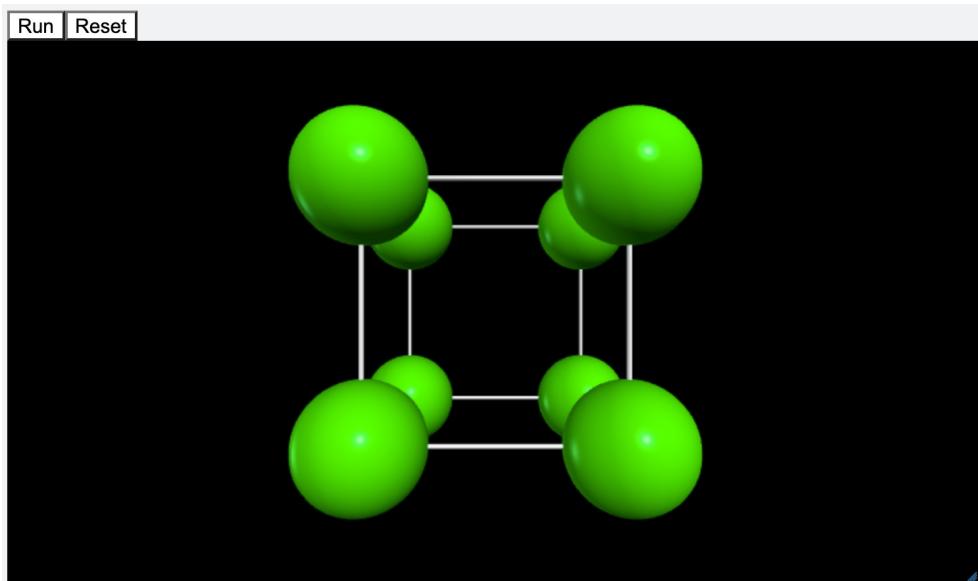
Before the class: Look through these concepts

# Applications: Design simple cubic and face-center cubic materials

# Ex1 - Simple Cubic: Metal Polonium (Po)



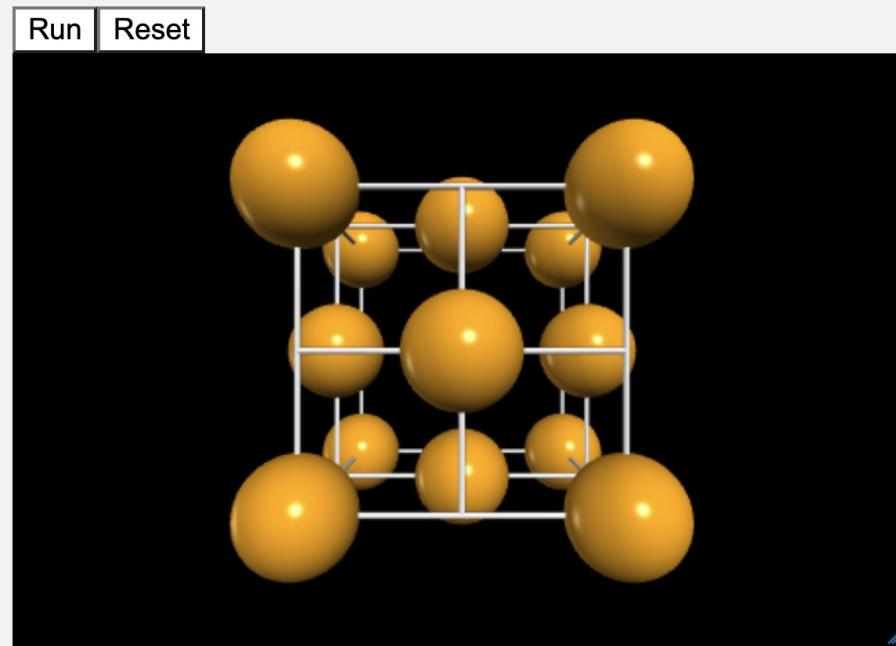
- Polonium is a rare and **highly radioactive** metal.
- This structure consists of the smallest repeating pattern of the cube with one lattice point on each corner of the cube.



# 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



## Parameters:

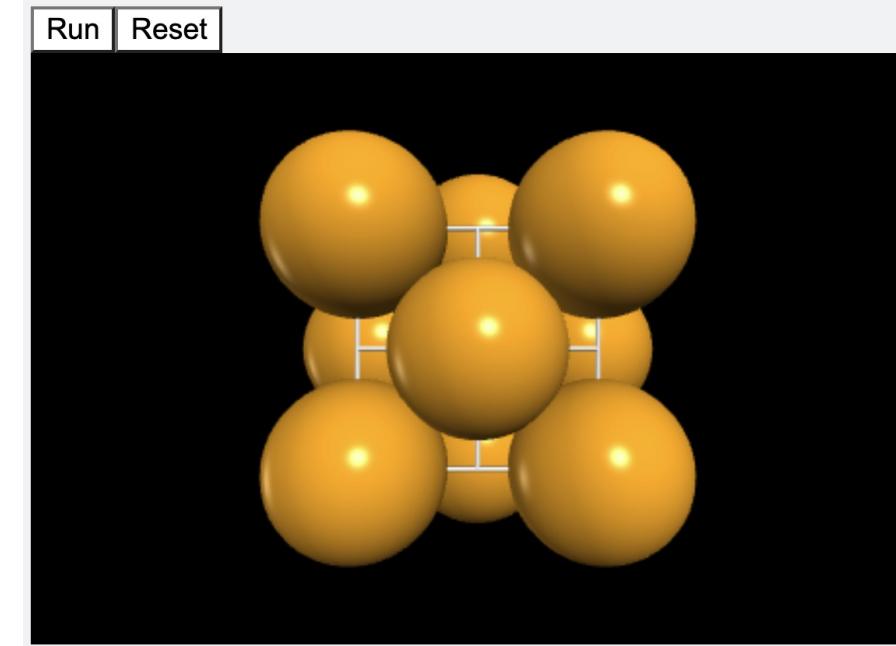
Adjust the parameters below to build up another fcc material.  
Press **Enter key** after **every** change to take effect.

L:

a:  Å

ra:  Å

scale:  ( Input a number between 0 and 1 )



## Parameters:

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

L:

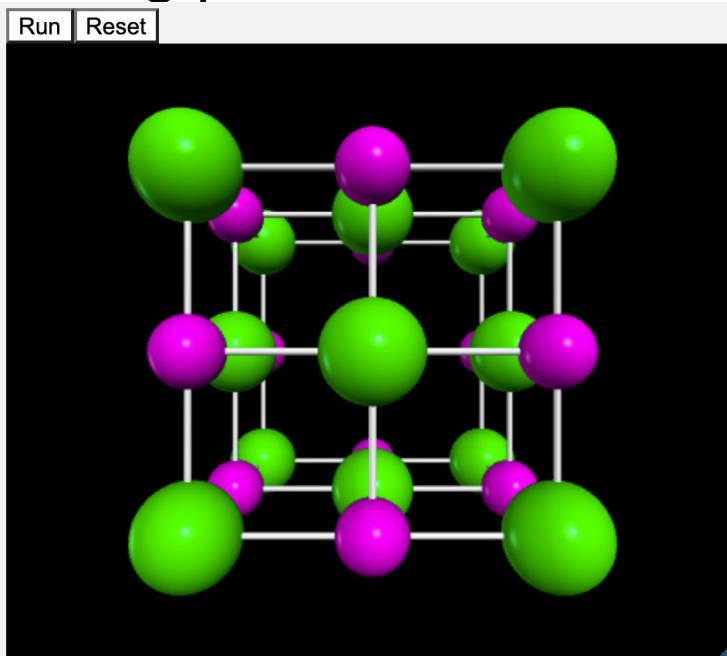
a:  Å

ra:  Å

scale:  ( 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.

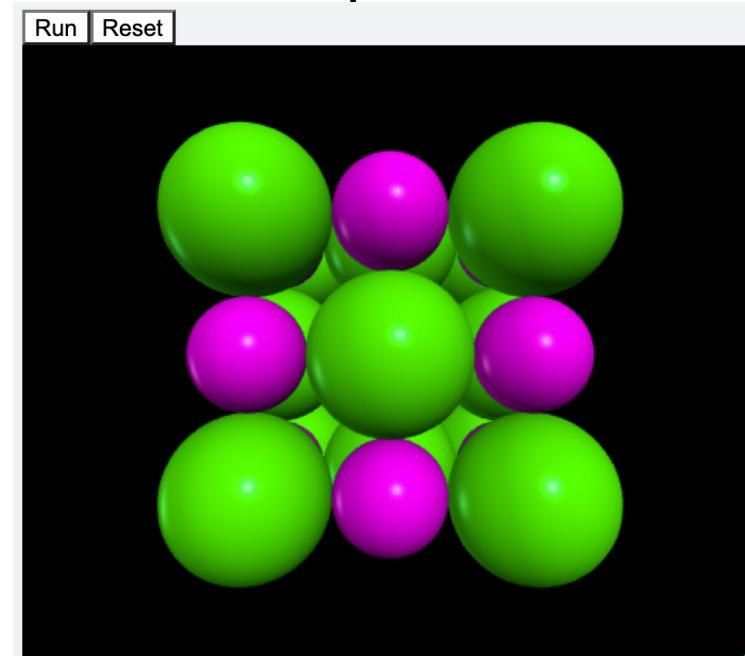


#### Parameters:

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

L:  Å  
a:  Å  
ra:  Å  
rb:  Å

scale:  ( Input a number between 0 and 1 )



#### Parameters:

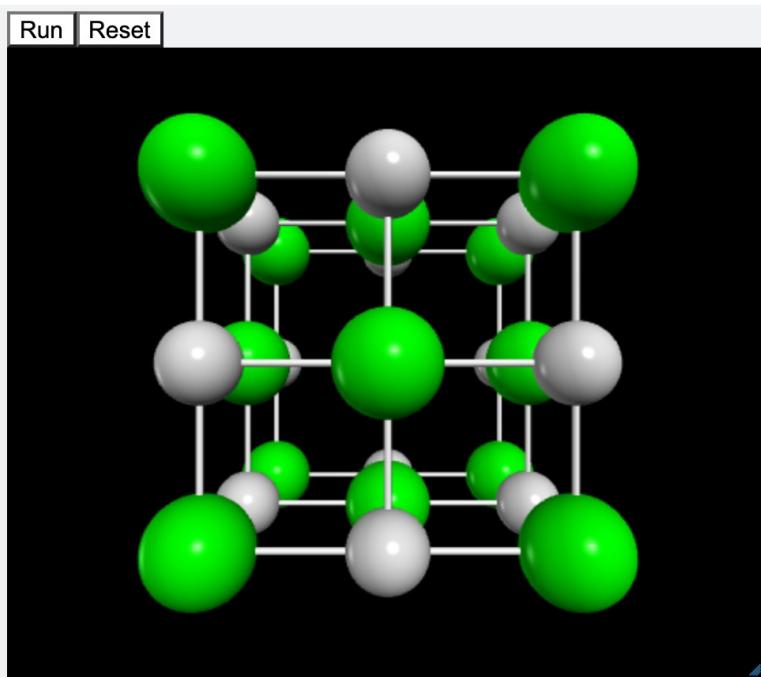
Adjust the parameters below to build up another fcc material.  
Press **Enter key** after **every** change to take effect.

L:  Å  
a:  Å  
ra:  Å  
rb:  Å

scale:  ( Input a number between 0 and 1 )

# Ex4 - Face-centered Cubic: AgCl

- The solid adopts the fcc NaCl structure
  - But Ag<sup>+</sup> ions replace Na<sup>+</sup> ions



#### Parameters:

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

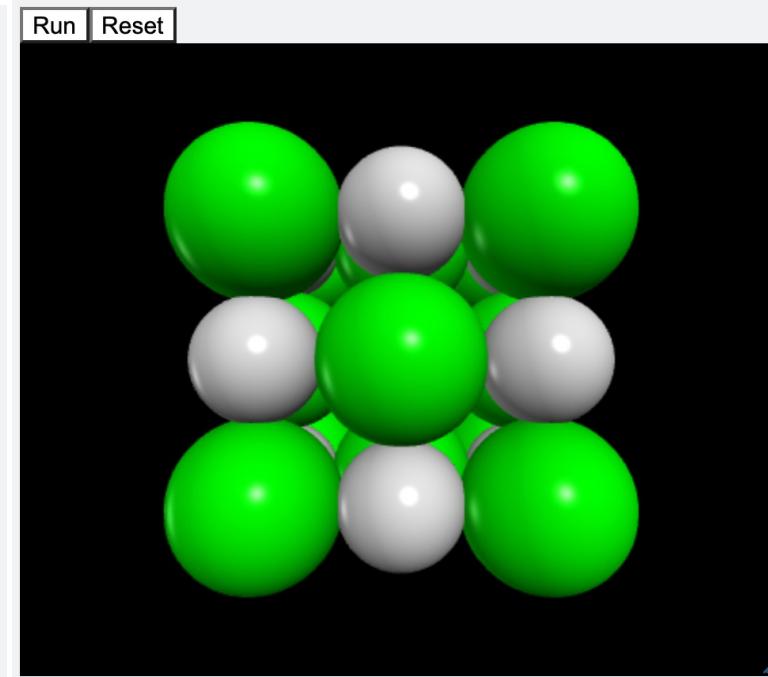
L:

a: 5.55 (Å)

ra: 1.26 (Å)

rb: 1.67 (Å)

scale:  ( Input a number between 0 and 1 )



#### Parameters:

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

L:

a: 5.55 (Å)

ra: 1.26 (Å)

rb: 1.67 (Å)

scale:  ( 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 \(data page\)](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 (Å)	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

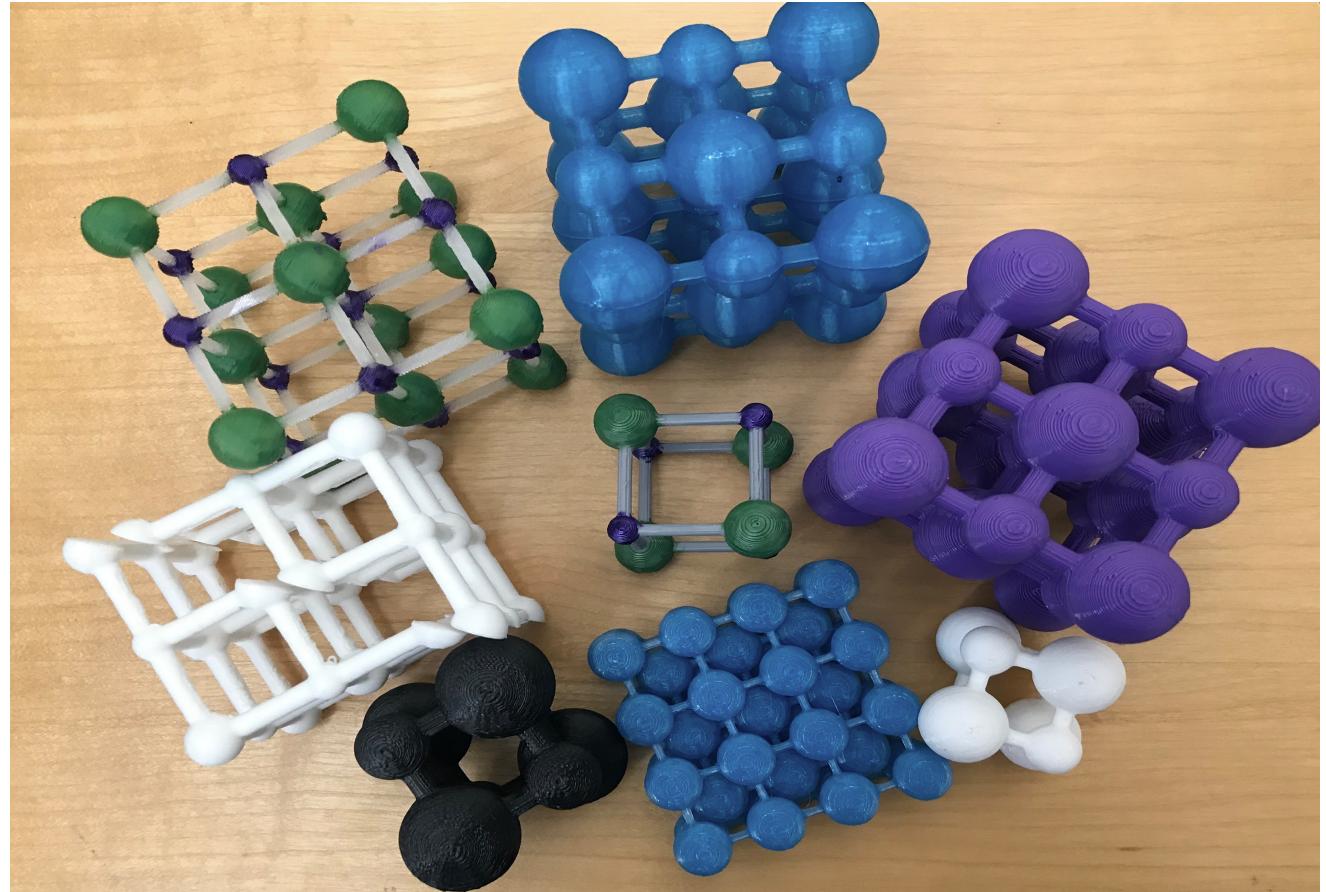
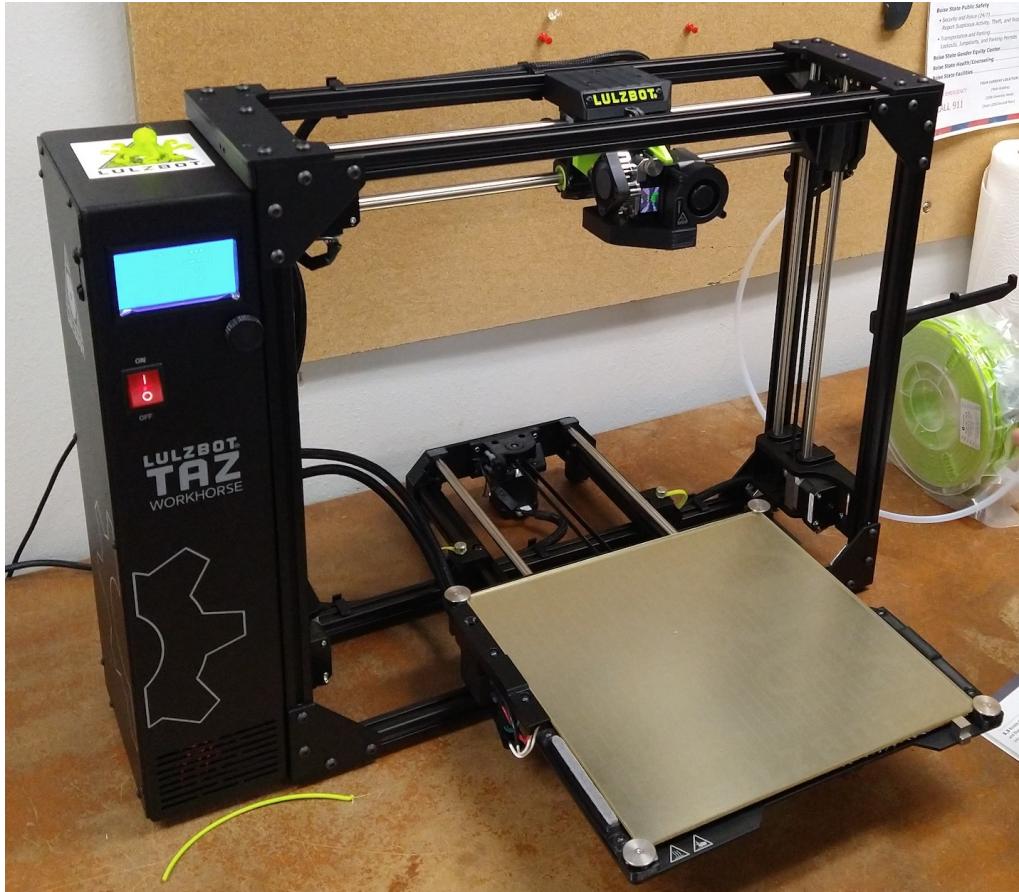
Material	a (Å)	Ionic ra(Å)	Ionic rb(Å)
KF	5.34	1.52	1.19
KCl	6.29	1.52	1.67
KBr	6.60	1.52	1.82
KI	7.07	1.52	2.06
RbF	5.65	1.66	1.19
RbCl	6.59	1.66	1.67
RbBr	6.89	1.66	1.82
RbI	7.35	1.66	2.06
CsF	6.02	1.81	1.19
AgF	4.92	1.29	1.19
AgCl	5.55	1.29	1.67
AgBr	5.77	1.29	1.82

# Practice and Work Sheet Time

- Access the online toolkit
- Observe simple and fcc structures.
- Answer questions in Work Sheet.

