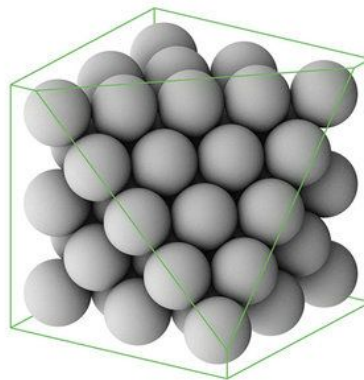
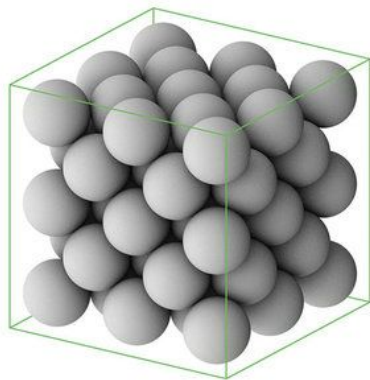
The background is a dark blue-grey color. It is decorated with various geometric shapes in orange and white. There are circles, hexagons, and triangles. Some shapes are solid, while others are outlines or filled with a pattern of small white dots. The overall design is modern and technical.

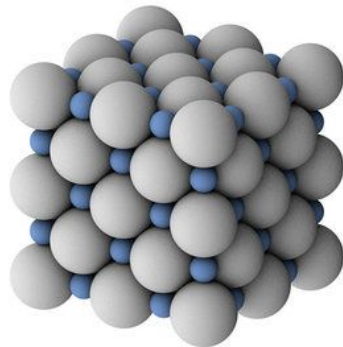
# Machine Learning Approaches for the Classification of Materials' Crystalline Structures

Mishek Musa  
PhD Student in Mechanical Engineering  
University of Arkansas, Fayetteville

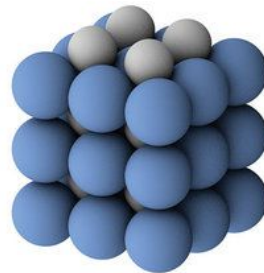
# What are Crystalline Structures?



**NaCl**

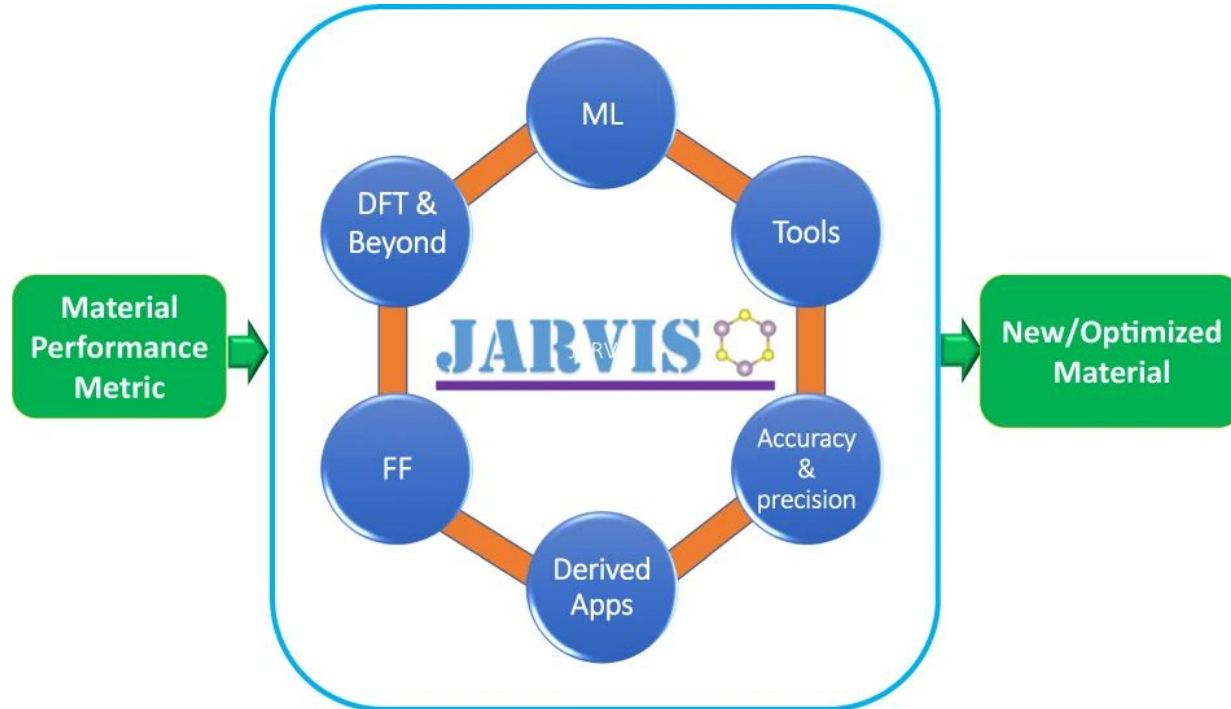


**CsCl**



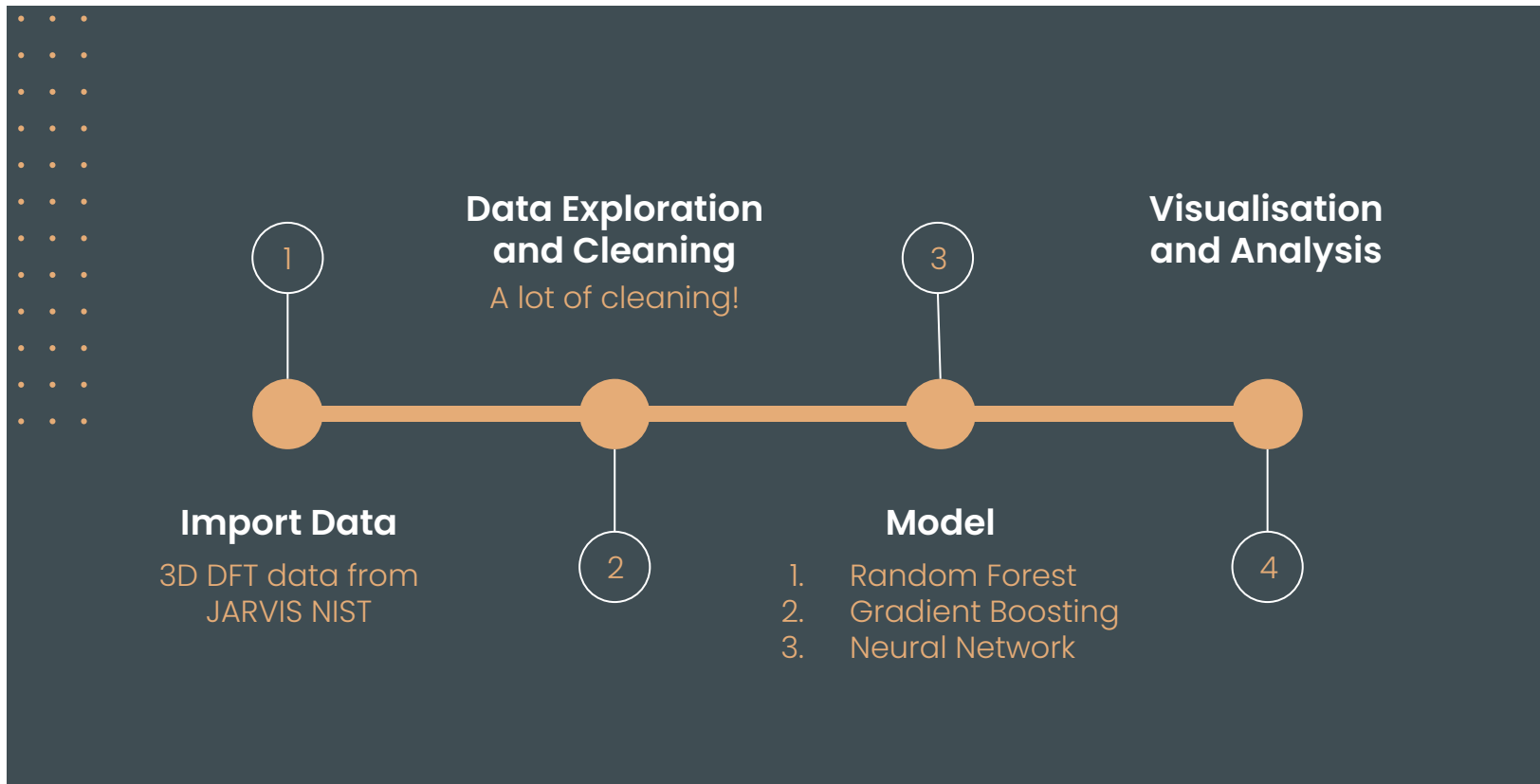
# Dataset

Joint Automated Repository for Various Integrated Simulations



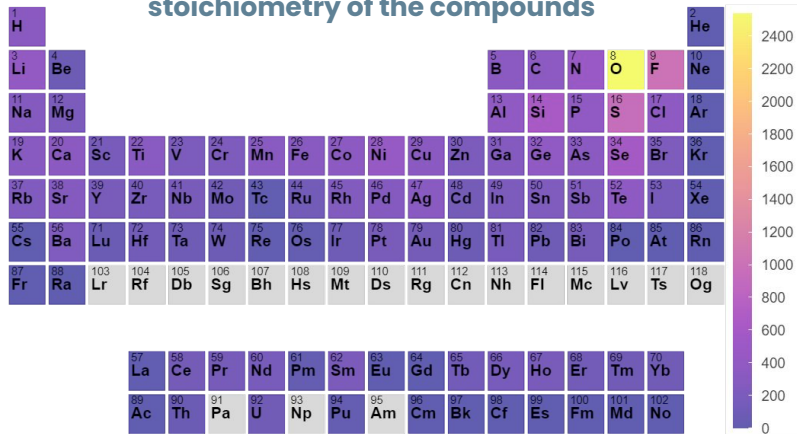
# Methodology

ML can be used to predict the crystalline structure of a material given DFT material properties