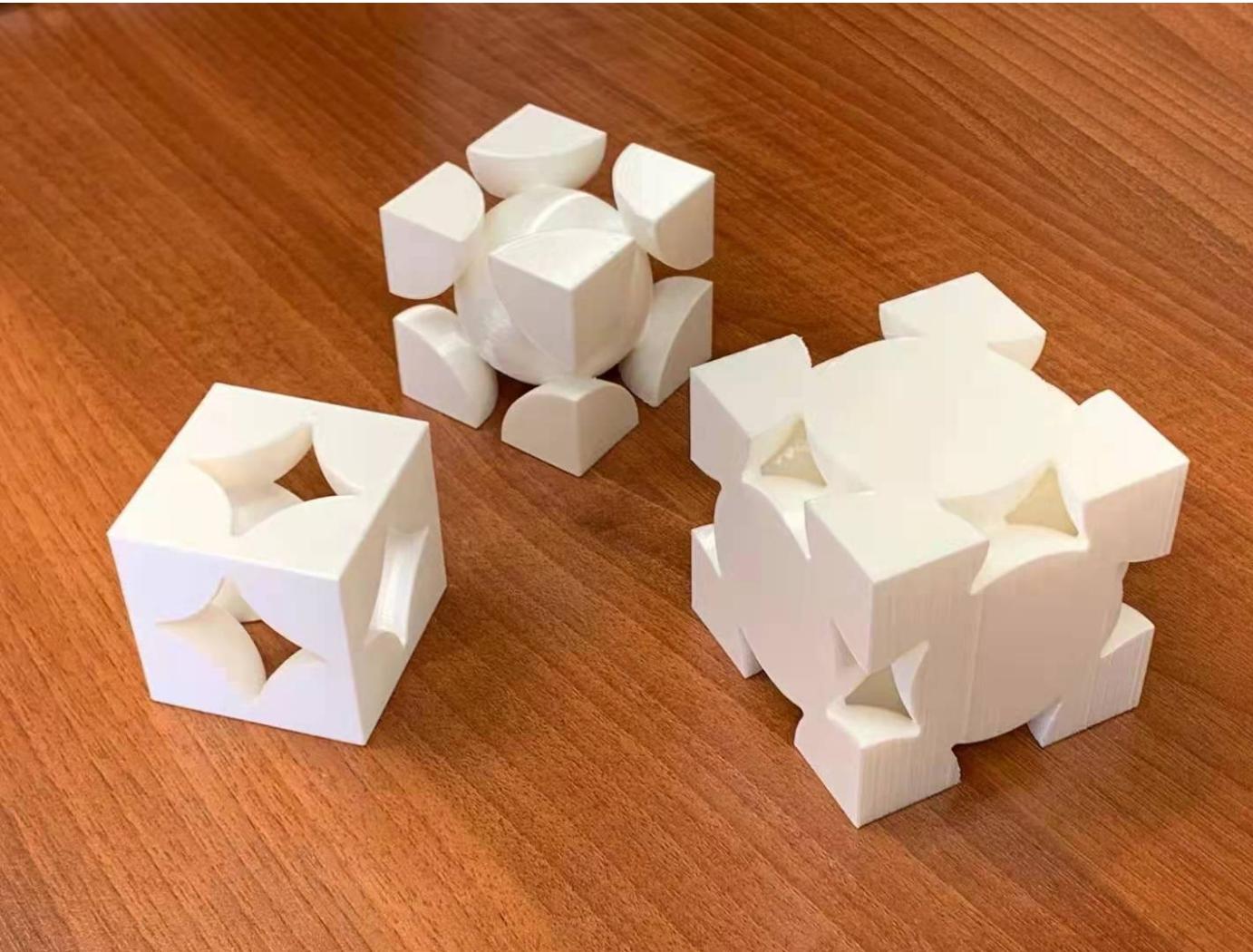
# Print it (Next Class)!

- 3D Printing



# Print it (Next Class)!

- 3D Printing



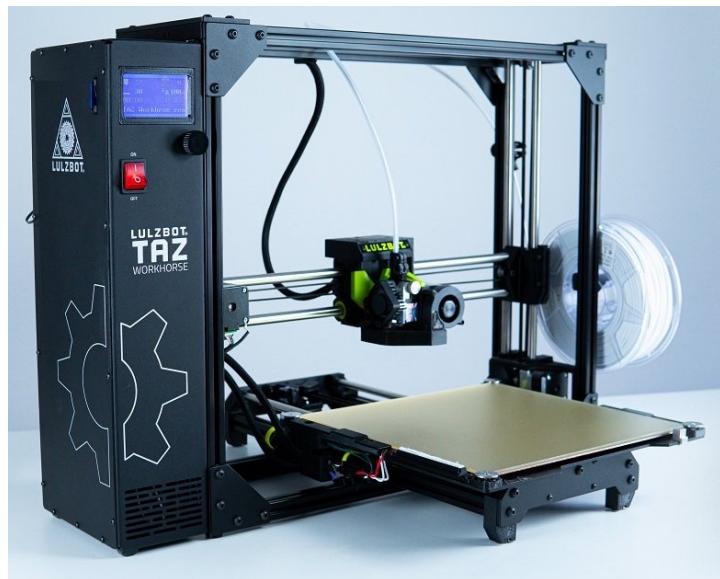
# Summary: Geometrical Concepts

- **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  $N \times A$  units of the first quantity,  $N \times B$  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.

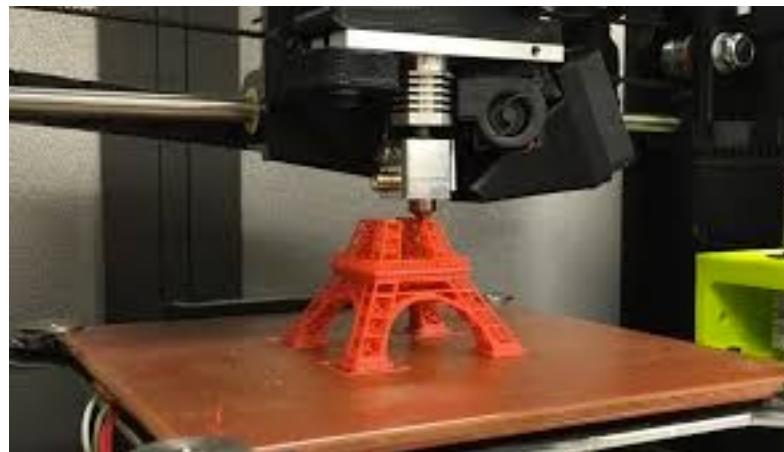
# Lecture 2: Introduction to 3D Printing

# Outline

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



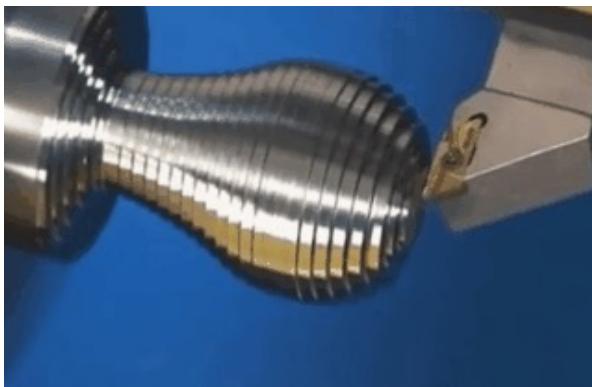
Lulzbot Workhorse



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

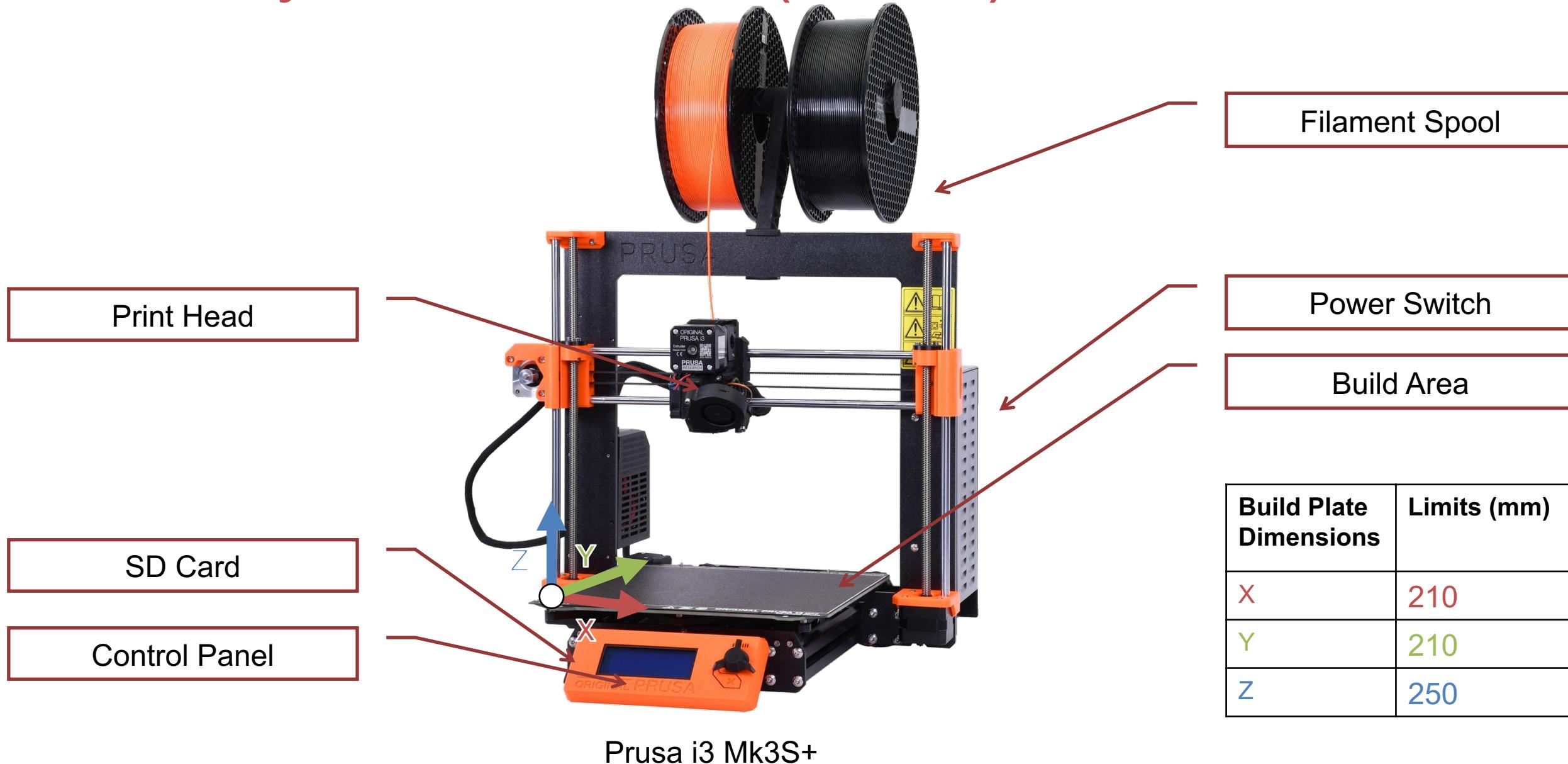


# Anatomy of 3D Printer (LulzBot)



LulzBot Workhorse 3D Printer

# Anatomy of 3D Printer (Prusa)



# 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/Mini/2.0.4/sample_prints/Octopus/)
    - [https://download.lulzbot.com/3D\\_Models/TAZ\\_Workhorse\\_Samples/](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/octo_gear_v1.stl)
    - <http://cs.boisestate.edu/~mlong/3dprinting/OctopusRev06.stl>

← → ⌂ download.lulzbot.com/Mini/2.0.4/sample\_prints/Octopus/

## Index of /Mini/2.0.4/sample\_prints/Octopus

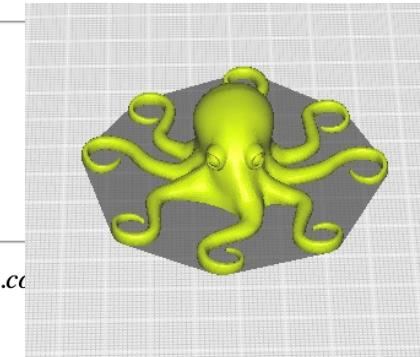
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License.txt 2018-10-17 13:24 178

OctopusRev06.stl 2018-10-17 13:24 2.1M



Apache/2.4.29 (Ubuntu) Server at download.lulzbot.co

← → ⌂ download.lulzbot.com/3D\_Models/TAZ\_Workhorse\_Samples/

## Index of /3D\_Models/TAZ\_Workhorse\_Samples

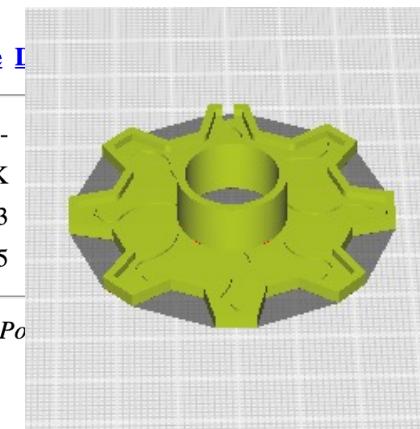
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octo\_gear\_v1\_License.txt 2019-07-30 20:34 185



Apache/2.4.29 (Ubuntu) Server at download.lulzbot.com Po

# 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>



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

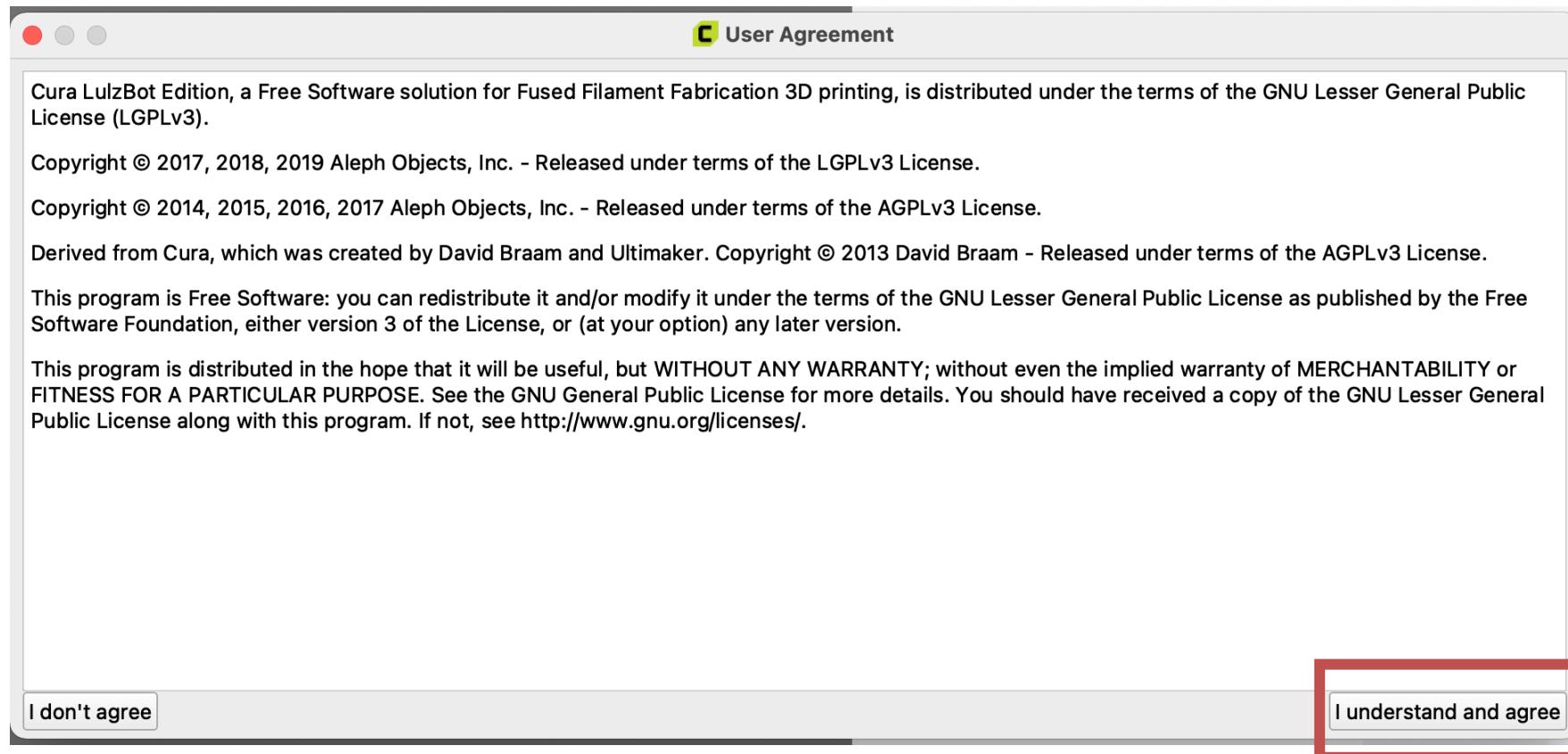
Find links and instructions based on your operating system in the tutorials below.

Current Version: 3.6.25 - 10



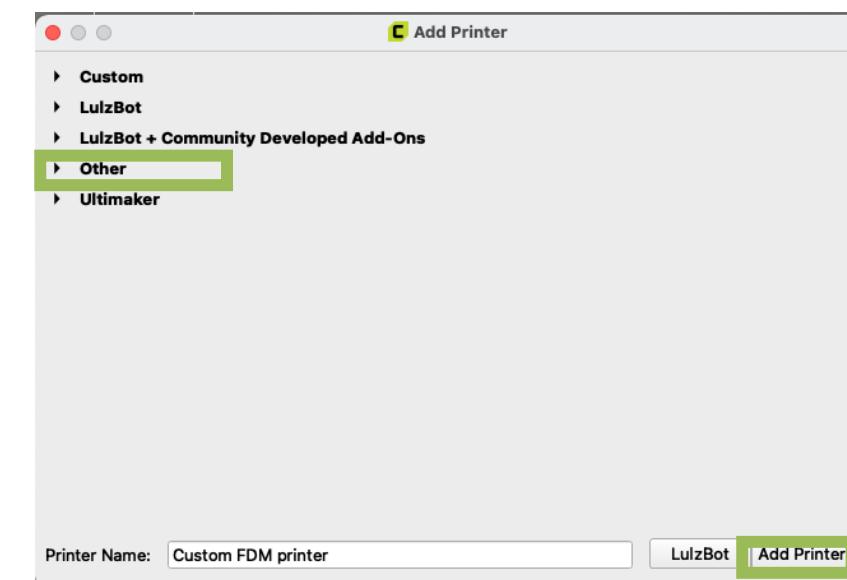
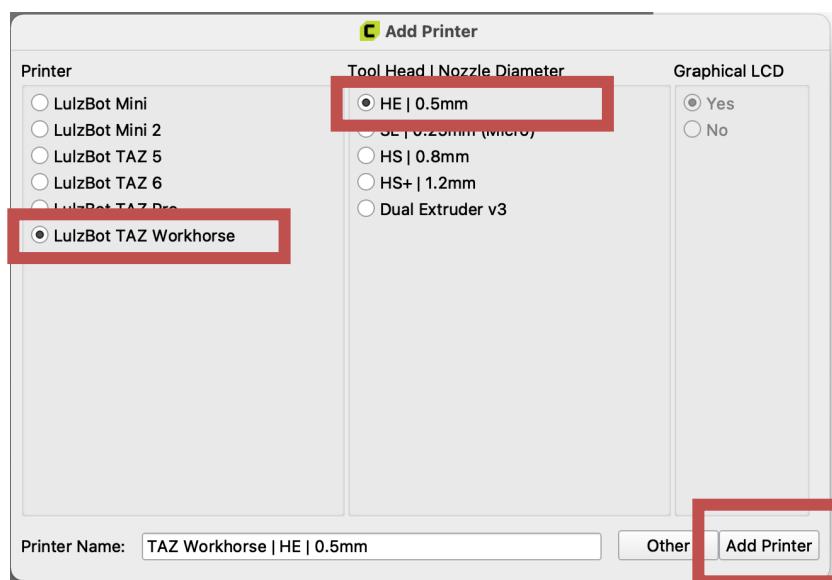
# Step 2. Access Cura LulzBot: first time user

- User Agreement:
  - Select “I understand and agree”



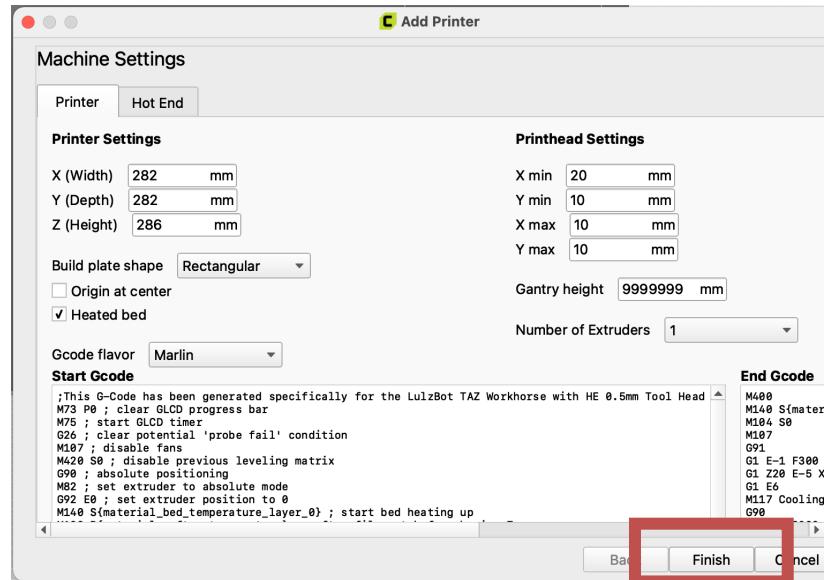
# Step 2. Access Cura LulzBot: first time user