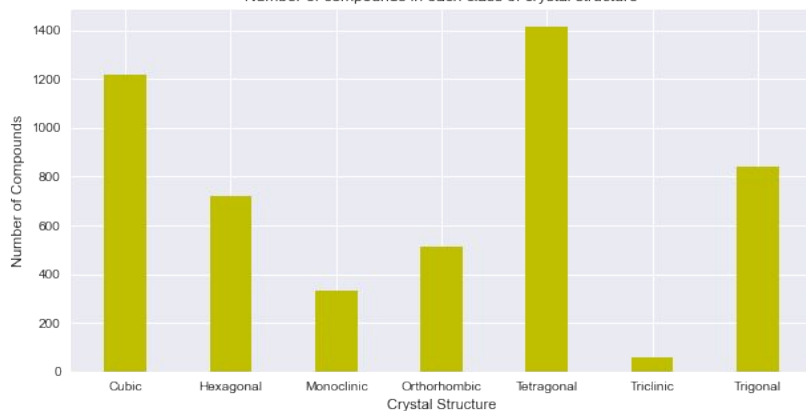


# Cleaning the Data

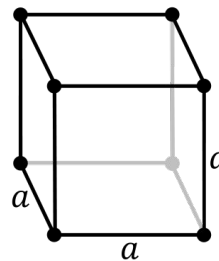
Heat map of the quantity of elements based on the stoichiometry of the compounds



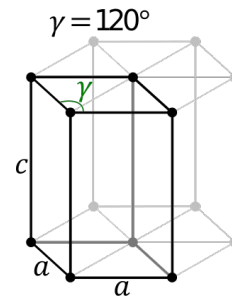
Number of compounds in each class of crystal structure



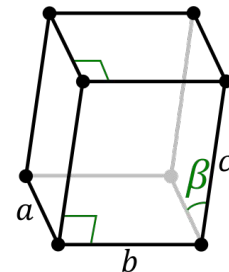
cubic



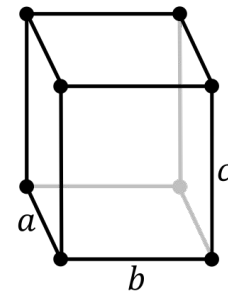
hexagonal



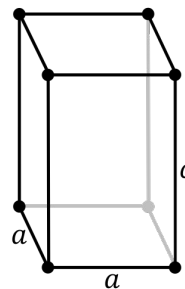
monoclinic



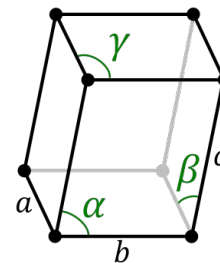
orthorhombic



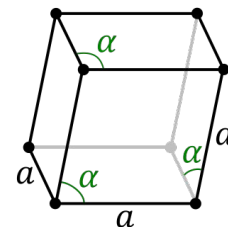
tetragonal



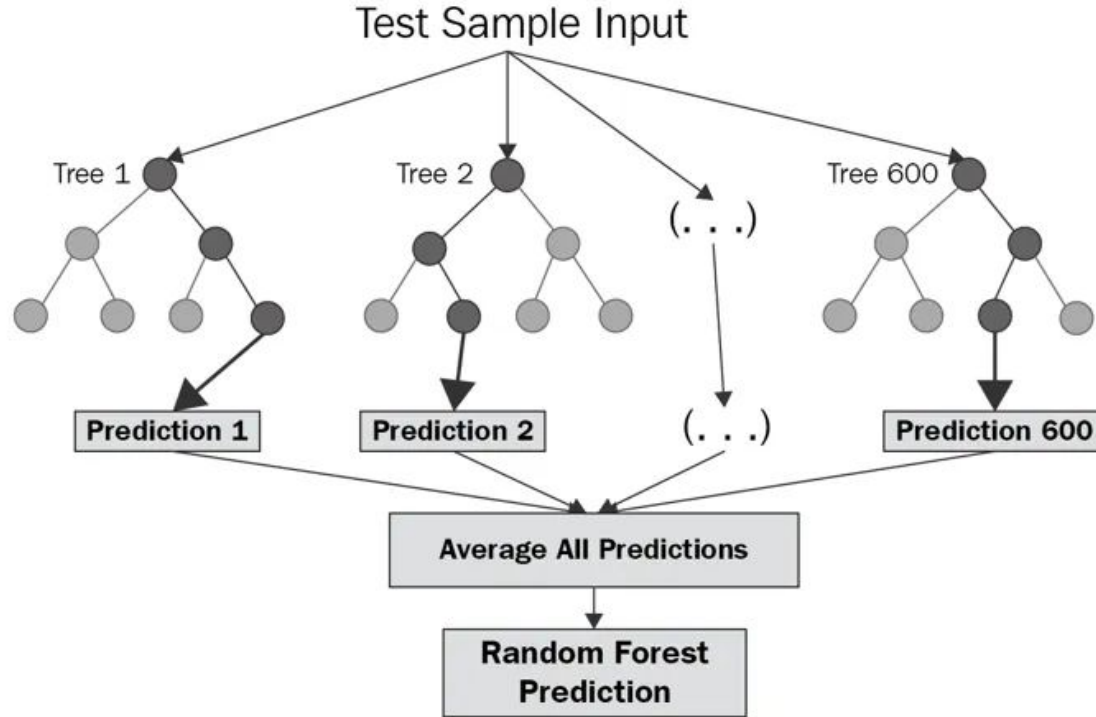