- Add a printer
  - For **Lulzbots**, 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**

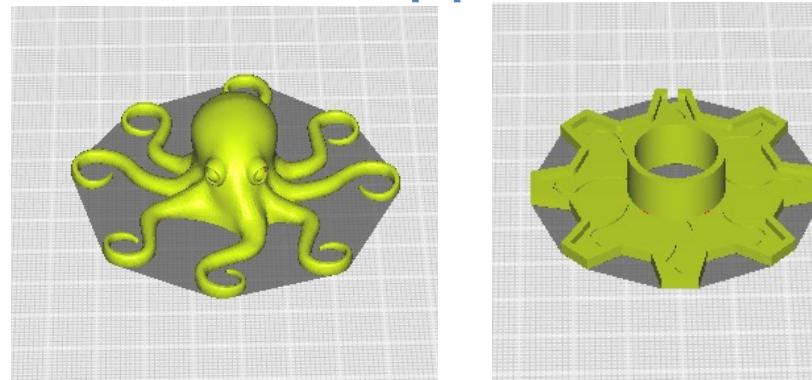


# Step 2. Access Cura LulzBot: first time user

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

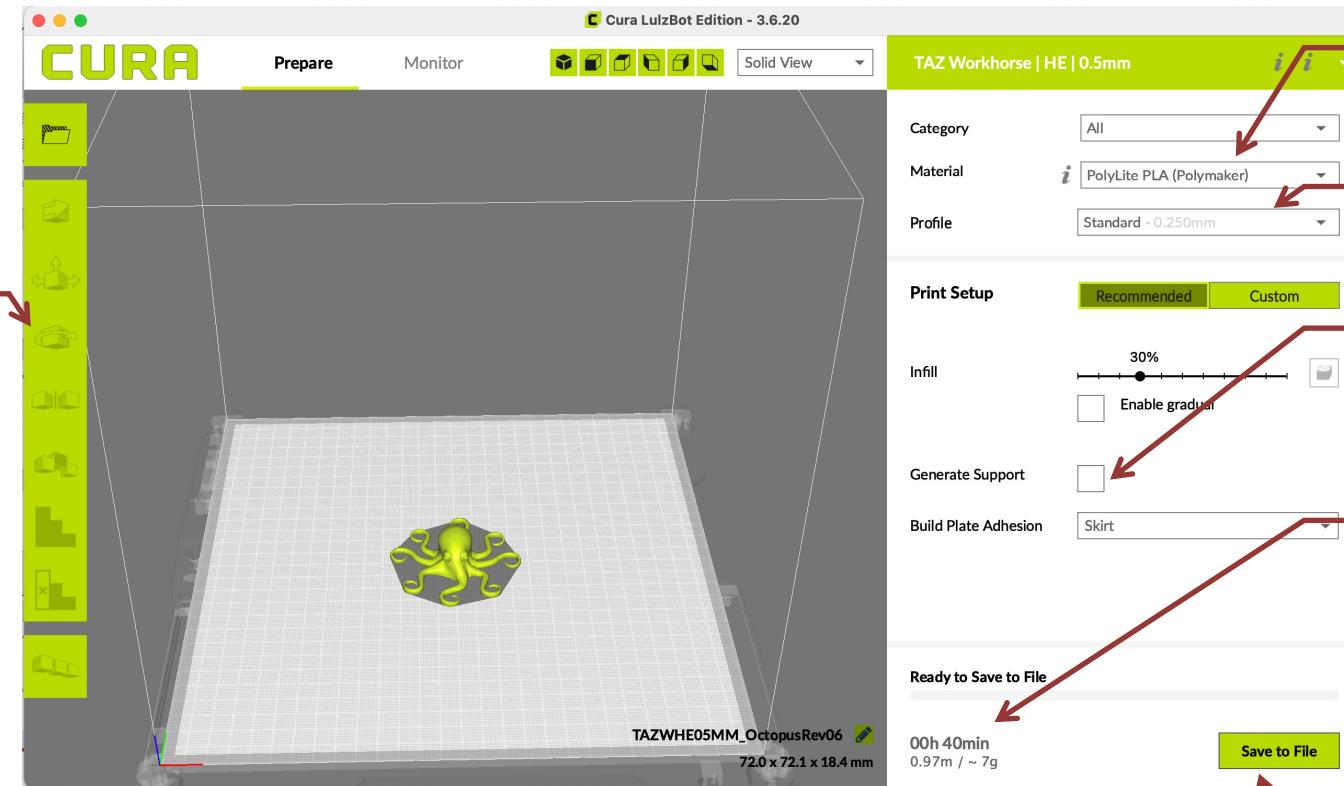


- A built-in Octopus or Gear will appear in the build area.



# 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)

Print Setup

Recommended

Custom

Search...

Infill	215	°C
Material	215	°C
Default Printing Temperature	215	°C
Printing Temperature	215	°C
Probe Temperature	160	°C
Soften Temperature	180	°C
Wipe Temperature	170	°C
Printing Temperature Initial Layer	210	°C
Initial Printing Temperature	210	°C
Final Printing Temperature	210	°C
Build Plate Temperature	45	°C
Part Removal Temperature	35	°C
Keep Heating	<input checked="" type="checkbox"/>	
Build Plate Temperature Initial Layer	55	°C
Diameter	2.85	mm
Flow	100	%
Initial Layer Flow Rate	100	%
Enable Retraction	<input checked="" type="checkbox"/>	
Retract at Layer Change	<input checked="" type="checkbox"/>	
Retraction Distance	1.5	mm

Before

Print Setup

Recommended

Custom

Search...

Infill	220	°C
Material	220	°C
Default Printing Temperature	220	°C
Printing Temperature	220	°C
Probe Temperature	140	°C
Soften Temperature	140	°C
Wipe Temperature	140	°C
Printing Temperature Initial Layer	225	°C
Initial Printing Temperature	210	°C
Final Printing Temperature	205	°C
Build Plate Temperature	75	°C
Part Removal Temperature	35	°C
Keep Heating	<input checked="" type="checkbox"/>	
Build Plate Temperature Initial Layer	55	°C
Diameter	2.85	mm
Flow	100	%
Initial Layer Flow Rate	100	%
Enable Retraction	<input checked="" type="checkbox"/>	
Retract at Layer Change	<input checked="" type="checkbox"/>	
Retraction Distance	1.5	mm

After

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

The screenshot shows the CURA software interface for 3D printing preparation. On the left, there's a vertical toolbar with icons for various functions. Three specific icons are highlighted with colored arrows pointing to callout boxes:

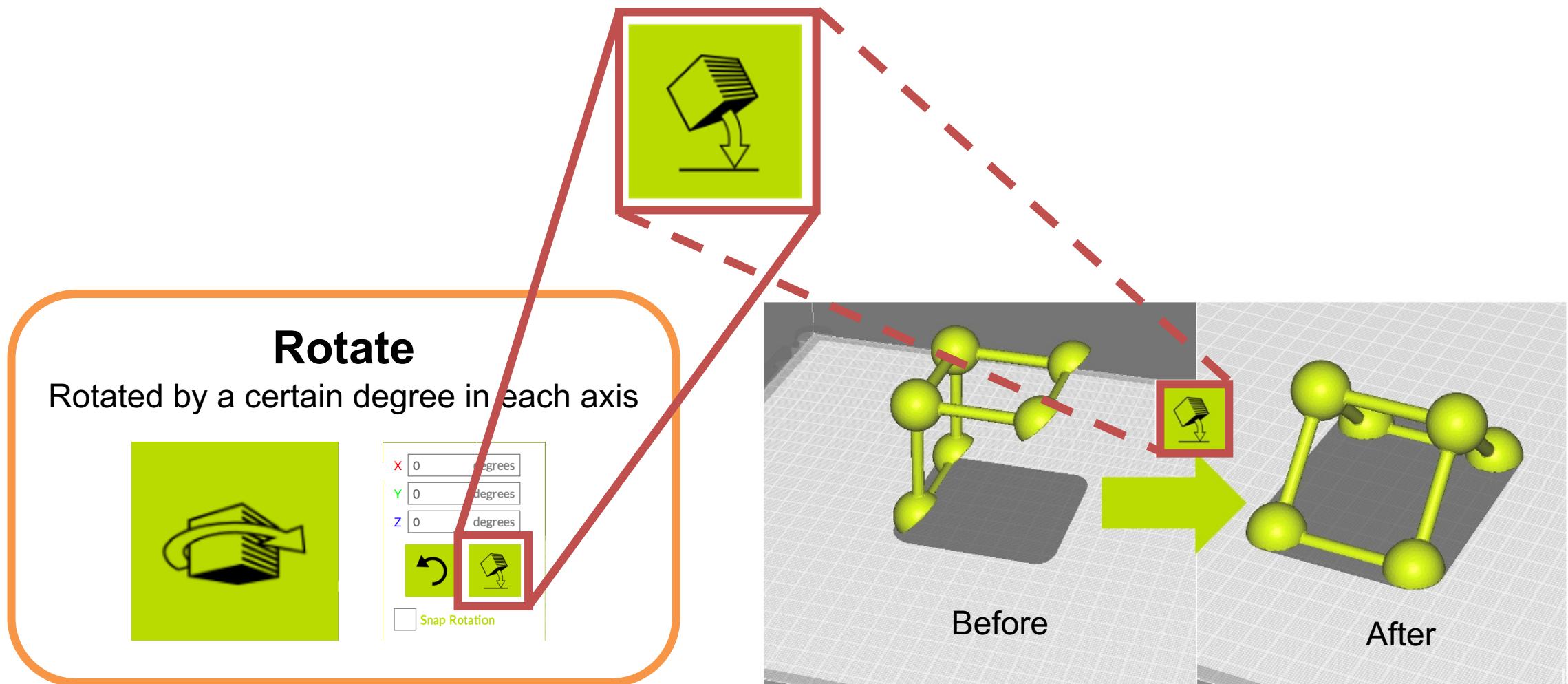
- Translation**: Moved by a distance. This tool allows you to move the model in 3D space. The interface shows input fields for X, Y, and Z coordinates in mm, and a checkbox for "Lock Model".
- Scaling**: Scaled by a value. This tool allows you to scale the model. It shows current scaling factors (X: 72.0108 mm, Y: 72.1426 mm, Z: 18.4353 mm) relative to 100%, and checkboxes for "Snap Scaling" and "Uniform Scaling".
- Rotate**: Rotated by a certain degree. This tool allows you to rotate the model. It shows input fields for rotation angles in degrees for X, Y, and Z axes, and a checkbox for "Snap Rotation".

The right side of the interface displays the print profile settings:

- Profile**: Set to TAZ Workhorse | HE | 0.5mm.
- Category**: All.
- Material**: PolyLite PLA (Polymaker).
- Profile**: Standard - 0.250mm.
- Print Setup**: Set to Recommended.
- Infill**: Infill level is set to 30%.
- Generate Support**: Option to generate support structures is available.
- Build Plate Adhesion**: Skirt is selected.
- Ready to Save to File**: Status message indicating preparation is complete.
- 00h 40min**: Total print time estimated.
- 0.97m / ~ 7g**: Total filament length and weight estimated.
- Save to File**: Button to save the prepared file.

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

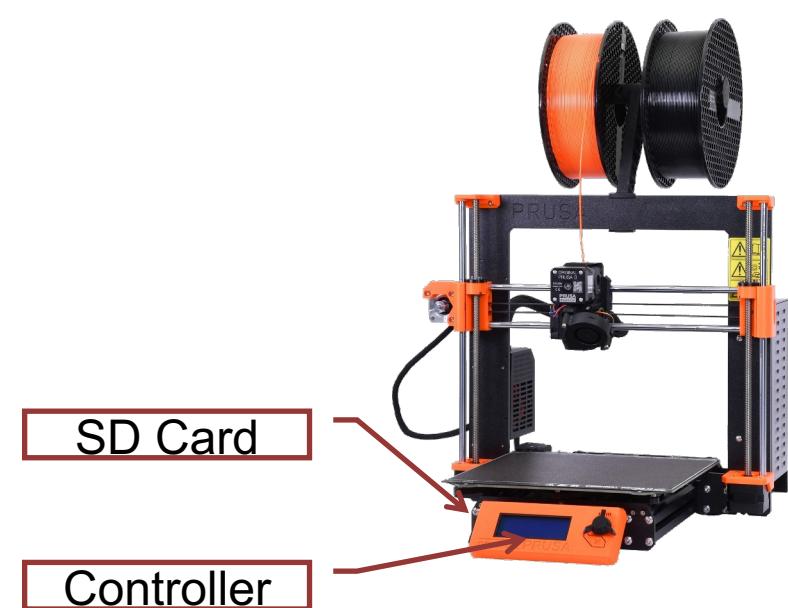
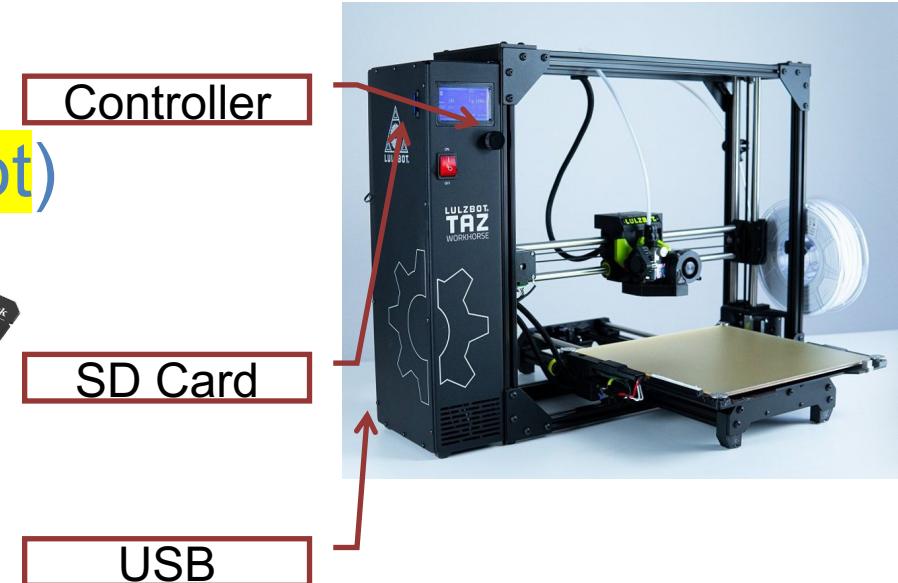
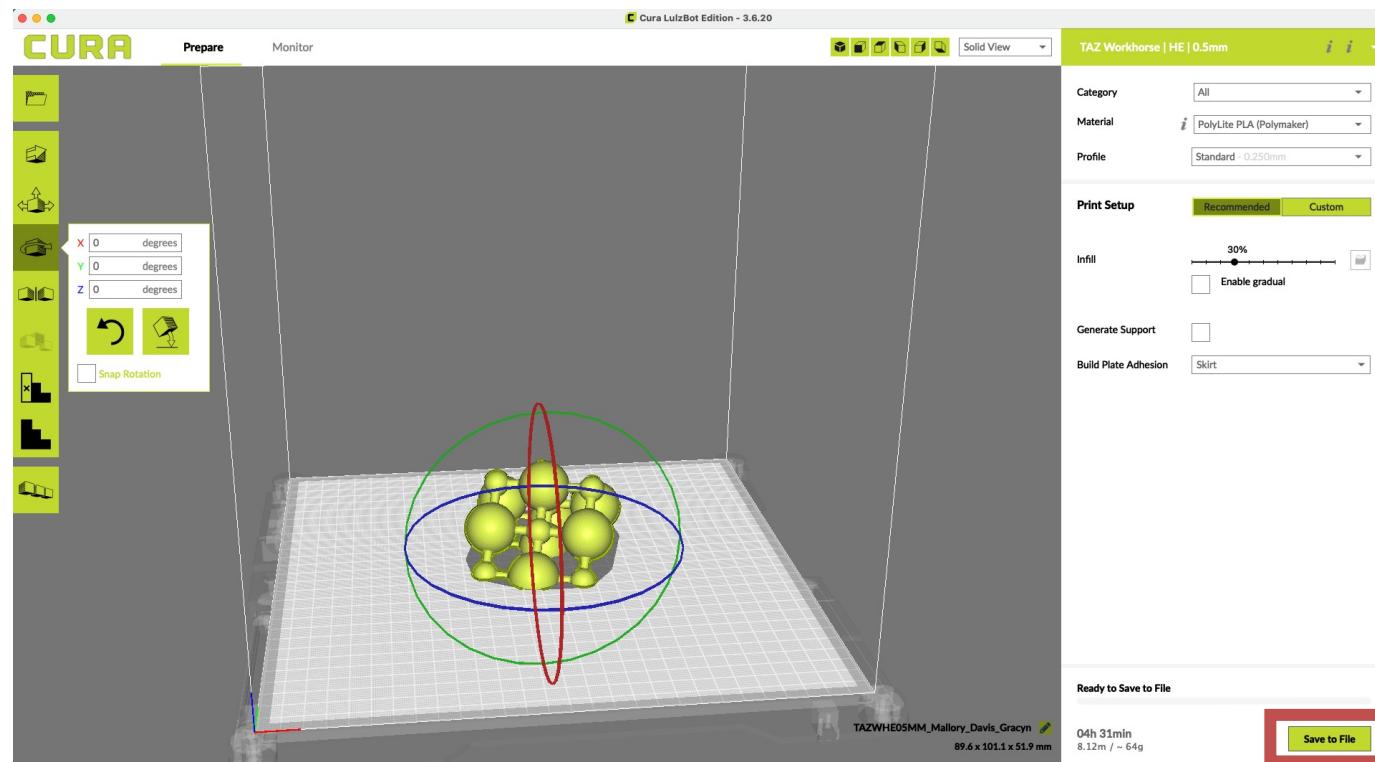
- For the rotation, we **highly** recommend using the “Lay Flat” button.



# Step 4. 3D Printing Time!

## • Option 1: Print through SD card (Prusa/Lulzbot)

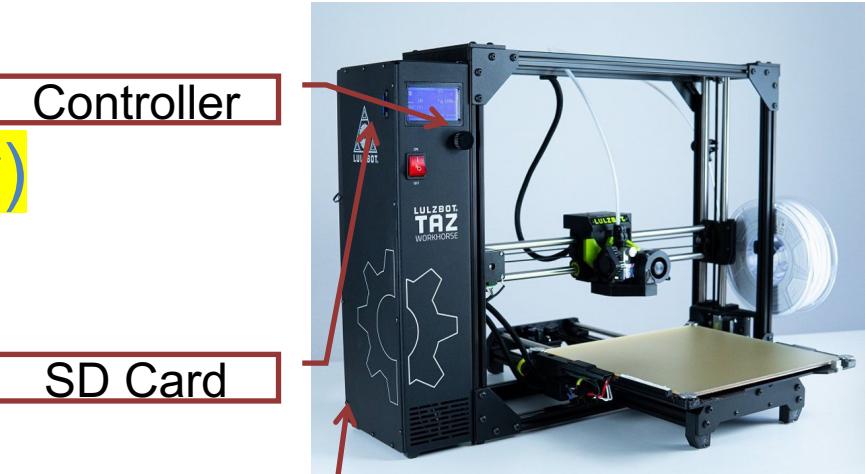
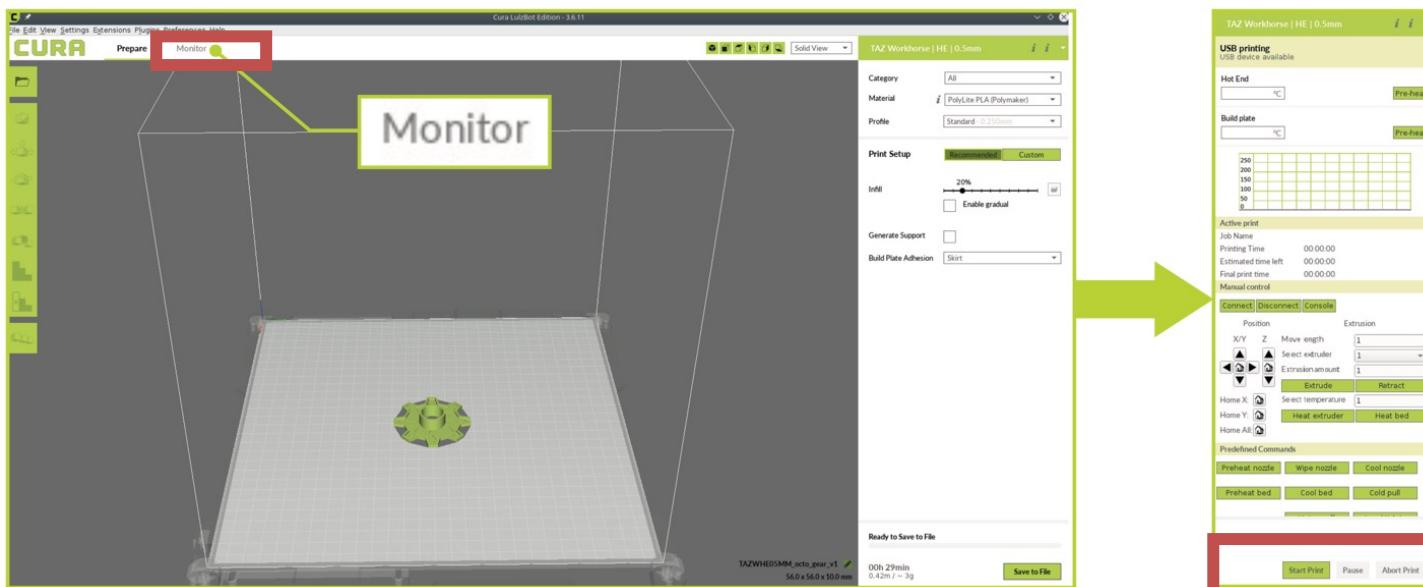
- Click **Save to File** in Cura
  - Save the model in .Gcode format to a SD card
- Use printer's control panel for printing



# Step 4. 3D Printing Time!

- Option 2: Print through Computer (Lulzbot only)

- Click “Monitor” in Cura
- Click “Start Print”



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.

Sign Up

Already have an account? [Log in here](#) to respond to the invitation.

First Name  Last Name

Email

Phone

Password

Sector

I agree to the [Terms of Use](#) and [Privacy Policy](#).

- 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.

The screenshot shows the ClusterMarket.com platform's equipment management section. On the left, there is a sidebar with a 'Equipment' header, followed by 'Overview' (which is highlighted with a blue background), 'Bookings', and 'Add Equipment'. Below this is a 'Services' section with a downward arrow. The main area has a header 'Equipment' with dropdown arrows for sorting by 'Visibility', 'Room', 'Rating', and 'Status'. There are two entries in the table:

Equipment	Visibility	Room	Rating	Status	
LulzBot TAZ Workhorse #1	internal	-	0 Reviews	Available	<input type="button" value=""/>
LulzBot TAZ Workhorse #2	internal	-	0 Reviews	Available	<input type="button" value=""/>

# Step 5: Lab Scheduling Management (Optional)

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



Announcements My booking Member booking External booking Not available

Booking details

Dates	Time	Quantity
05/09/2021	10:15 - 11:45	1.5 hrs

Notes

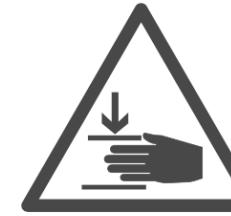
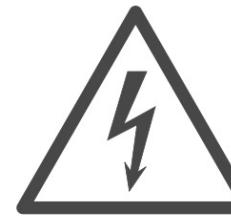
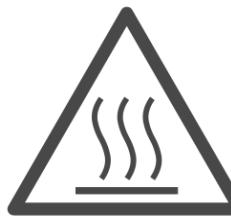
Write your notes

**Book**

# 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](#)

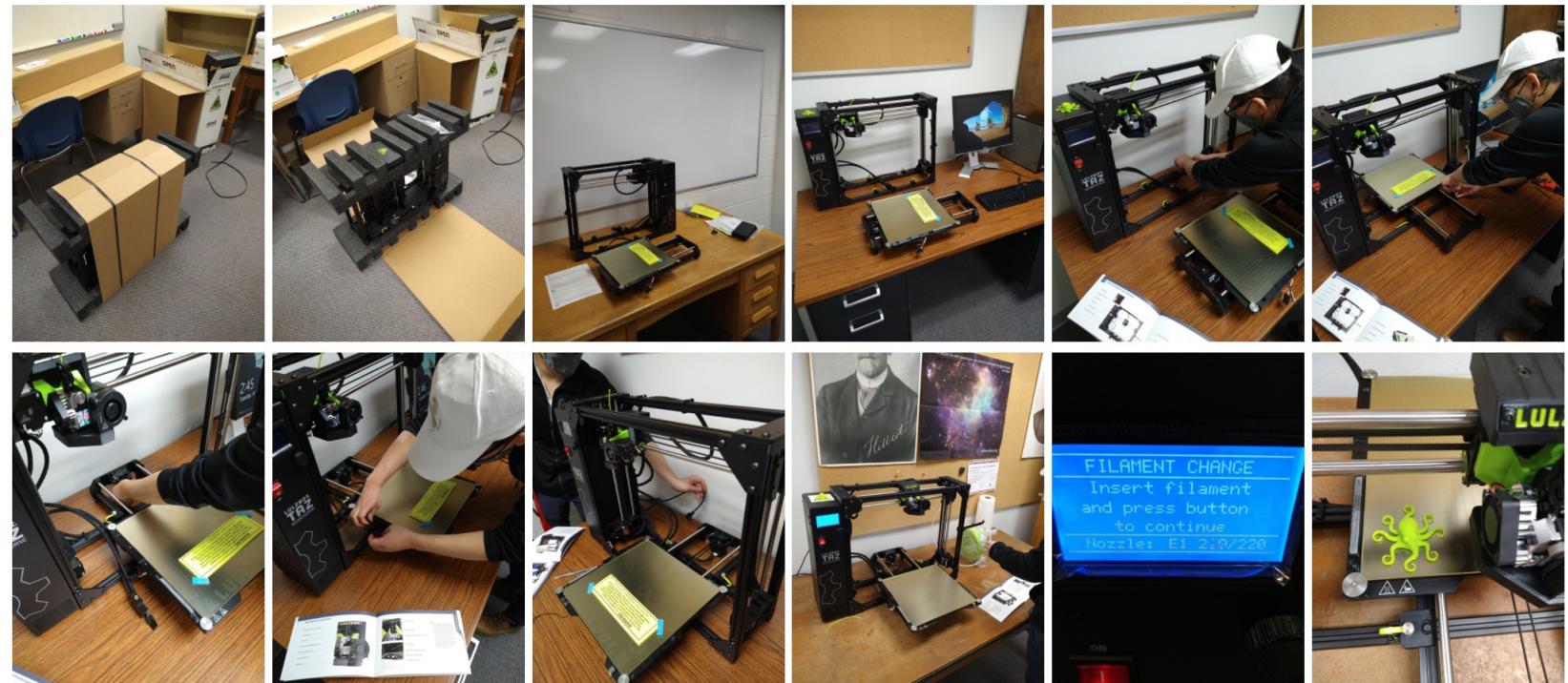


**3D Printer 2: Lulzbot Workhorse (Use with caution. Hot end jam happens frequently)**

[Quick Start Guide](#)

[User Manual](#)

[Test Printing](#)



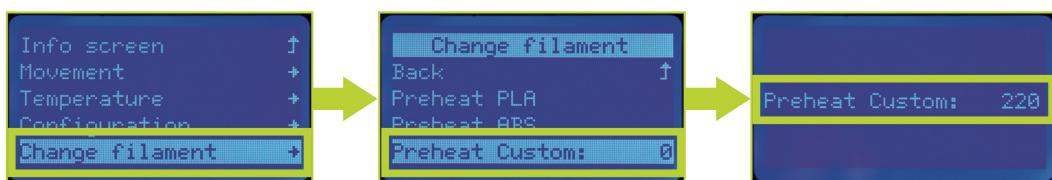
# How to do Filament Change

- Follow User's Guide, Section 5
  - TAZ\_Workhorse\_QuickStartGuide\_08-2019.pdf
  - Available at our website

## 5 Preparing Your LulzBot TAZ Workhorse to Print

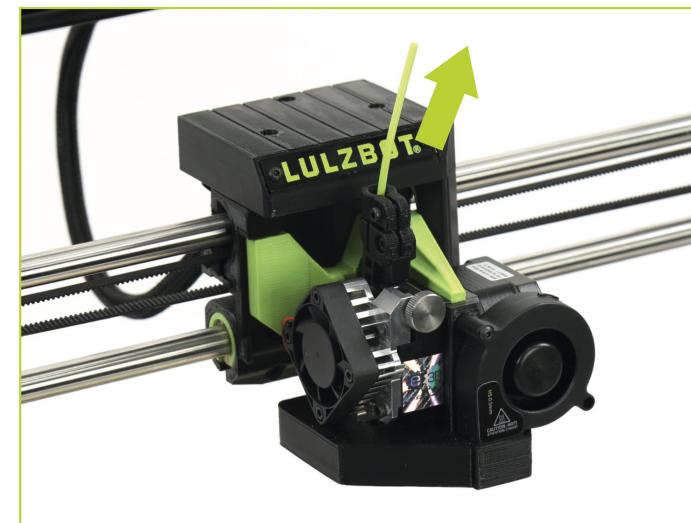
*i* Your LulzBot TAZ Workhorse was tested for quality assurance before being packaged. You will need to remove the remaining filament left in the tool head from this process before loading new filament for your next print. Follow the steps below to remove or change filament.

**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.



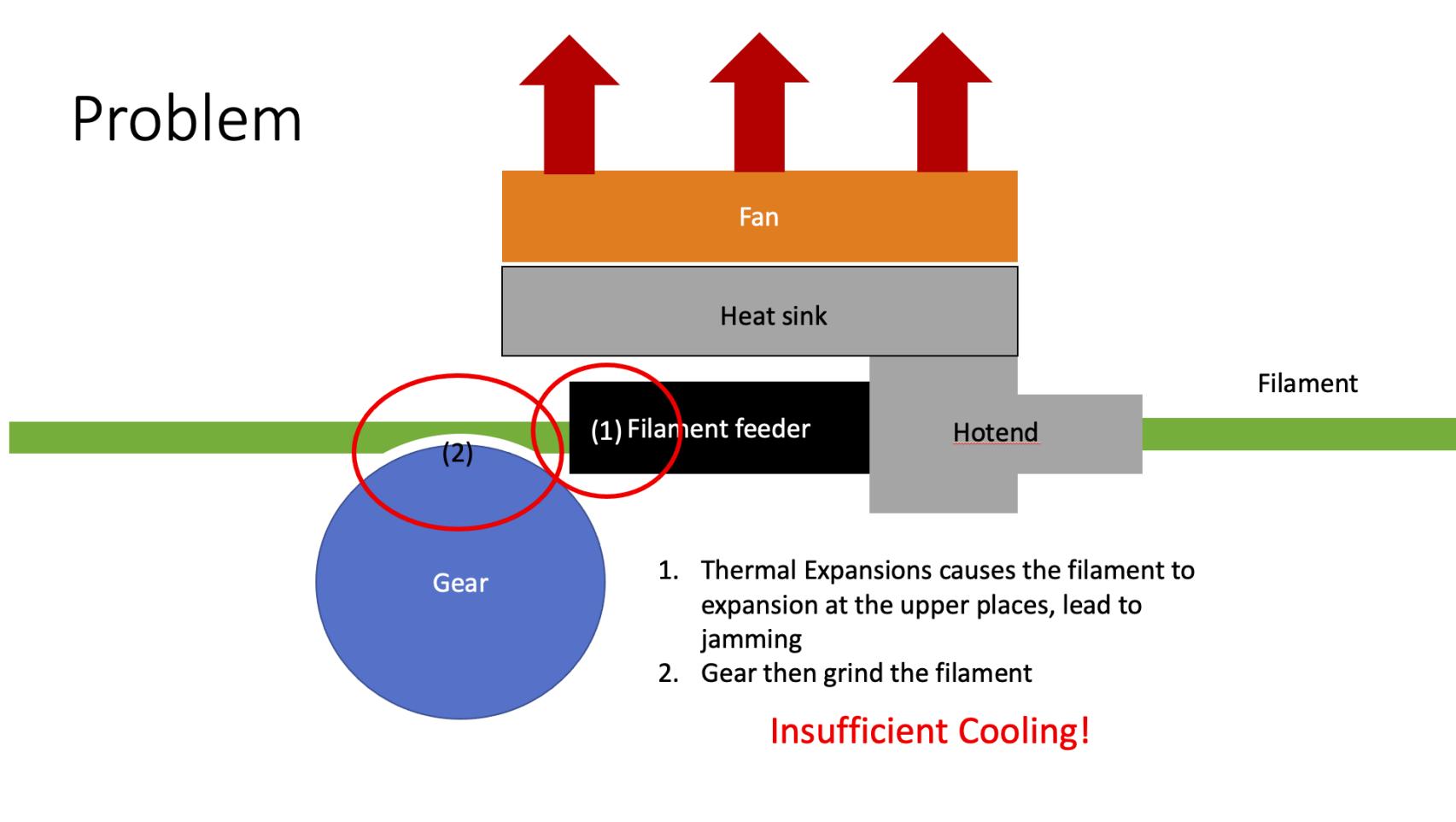
### 5 Preparing to Print

**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.



# Potential “Hotend Jam” Issues in Lulzbot Printer

- An intrinsic design problem
- We are working on workarounds



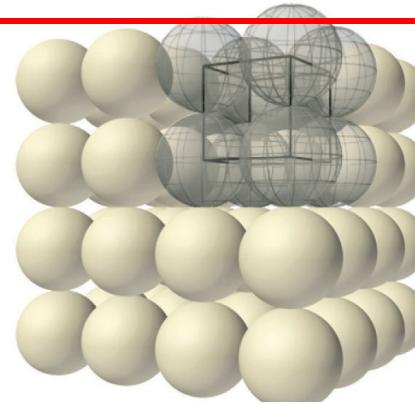
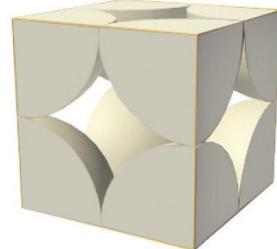
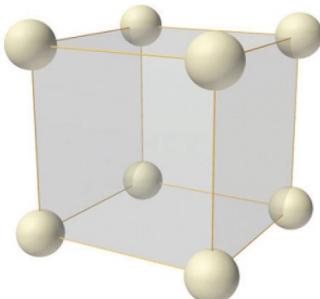
# Lecture 3: Printing Simple and FCC Materials

# 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

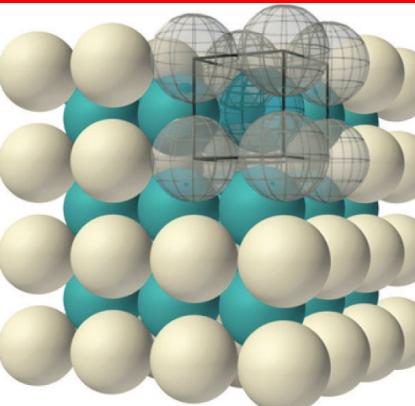
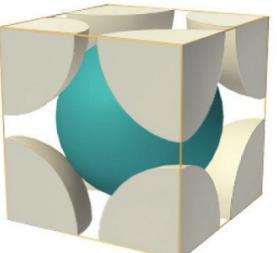
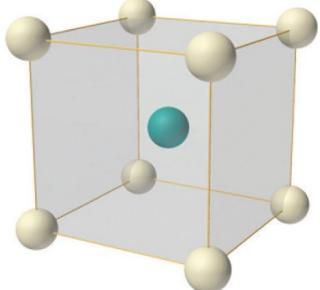
# Crystal Structures – Let's print them

Simple Cubic



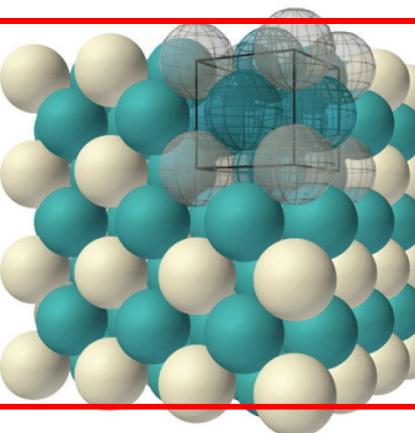
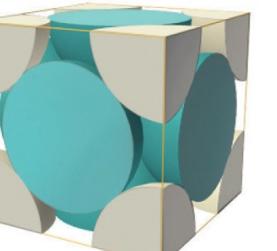
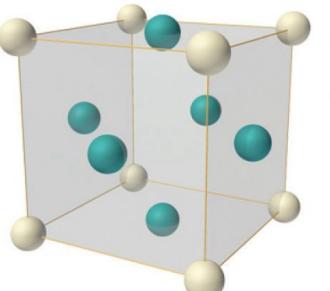
Polonium

Body-centered  
Cubic



Iron

Face-centered  
Cubic



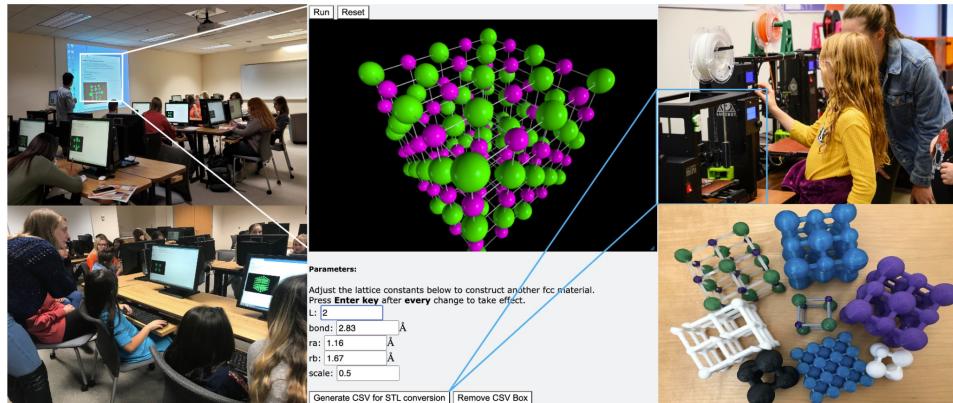
# Access Online Toolkit

- 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, visualization 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 \(Salt\)](#)

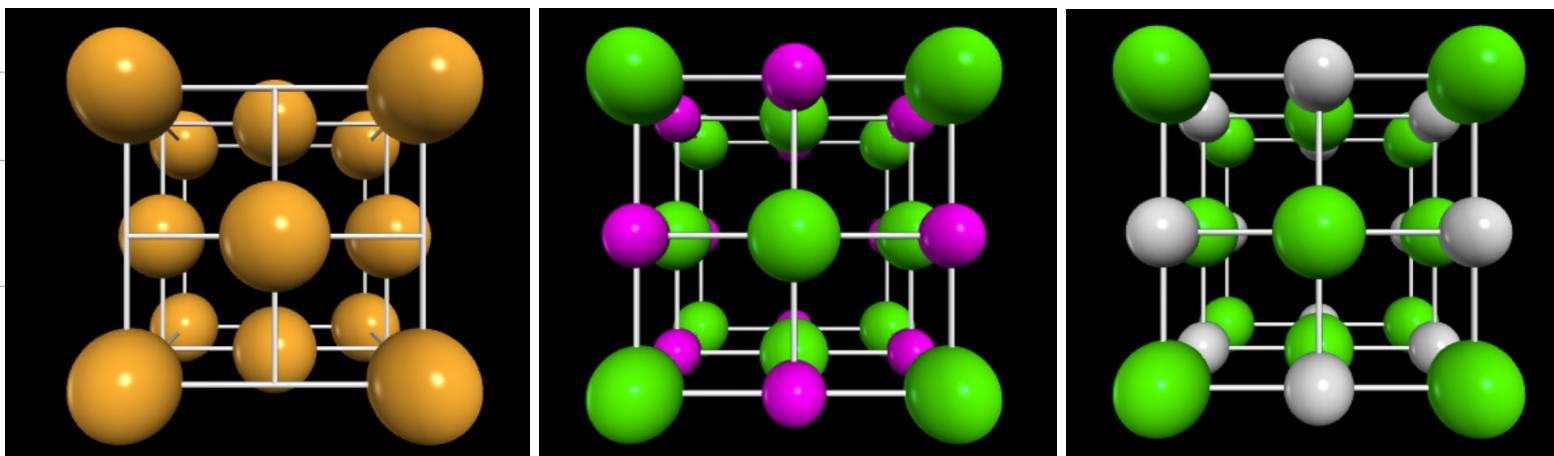
[AgCl \(Silver Chloride\)](#)

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**.



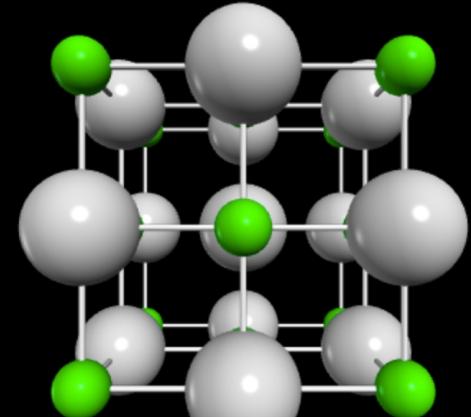
# Optional: Create Your Own fcc Material

- 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<sup>+</sup> 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

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: 6 (Å)
ra: 2 (Å)
rb: 1 (Å)

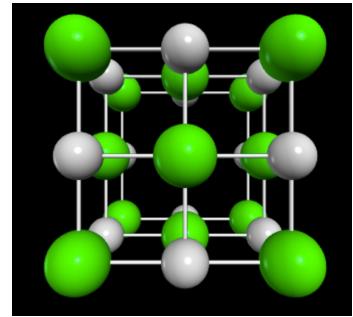
scale: 0.5 ( Input a number between 0 and 1 )

You can change those 3 numbers.  
We don't recommend to set L>1 because it will take very long time for printing.