triclinic



trigonal

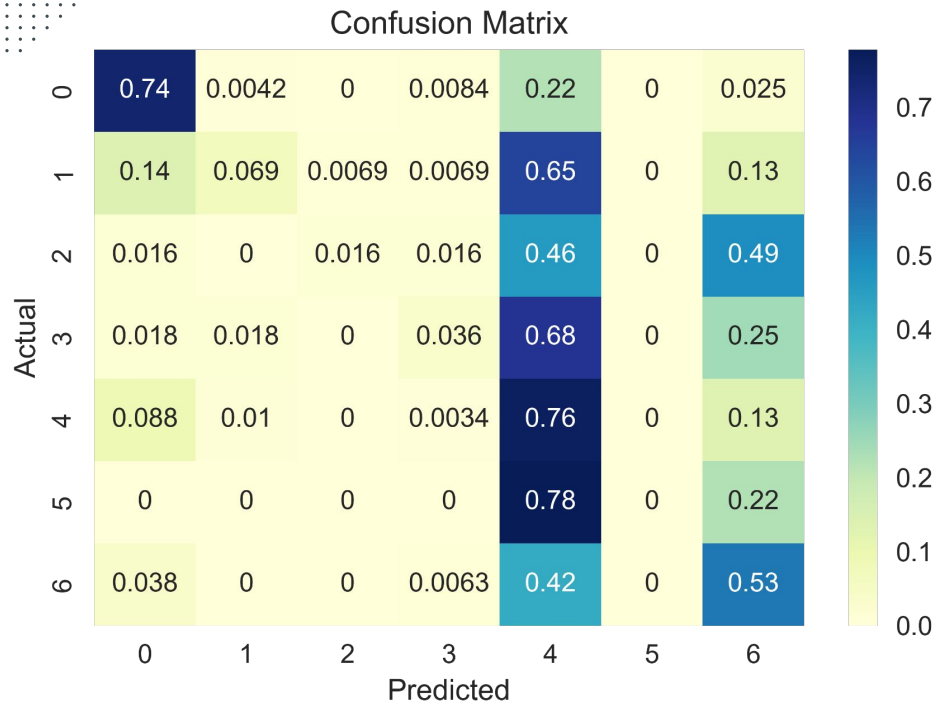


# Random Forest Classifier



# Method 1

## Random Forest Classifier



**Testing Accuracy: 47.1%**

0 - cubic

1 - hexagonal

2 - monoclinic

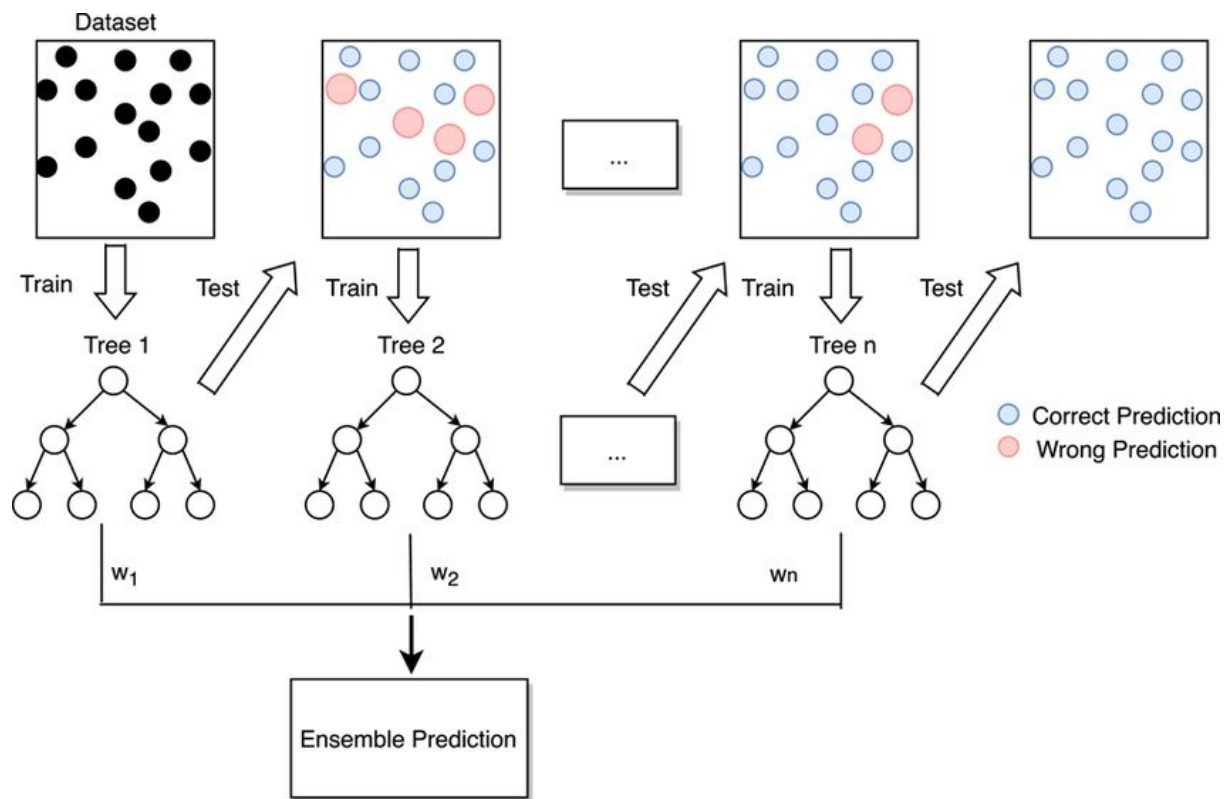
3 - orthorhombic

4 - tetragonal

5 - triclinic

6 - trigonal