Generate CSV for STL conversion Remove CSV Box

# 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

Generate CSV for STL conversion Remove CSV Box

2. Select all lines in the box

3. Right click and choose copy

```
#type,x,y,z,radius
#Type:AGCL#type,x,y,z,radius
0,-1,-1,0,0.22702702702702704
0,-1,0,-1,0.22702702702702704
0,-1,0,1,0.22702702702702704
0,-1,1,0,0.22702702702702704
0,0,-1,-1,0.22702702702702704
0,0,-1,0,0.22702702702702704
0,0,0,0,0.22702702702702704
0,0,1,-1,0.22702702702702704
0,0,1,0,-1,0.22702702702702704
0,1,0,-1,0.22702702702702704
0,1,0,1,0.22702702702702704
0,1,1,0,0.22702702702702704
0,-1,-1,-1,0.3009009009
0,-1,-1,1,0.3009009009
0,-1,0,0,0.3009009009
0,-1,1,-1,0.3009009009
0,-1,1,1,0.3009009009
0,0,-1,0,0.3009009009
0,0,0,-1,0.3009009009
0,0,0,1,0.3009009009
0,0,1,0,0.3009009009
0,1,-1,-1,0.3009009009
0,1,-1,1,0.3009009009
0,1,0,0,0.3009009009
0,1,1,-1,0.3009009009
0,1,1,1,0.3009009009
#type,x,y,z,axis,length
1,-1,-1,-1,0,1
1,-1,-1,-1,1,1
1,-1,-1,-1,2,1
1,-1,-1,0,0,1
1,-1,-1,0,1,1
1,-1,-1,0,2,1
1,-1,-1,1,0,1
1,-1,-1,1,1,1
1,-1,-1,1,2,1
1,-1,-1,2,0,1
1,-1,-1,2,1,1
1,-1,-1,2,2,1
1,-1,0,0,1
1,-1,0,1,1
1,-1,0,2,1
```

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

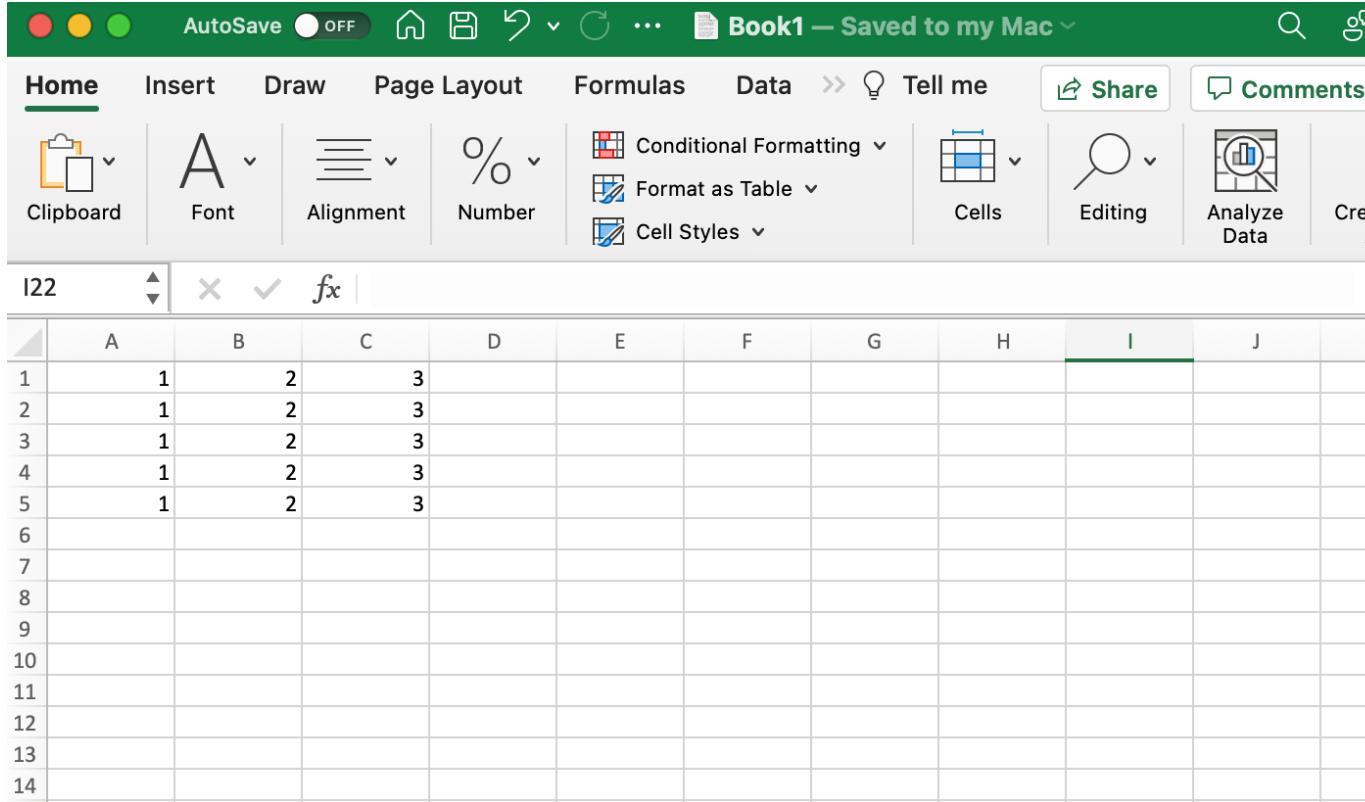
1 structure 1 file !

WORD

```
#type,x,y,z,radius
#Type:AGCL#type,x,Y,z,radius
0,-1,-1,0,0.22702702702702704
0,-1,0,-1,0.22702702702702704
0,-1,0,1,0.22702702702702704
0,-1,1,0,0.22702702702702704
0,0,-1,-1,0.22702702702702704
0,0,-1,1,0.22702702702702704
0,0,0,0,0.22702702702702704
0,0,1,-1,0.22702702702702704
0,0,1,0,0.22702702702702704
0,0,1,1,0.22702702702702704
0,1,0,-1,0.22702702702702704
0,1,0,1,0.22702702702702704
0,1,1,0,0.22702702702702704
0,-1,-1,-1,0.3009009009
0,-1,-1,1,0.3009009009
0,-1,0,0,0.3009009009
0,-1,1,-1,0.3009009009
0,-1,1,1,0.3009009009
0,0,-1,0,0.3009009009
0,0,0,1,0,0.3009009009
0,0,1,0,0.3009009009
0,1,-1,-1,0.3009009009
0,1,-1,1,0.3009009009
0,1,0,0,0.3009009009
0,1,1,-1,0.3009009009
0,1,1,1,0.3009009009
#type,x,y,z,axis,length
1,-1,-1,-1,0,1
1,-1,-1,-1,1,1
1,-1,-1,-1,2,1
1,-1,-1,0,0,1
1,-1,-1,0,1,1
1,-1,-1,0,2,1
1,-1,-1,1,0,1
1,-1,-1,1,1,1
1,-1,-1,1,2,1
1,-1,-1,2,0,1
1,-1,-1,2,1,1
1,-1,-1,2,2,1
1,-1,0,0,1
1,-1,0,1,1
1,-1,0,2,1
```

# A sample CSV file

- You've used CSV files before, indeed



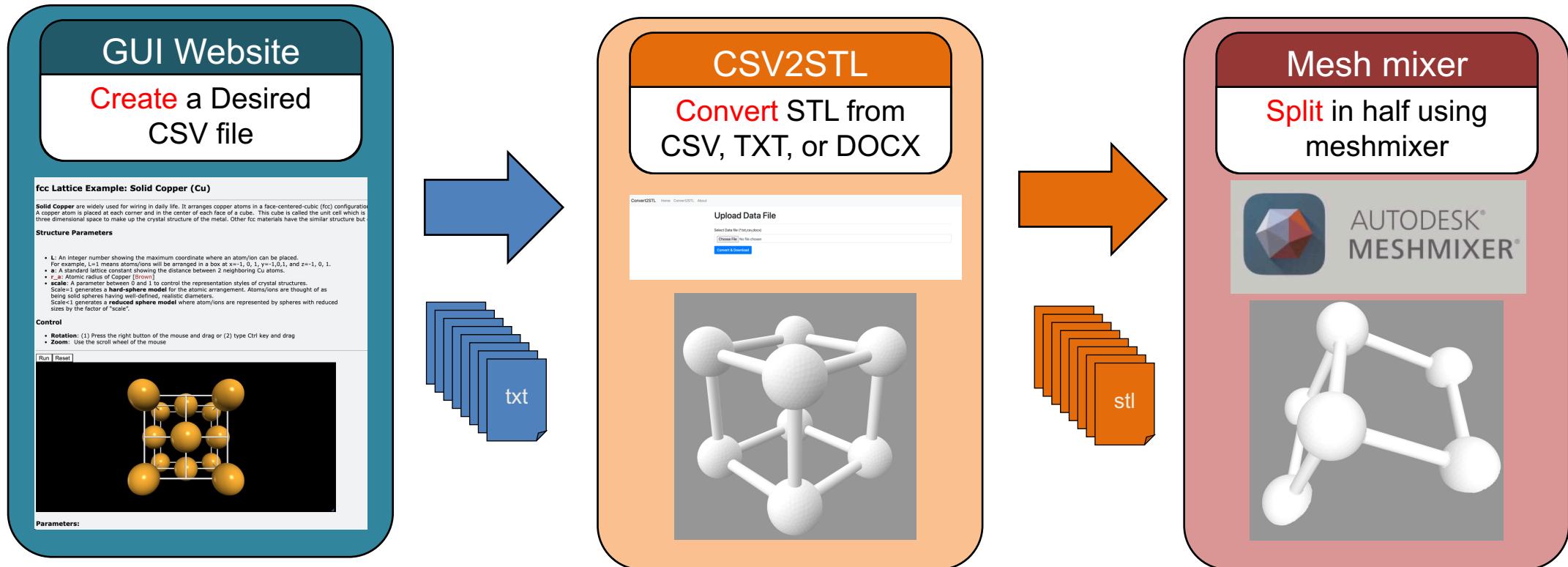
The screenshot shows a Microsoft Excel spreadsheet titled "Book1 — Saved to my Mac". The ribbon menu is visible at the top, and the Home tab is selected. The spreadsheet contains a single sheet with data from row 1 to 5 and columns A to C. The data is as follows:

1	1	2	3
2	1	2	3
3	1	2	3
4	1	2	3
5	1	2	3

```
[long@Cygnus:Downloads]$ more Book1.csv
<U+FEFF>1,2,3
1,2,3
1,2,3
1,2,3
1,2,3
Book1.csv (END)
```

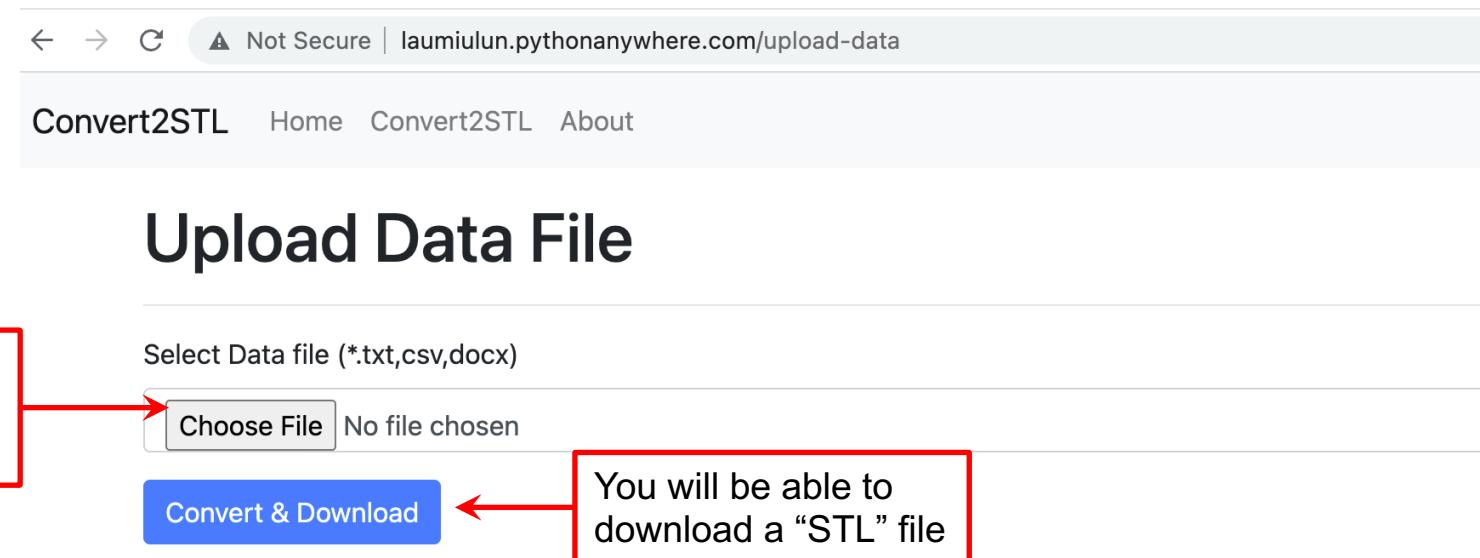
# What's Next?

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



# Convert the CSV file to a STL file for Printing

- <http://laumiulun.pythonanywhere.com/upload-data>



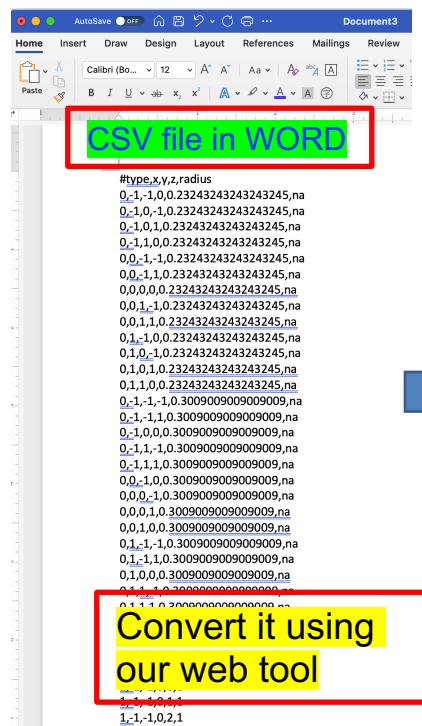
The screenshot shows a web browser window with the URL <http://laumiulun.pythonanywhere.com/upload-data> in the address bar. The page title is "Convert2STL". The main heading is "Upload Data File". On the left, a red box contains the text "You can upload your txt, csv, docx files of crystal structures here". An arrow points from this box to the "Choose File" button. To the right of the button, the text "No file chosen" is displayed. Below the button is a blue "Convert & Download" button. To the right of the download button, another red box contains the text "You will be able to download a “STL” file". An arrow points from this box back towards the "Convert & Download" button.

- Note: We have a **free account** on [pythonanywhere.com](http://pythonanywhere.com)
  - It can support a limited number of hits per day.
- So if you can't access it due to overloading, you can
  - contact us
  - Or visit it the next day.

# What's a STL file?

- **STL format**

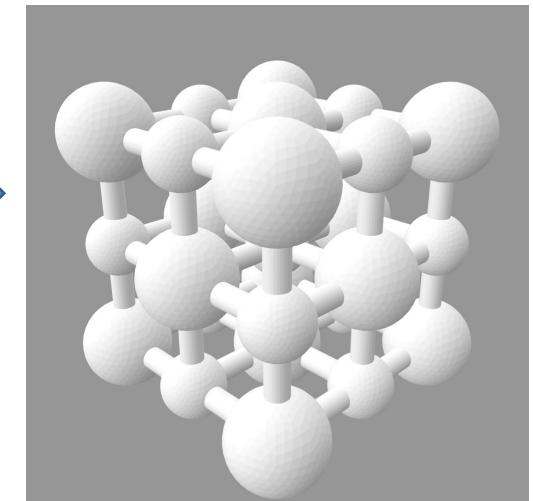
- A file format native to the **STereoLithography** CAD software for 3D Systems
- Referred to as "**Standard Tessellation Language**" or "**Standard Triangle Language.**"
- Describe the surface geometry of a 3D object



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  
...

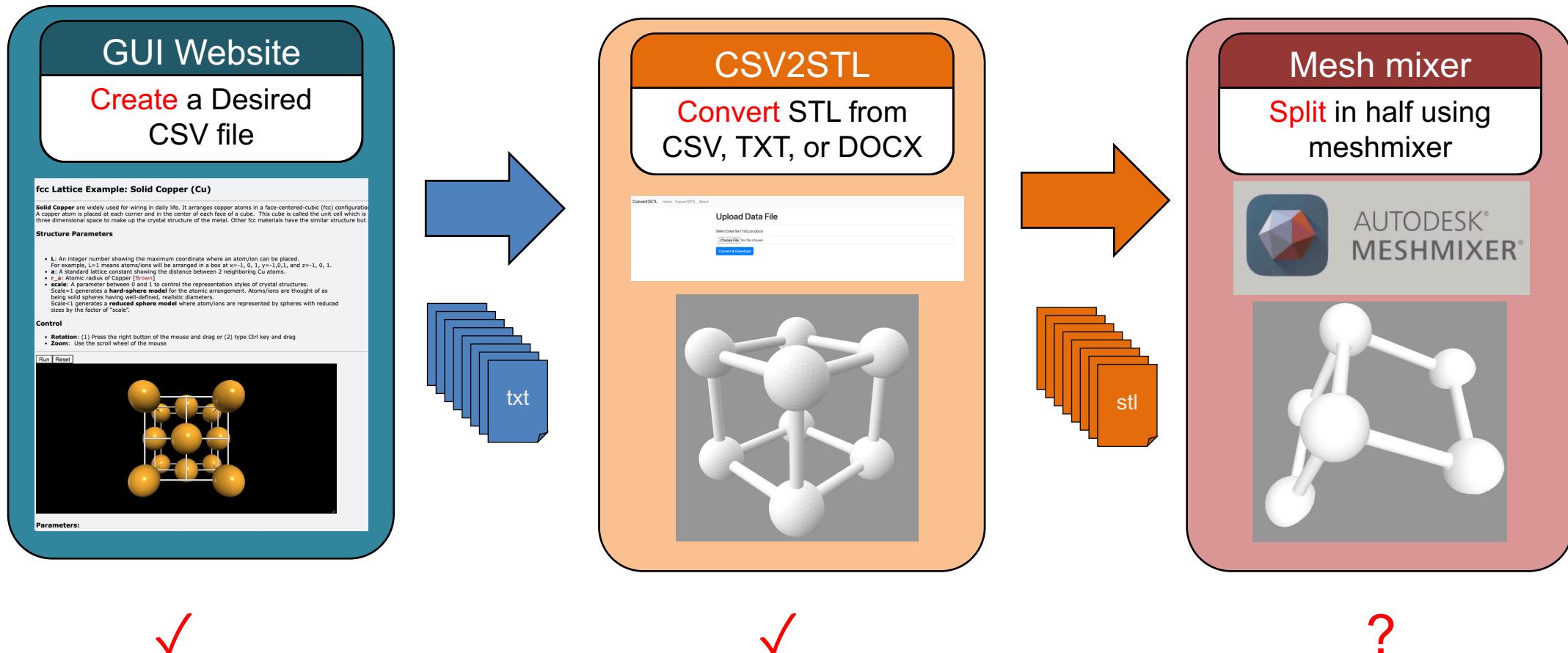
A red box highlights the first line 'solid Group\_1\_AgCl.stl' with the label 'A STL file'. Another red box highlights the text 'This is what you will get' at the bottom.

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



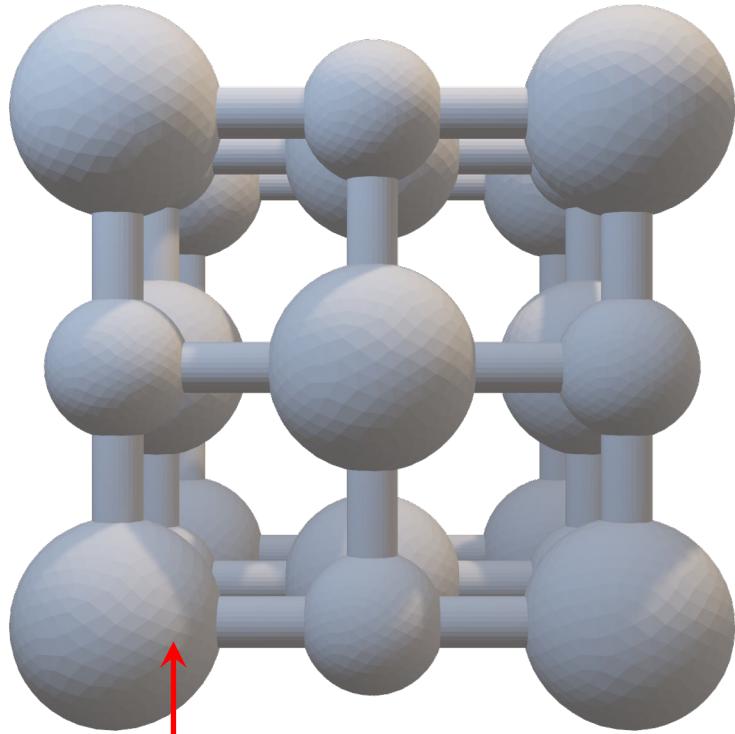
# Last Step: Split STL in Half for Stable Printing

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



# Split STL file in Half for Stable Printing

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



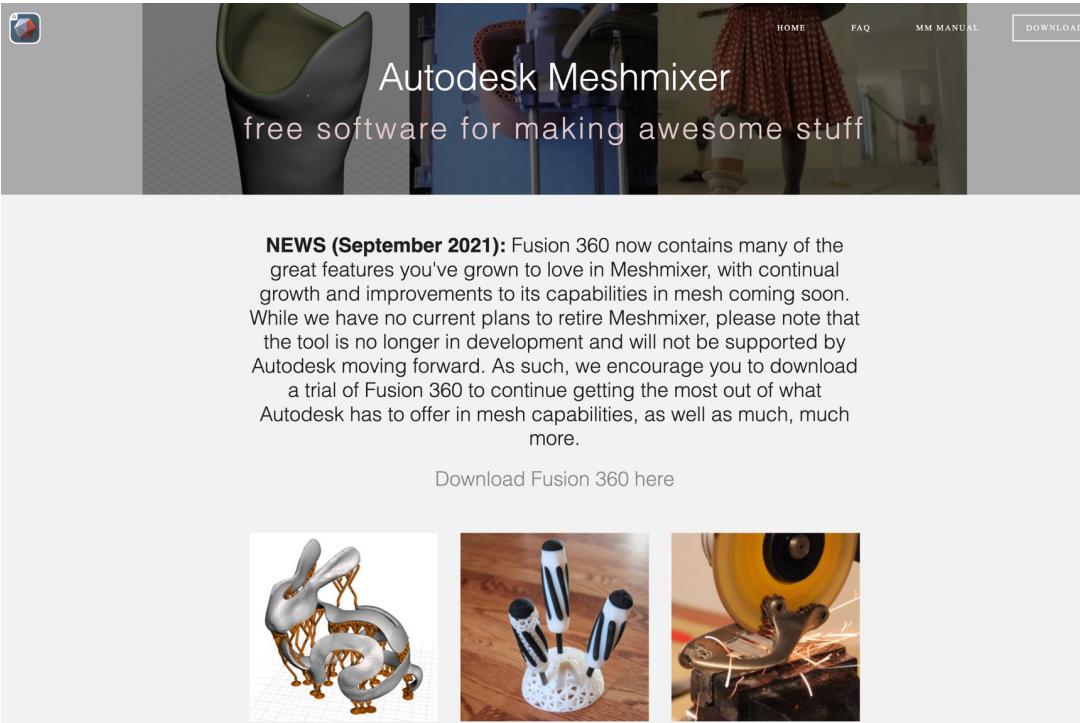
**Unstable** for printing: Melt plastics in bottom layers may not be strong enough to support top layers.



**Stable** for printing: Sufficient support from bottom layers.

# How to Split?

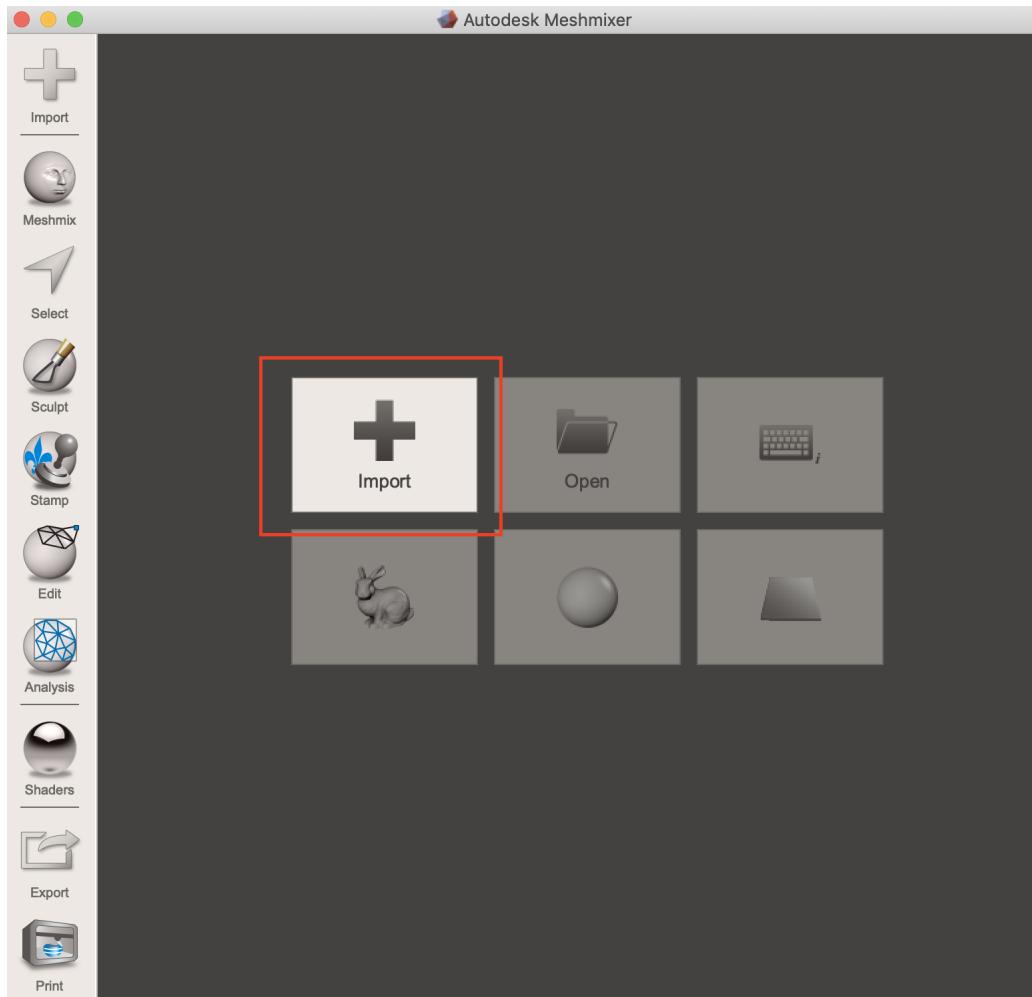
- 1. Do by yourself
  - Download Autodesk Meshmixer from [meshmixer.com](http://meshmixer.com)
  - It should be already installed in lab PC at Boise State



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

# Method 1: Use MeshMixer by yourself

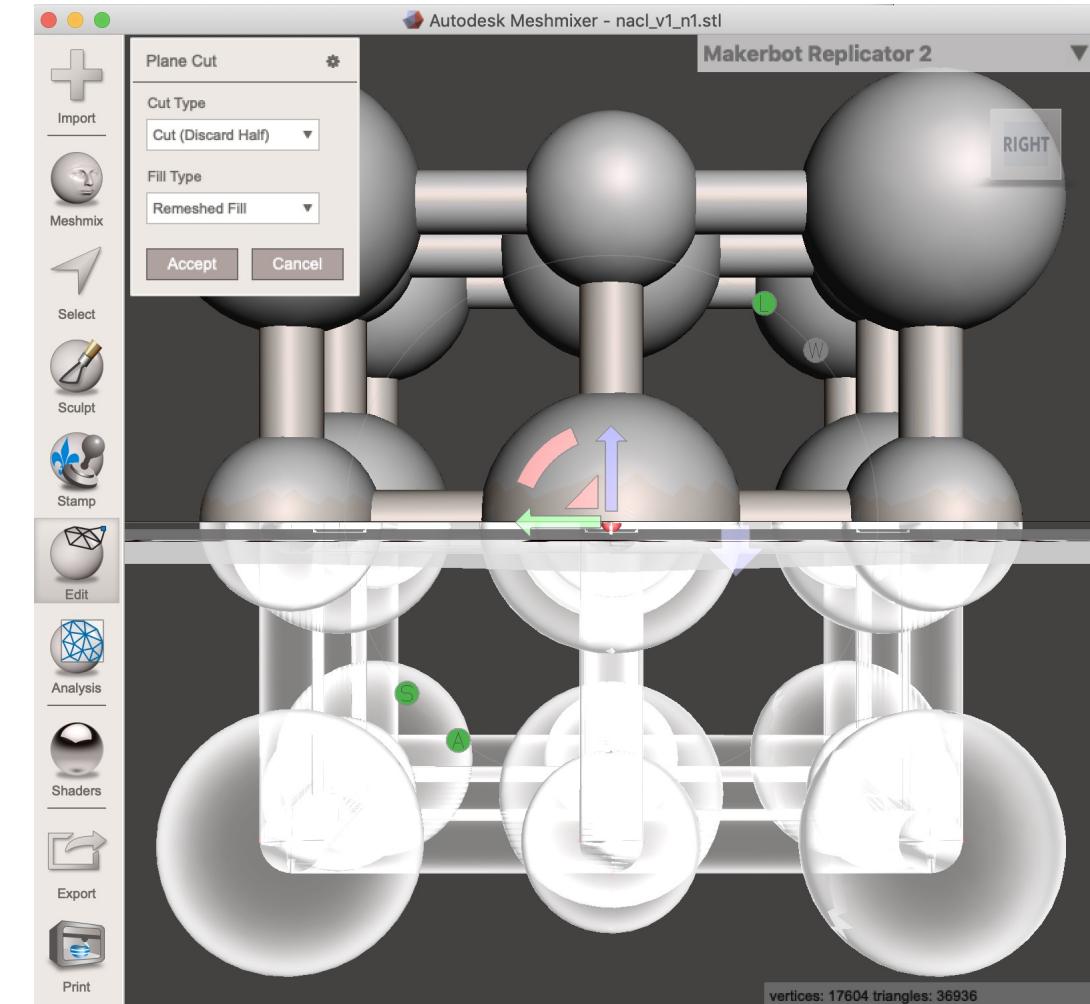
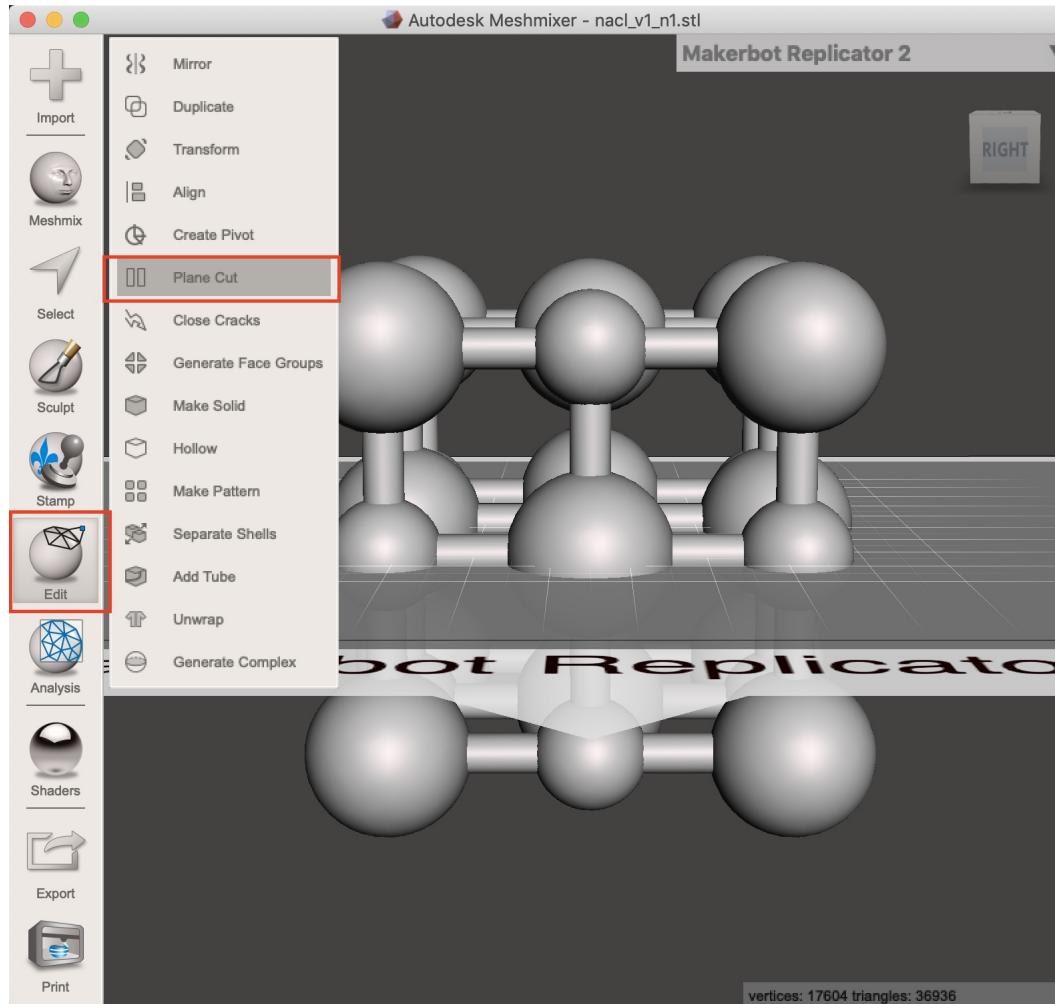
- Step 1: Open Mesh Mixer in the File Browser. Once *MeshMixer* is open, select **Import** and navigate it to the desired STL file



# 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



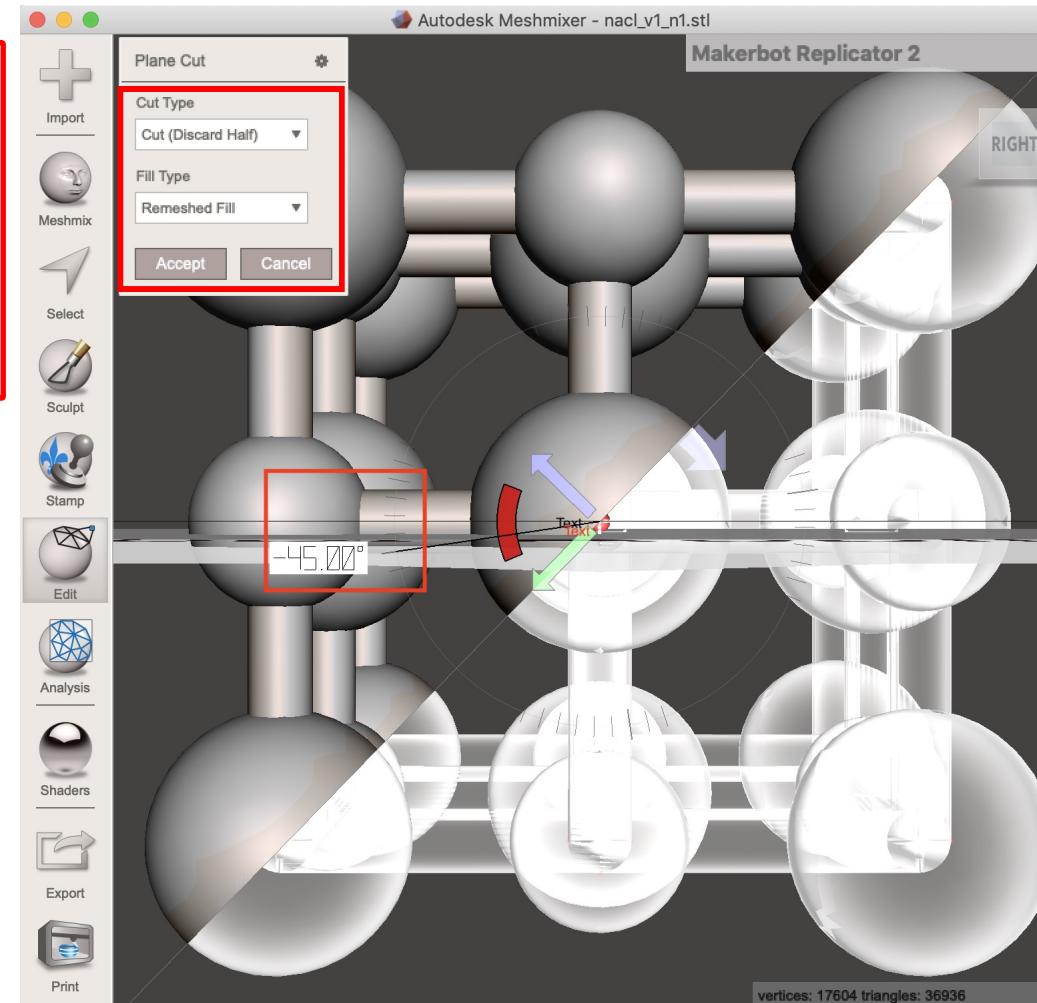
# Method 1: Use MeshMixer by yourself

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

Enable those options:

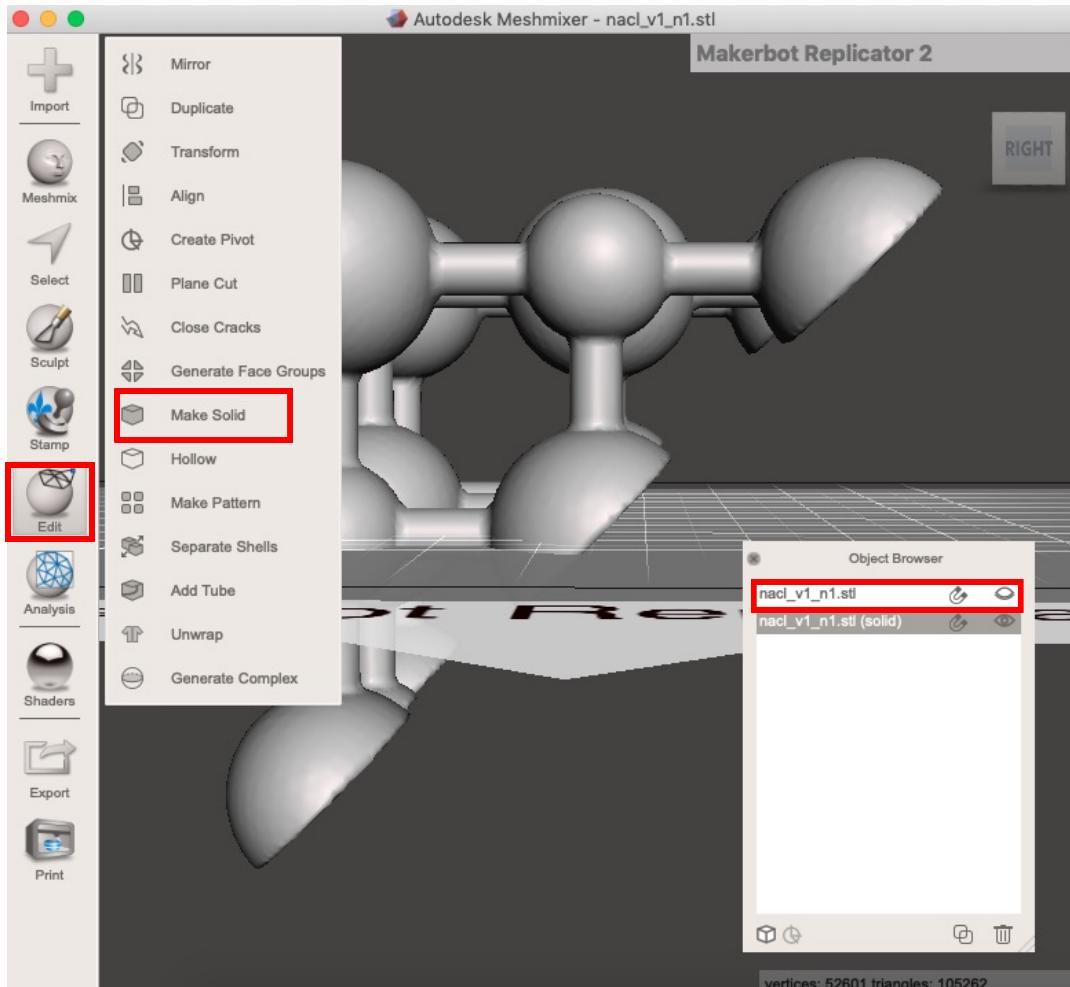
Cut type: **Cut (Discard Half)**  
Fill type is **Remeshed Fill**

Then click **Accept**.



# Method 1: Use MeshMixer by yourself

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

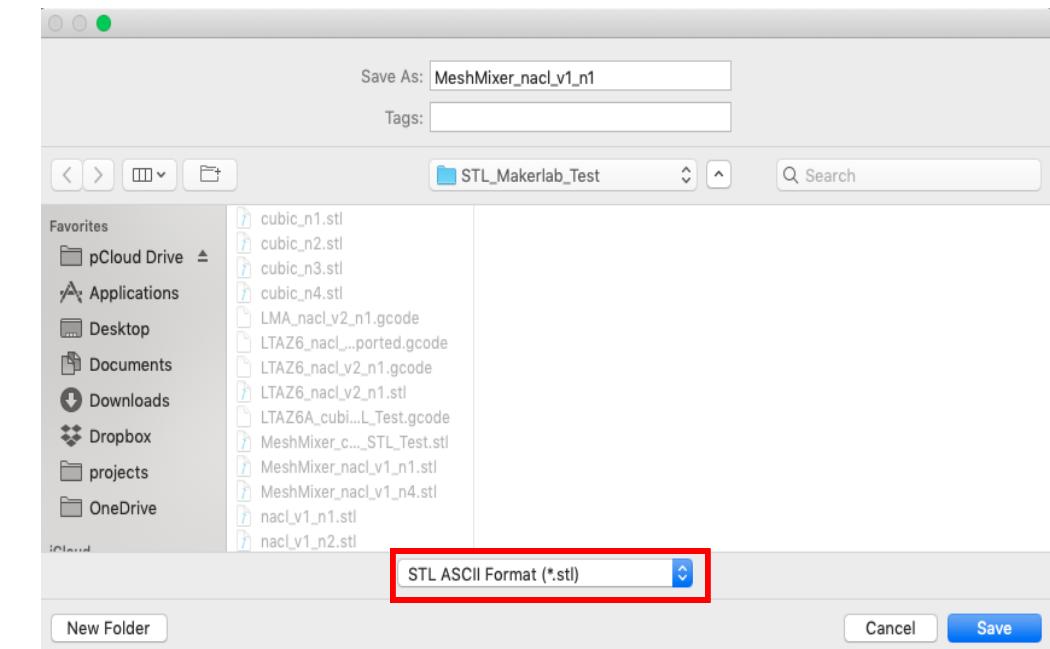
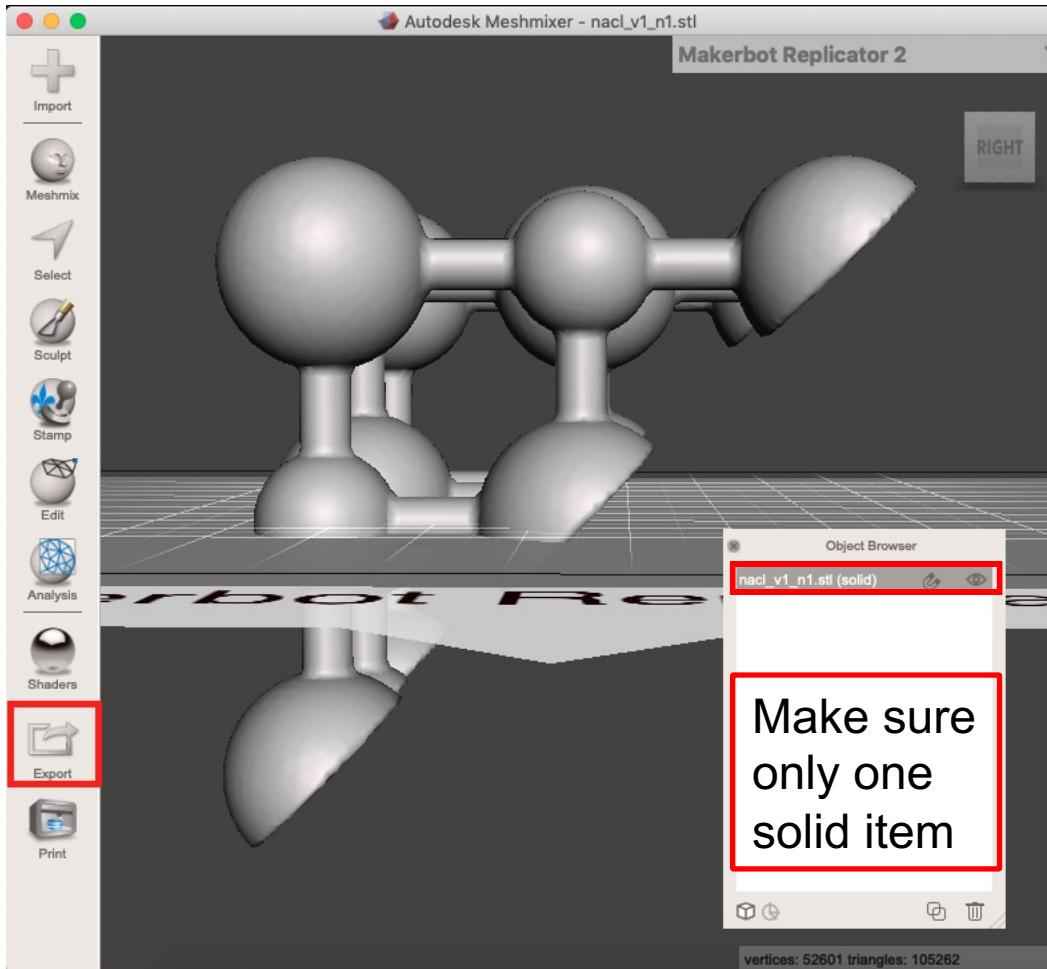


After you make the object solid, there should be a new menu **Object Browser**.

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)

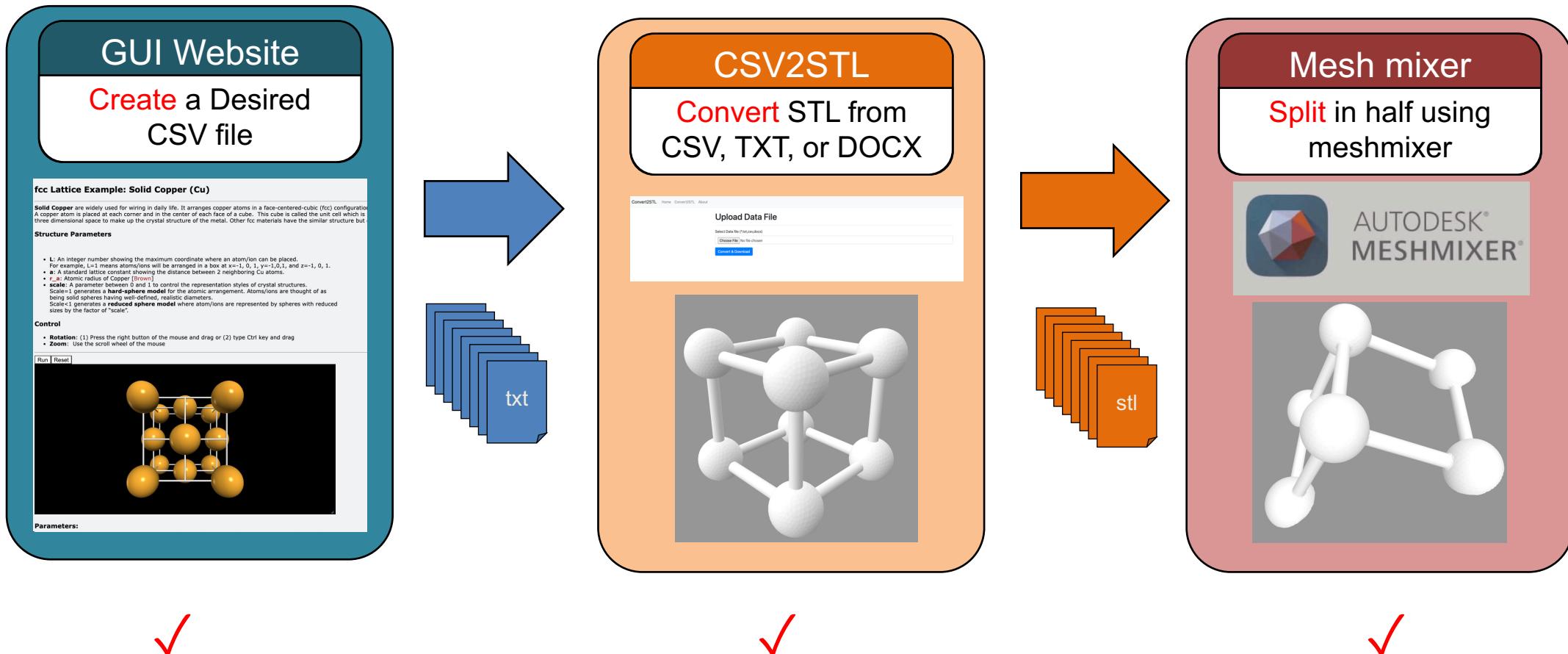
- Section 1
  - <https://drive.google.com/drive/folders/1fH6CuWyXZ0aIDGhqT0HjvHOAyyoVRHqn?usp=sharing>
- Section 2
  - <https://drive.google.com/drive/folders/1GuHV2k84seBOZ--wLyJE7zkPJXz1DA68>
- Links will also be posted on Canvas
- One group sends 2 stl file (Or talk to Dr. Wang if want to print more)
  - 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/1LozcoP6GN8mLxdYmBid264rZIn3K4AJtY>
  - Shared with [herve@hawaii.edu](mailto:herve@hawaii.edu), [jdf8043@hawaii.edu](mailto:jdf8043@hawaii.edu), and [marye@hawaii.edu](mailto:marye@hawaii.edu)
- UTSA
  - [https://drive.google.com/drive/folders/1S5YBsR\(cxMabeF19HmHUU6I4PS6loruY](https://drive.google.com/drive/folders/1S5YBsR(cxMabeF19HmHUU6I4PS6loruY)
  - Shared with Prof. Su and [jessica.gehrtz@utsa.edu](mailto:jessica.gehrtz@utsa.edu)
- Augusta
  - <https://drive.google.com/drive/folders/1eQApYHBqBMGETVaXeTSRs3luCQuhDL6>
  - Shared with Prof. He and [mfreitag@augusta.edu](mailto:mfreitag@augusta.edu)

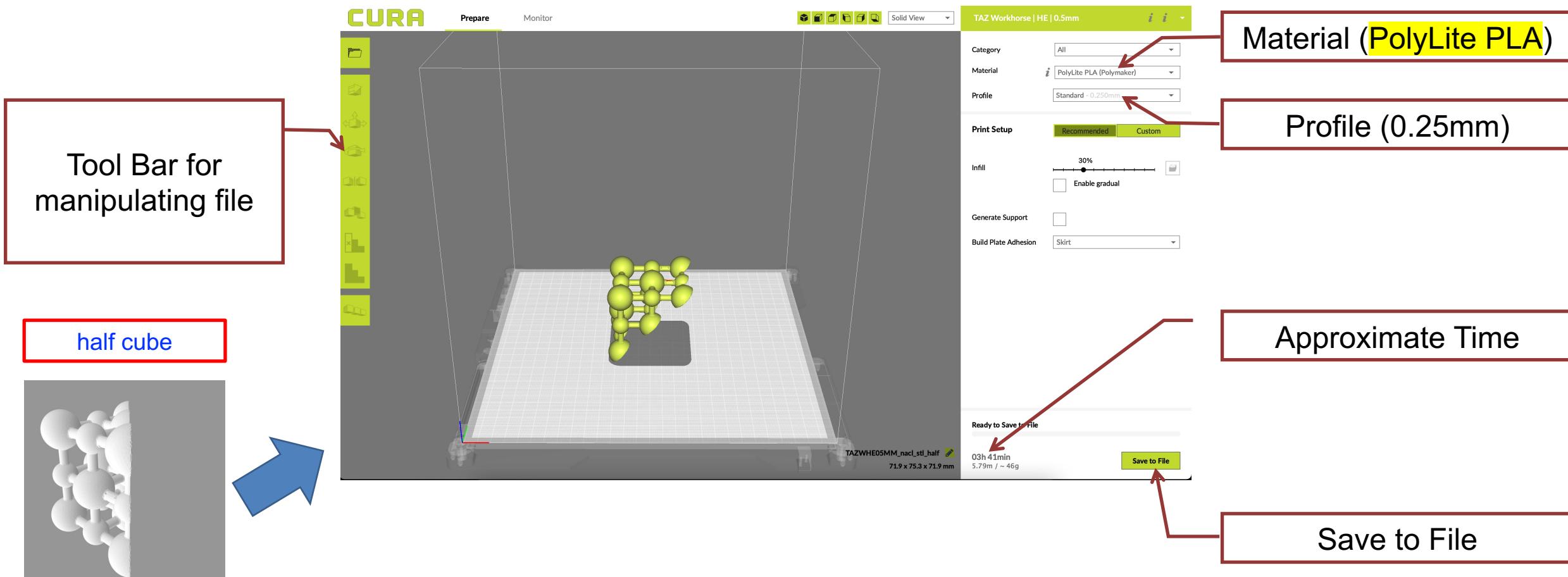
# Ready for Print

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



# Go to Lab for Printing

- Bring the “Group\_1\_AgCl.stl” to Lab
- Load it in Cura



# Adjust Parameters (for Lulzbot only)

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

Print Setup

Recommended

Custom

Search...

Infill	215	°C
Material	215	°C
Default Printing Temperature	215	°C
Printing Temperature	160	°C
Probe Temperature	180	°C
Soften Temperature	170	°C
Wipe Temperature	210	°C
Printing Temperature Initial Layer	210	°C
Initial Printing Temperature	210	°C
Final Printing Temperature	210	°C
Build Plate Temperature	45	°C
Part Removal Temperature	35	°C
Keep Heating	<input checked="" type="checkbox"/>	
Build Plate Temperature Initial Layer	55	°C
Diameter	2.85	mm
Flow	100	%
Initial Layer Flow Rate	100	%
Enable Retraction	<input checked="" type="checkbox"/>	
Retract at Layer Change	<input checked="" type="checkbox"/>	
Retraction Distance	1.5	mm

Before

Print Setup

Recommended

Custom

Search...

Infill	220	°C
Material	220	°C
Default Printing Temperature	140	°C
Printing Temperature	140	°C
Probe Temperature	225	°C
Soften Temperature	210	°C
Wipe Temperature	205	°C
Printing Temperature Initial Layer	75	°C
Initial Printing Temperature	35	°C
Final Printing Temperature	<input checked="" type="checkbox"/>	
Build Plate Temperature	<input checked="" type="checkbox"/>	
Part Removal Temperature	<input checked="" type="checkbox"/>	
Keep Heating	<input checked="" type="checkbox"/>	
Build Plate Temperature Initial Layer	55	°C
Diameter	2.85	mm
Flow	100	%
Initial Layer Flow Rate	100	%
Enable Retraction	<input checked="" type="checkbox"/>	
Retract at Layer Change	<input checked="" type="checkbox"/>	
Retraction Distance	1.5	mm

After

# Adjust Scaling and Rotate

The screenshot shows the CURA software interface with a model preview on the left and various settings on the right.

**Translation:** Moved by a distance

X: 0 mm  
Y: 0 mm  
Z: 0 mm  
 Lock Model

**Scaling:** Scaled by a value

X: 72.0108 mm 100 %  
Y: 72.1426 mm 100 %  
Z: 18.4353 mm 100 %  
 Snap Scaling  
 Uniform Scaling

**Rotate:** Rotated by a certain degree

X: 0 degrees  
Y: 0 degrees  
Z: 0 degrees  
 Snap Rotation

**Print Settings (Right Side):**

TAZ Workhorse | HE | 0.5mm

Category: All  
Material: PolyLite PLA (Polymaker)  
Profile: Standard - 0.250mm

Print Setup: Recommended

Infill: 30%  
 Enable gradual

Generate Support:

Build Plate Adhesion: Skirt

Ready to Save to File

00h 40min  
0.97m / ~ 7g

**Text Overlay:**

100% model takes 4 hours  
Use smaller scale if possible

**Tool Icons:**

- Translation: A 3D cube icon with a small arrow pointing from the center.
- Scaling: A 3D cube icon with three arrows pointing outwards from the faces.
- Rotate: A 3D cube icon with a large curved arrow around its vertical axis.

Arrows from the text boxes point to the corresponding icons on the left sidebar.

# Important: Use “Lay Flat”

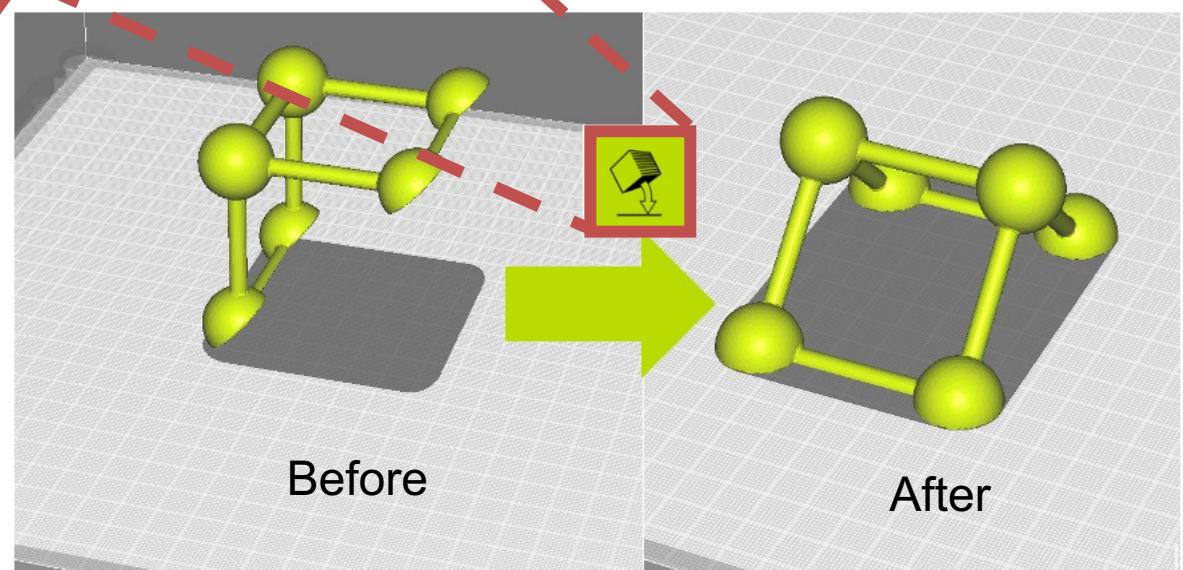
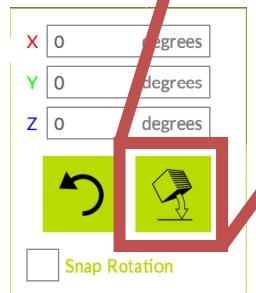
- To give the 3D object enough support during printing

You can use ‘Lay flat’ multiple times

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

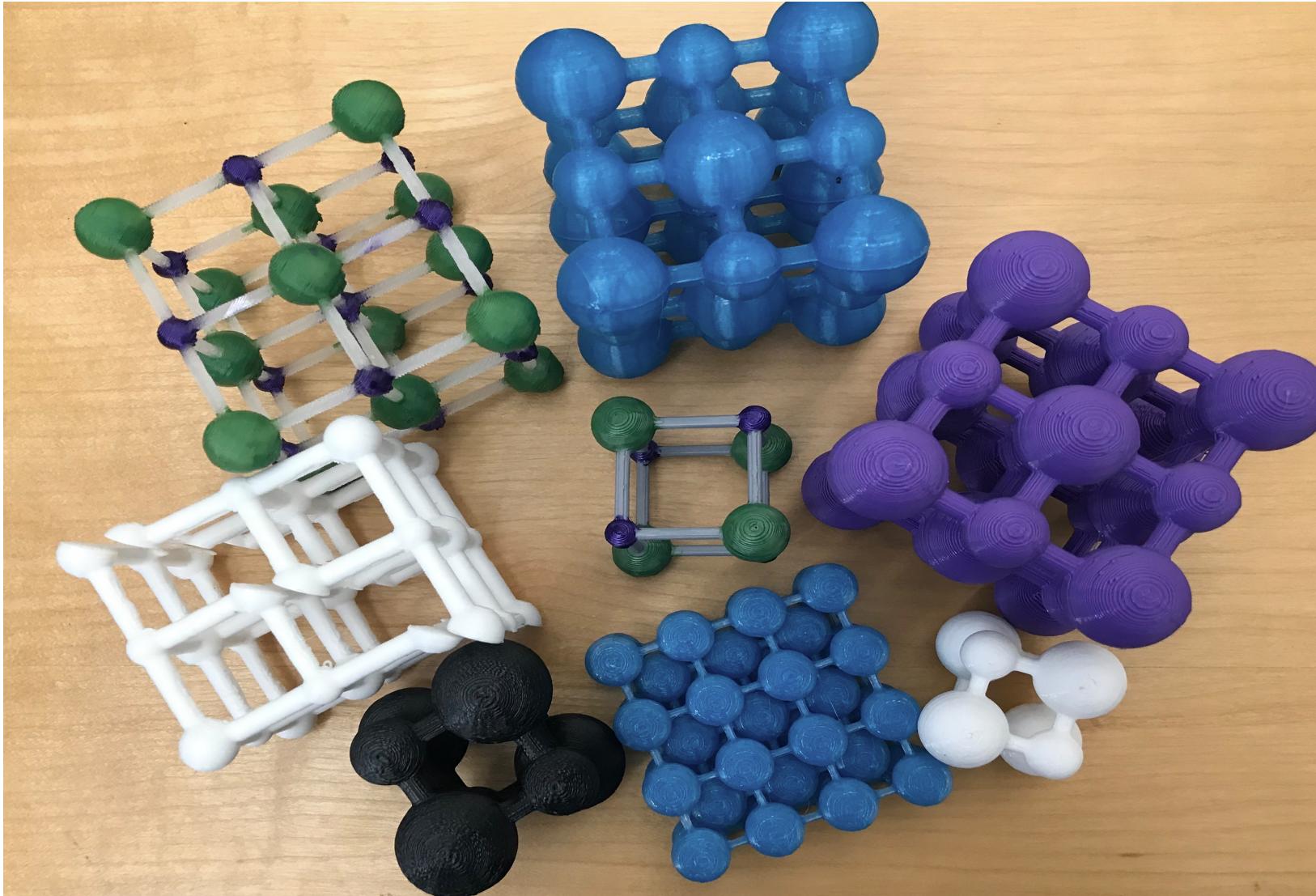
## Rotate

Rotated by a certain degree in each axis



# Enjoy printing your own materials!

- Examples

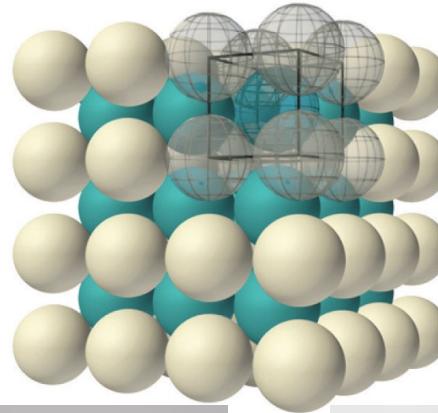
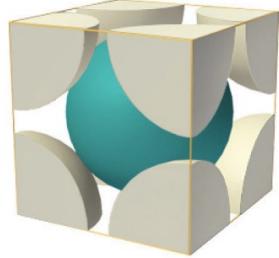
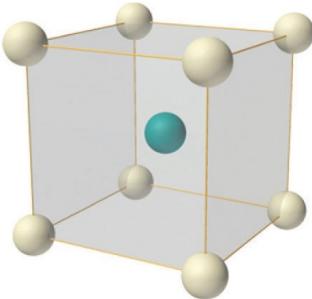


# Lecture 4: Design bcc and Perovskite Materials

# Outline

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

# Body-Centered Cubic



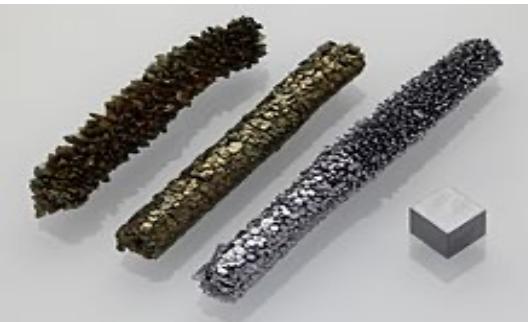
Iron (Fe)



Molybdenum (Mo)



Tungsten (W)



Vanadium (V)



Niobium (Nb)



Tantalum (Ta)

# Lattice Constants at 300K

- BCC Materials

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

# Visualization

- [https://cs.boisestate.edu/~mlong/GUI/crystal\\_html/fe\\_obs.html](https://cs.boisestate.edu/~mlong/GUI/crystal_html/fe_obs.html)

Run Reset

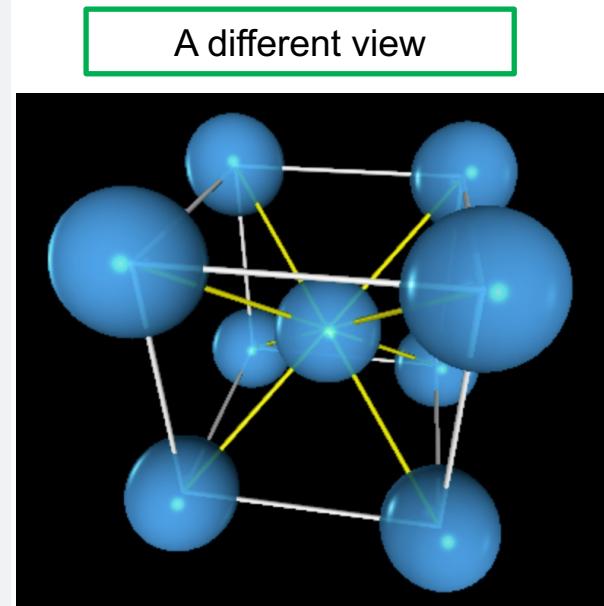
opacity: A parameter controlling the opacity of atom/ion spheres.

**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  
scale: 0.5 (Input a number between 0 and 1)  
opacity: 0.85 (Change opacity of atoms between 0 and 1)

Iron at room temperature

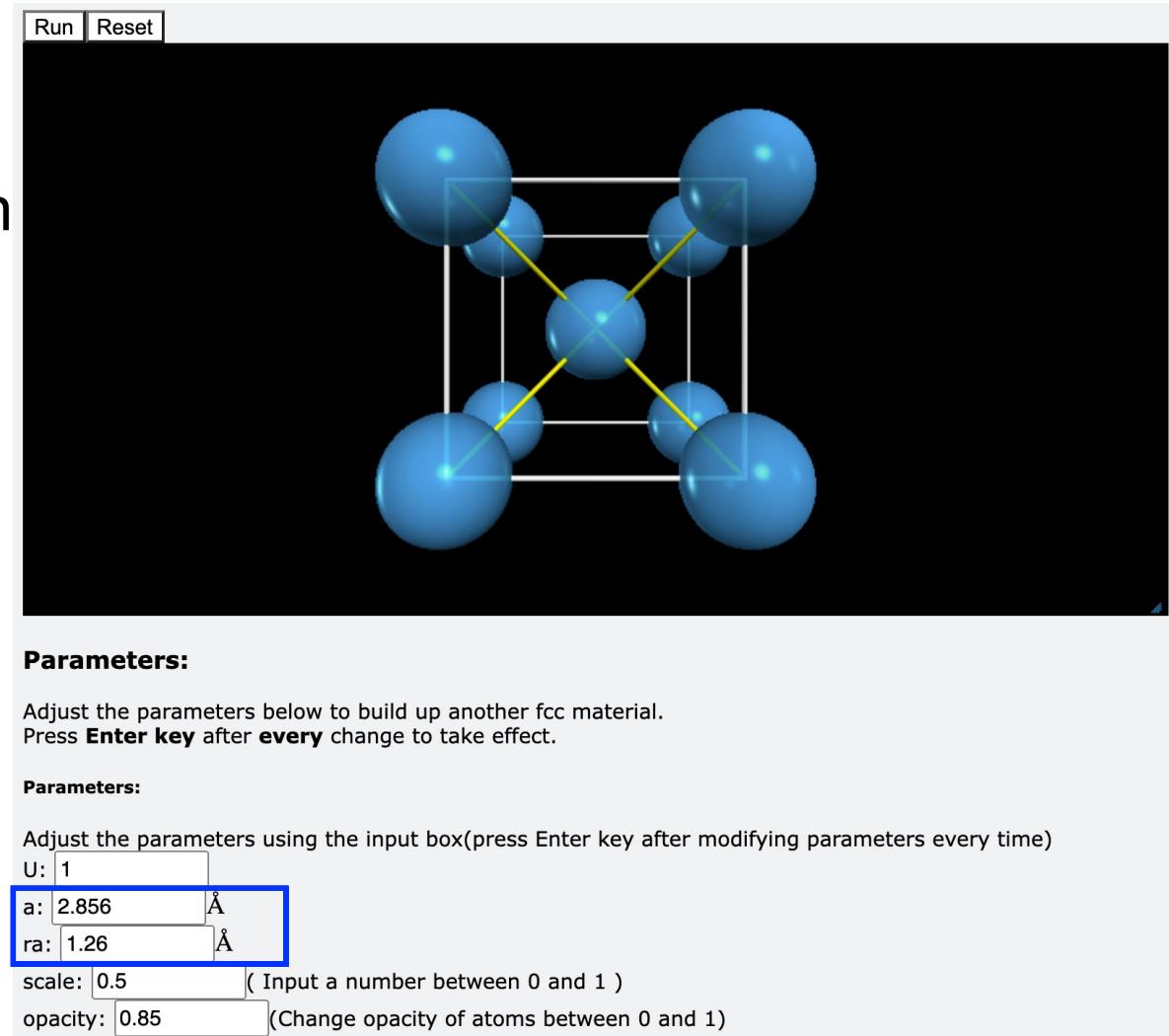


# Create another BCC Material

- **Changing Parameters**

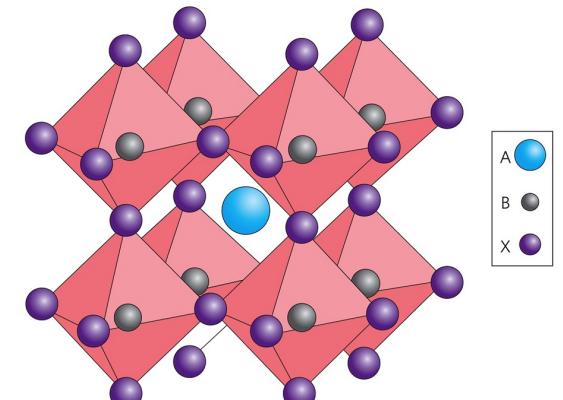
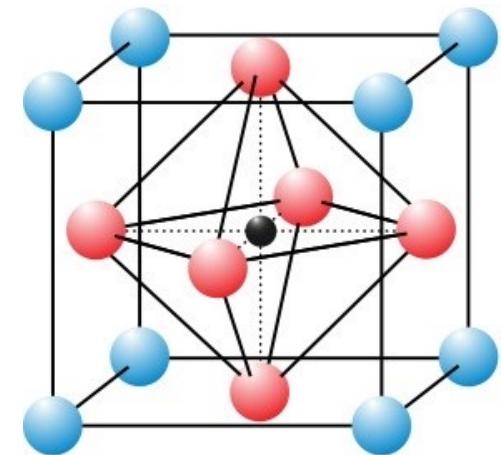
- **L**: An integer number showing the maximum coordinate where an atom/ion can be placed.
- **a**: A standard lattice constant showing the distance between 2 neighboring atoms/ions.
- **ra**: Atomic/ionic radius
- **scale**: A parameter between 0 and 1 to control the representation styles of crystal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

- Printing is not supported.



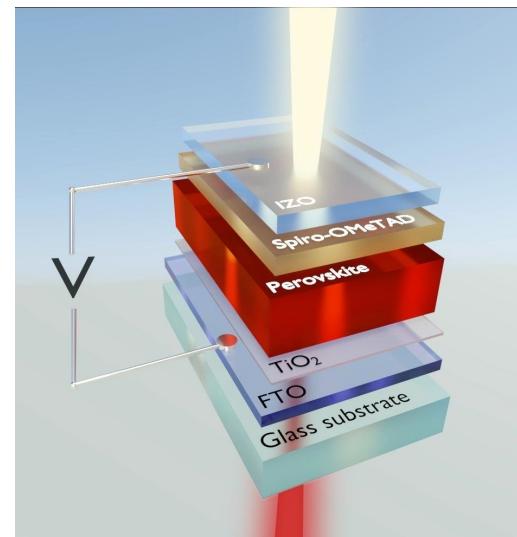
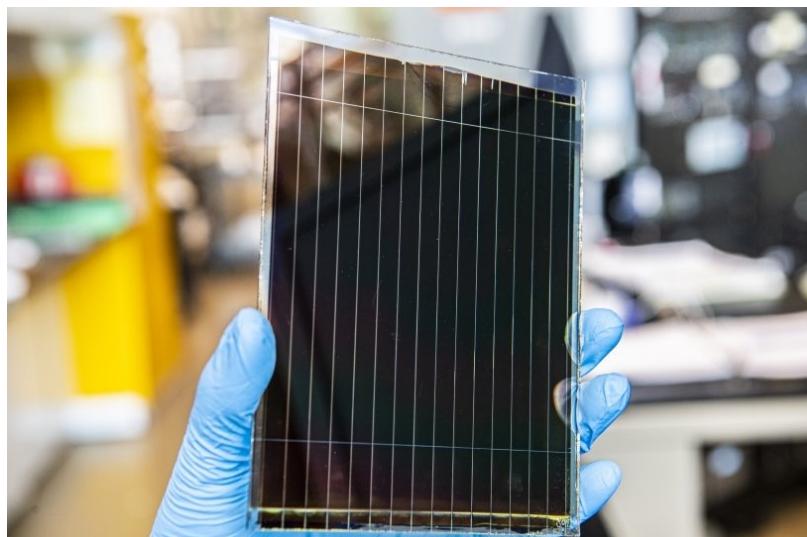
# Ideal Perovskite Structure

- Perovskites are referred to a family of materials
  - A Perovskite was first referred to a colorless mineral of Calcium Titanate with the chemical formula  $\text{CaTiO}_3$ .
  - who named it after a Russian mineralogist Lev Alexeievitch Perovskite.
- The general chemical formula is  $\text{ABX}_3$ ,
  - A is a metal cation (positively charged ion),
  - B is a cation and X is an anion (negatively charged ion).
  - A subgroup:  $\text{ABO}_3$
- Strontium Titanate is an ideal perovskite structure
  - $\text{SrTiO}_3$
  - No distortion
  - A diamond simulant



# Solar Cells with Perovskite Structures

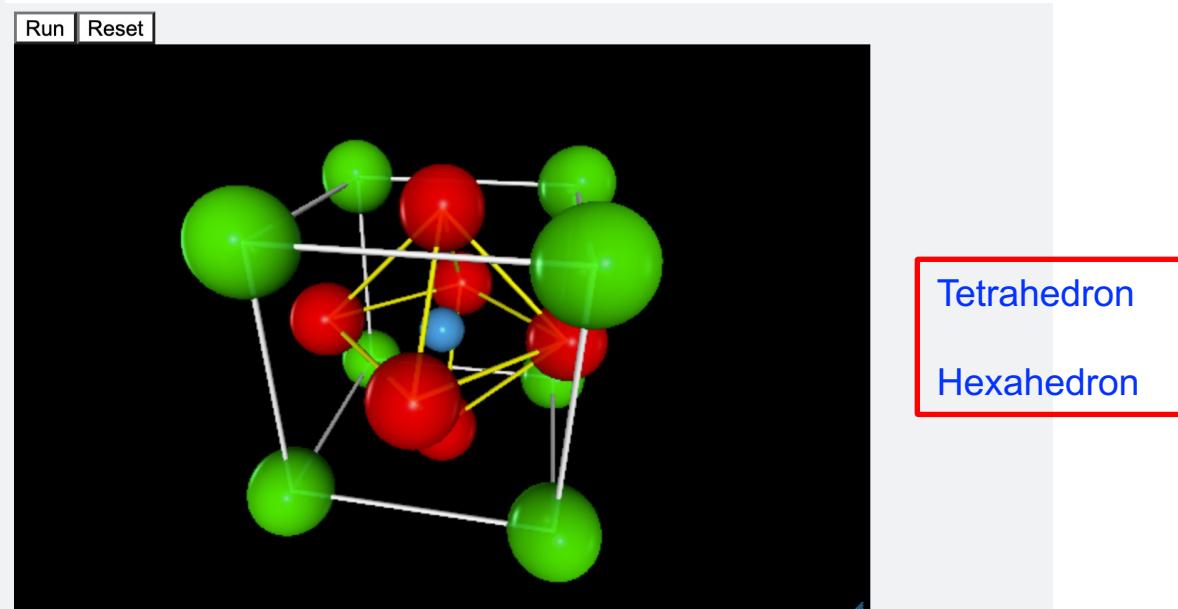
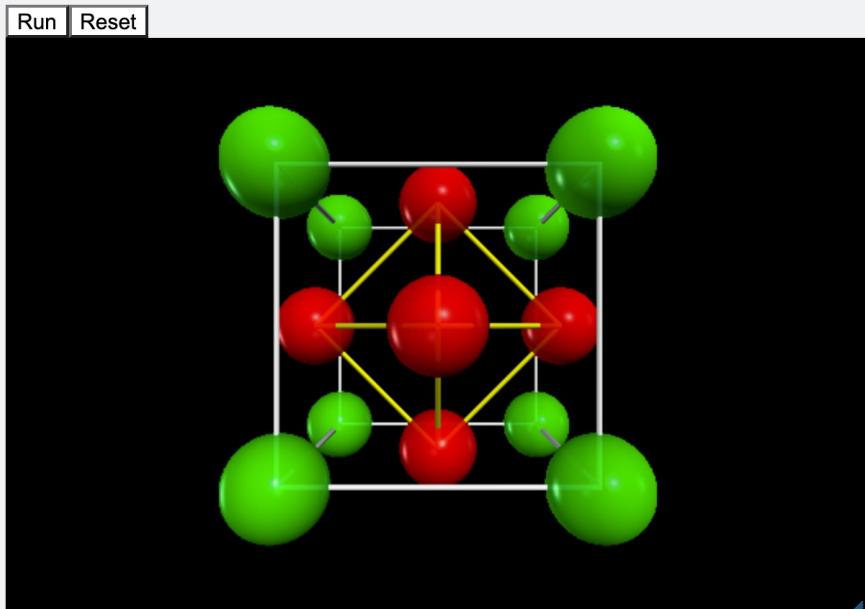
- High Energy Conversion Efficiency at Low Cost
  - Perovskite solar cells convert more than 20% of the incident light directly into usable current
    - Reports of about 3% in 2006 to over 25% in 2021
      - A peak efficiency of 25.6%: <https://doi.org/10.1038/s41586-021-03406-5>
      - Are thought 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.,  $\text{CH}_3\text{NH}_3\text{PbX}_3$ , where X = I, Br or Cl.



# Visualization of Ideal Perovskite: SrTiO<sub>3</sub>



- [https://cs.boisestate.edu/~mlong/GUI/crystal\\_html/srtio3\\_obs.html](https://cs.boisestate.edu/~mlong/GUI/crystal_html/srtio3_obs.html)



# Lattice Constants at 300K

- Ideal Perovskite Materials

Material	a (A)	Radius of Ionic A <sup>2+</sup> (A)	Radius of Ionic B <sup>4+</sup> (A)	Radius of Ionic O <sup>2-</sup> (A)
SrTiO <sub>3</sub>	3.98805	1.32	0.745	1.26
KTaO <sub>3</sub>	3.9885	1.52	0.82	1.26
EuTiO <sub>3</sub>	7.810	1.31	0.745	1.26
SrVO <sub>3</sub>	3.838	1.32	0.72	1.26
CaVO <sub>3</sub>	3.767	1.14	0.72	1.26

- [https://en.wikipedia.org/wiki/Ionic\\_radius](https://en.wikipedia.org/wiki/Ionic_radius)
  - “Crystal ionic radii”

# Goal: Learning Math in STEM Context

# Summary of STEM Concepts

- Math

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

- Materials

- Atoms
- Crystal Structures
- Crystalline

- Programming

- Class
- Object
- Attribute

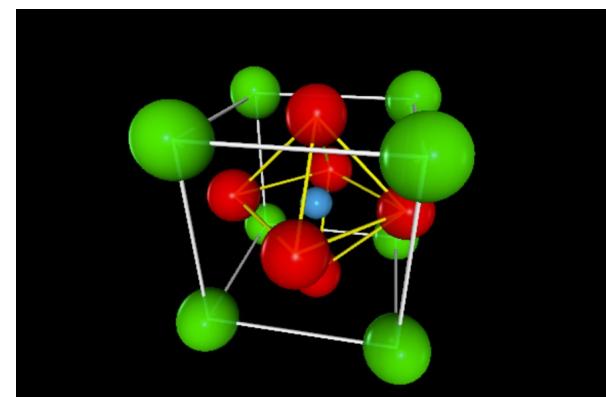
After the class: Review these concepts

# 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  $N \times A$  units of the first quantity,  $N \times B$  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

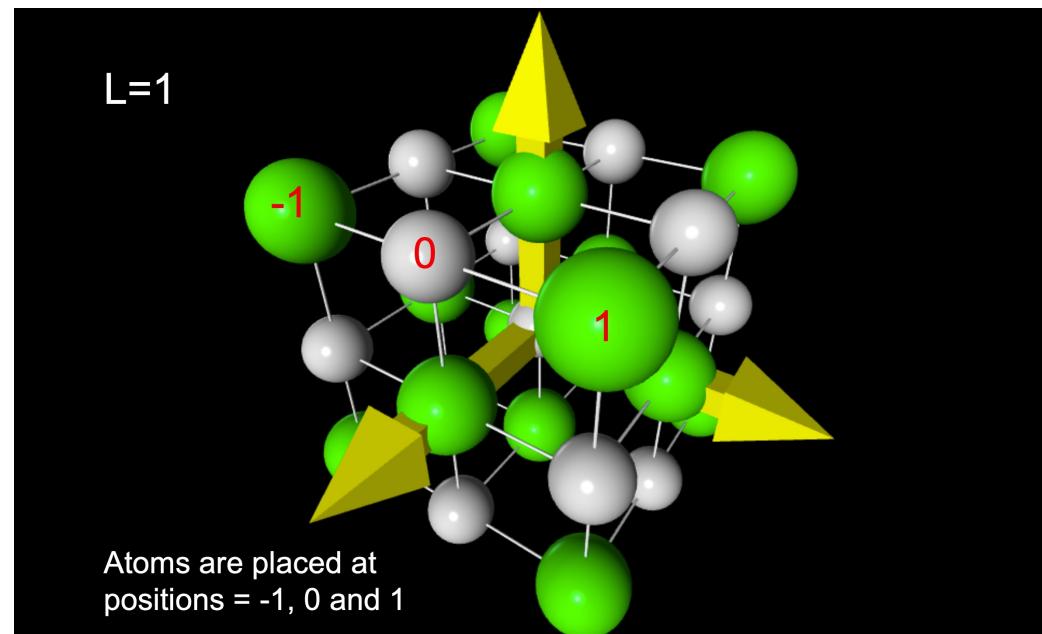


# Summary: Computer Science Concepts

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

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

Make it is possible to program complex problems.



**Let's discover Math in Patterns.**

Questions?