# Gradient Boosting Classifier





## Method 2

# Gradient Boosting Classifier

**Testing Accuracy: 62.3%**

0 - cubic

1 - hexagonal

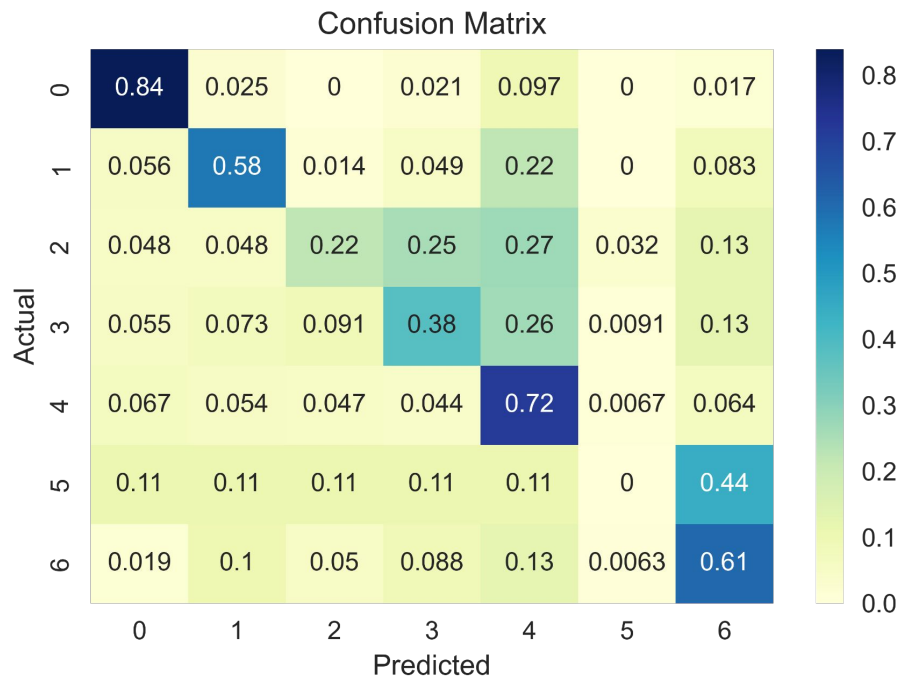
2 - monoclinic

3 - orthorhombic





4 - tetragonal

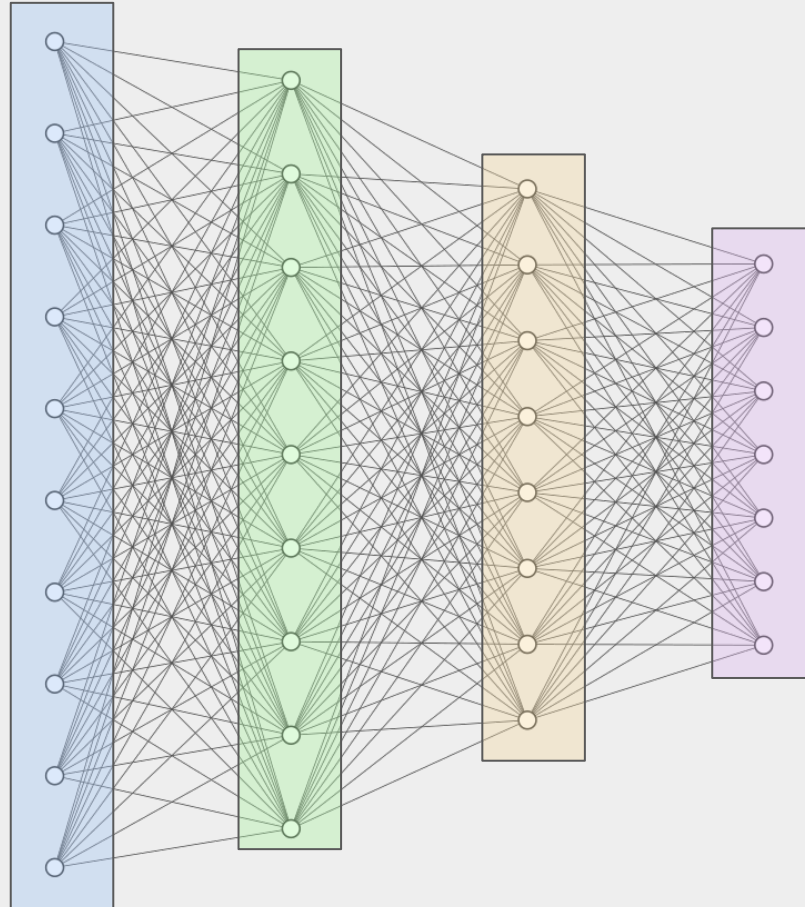
5 - triclinic

6 - trigonal



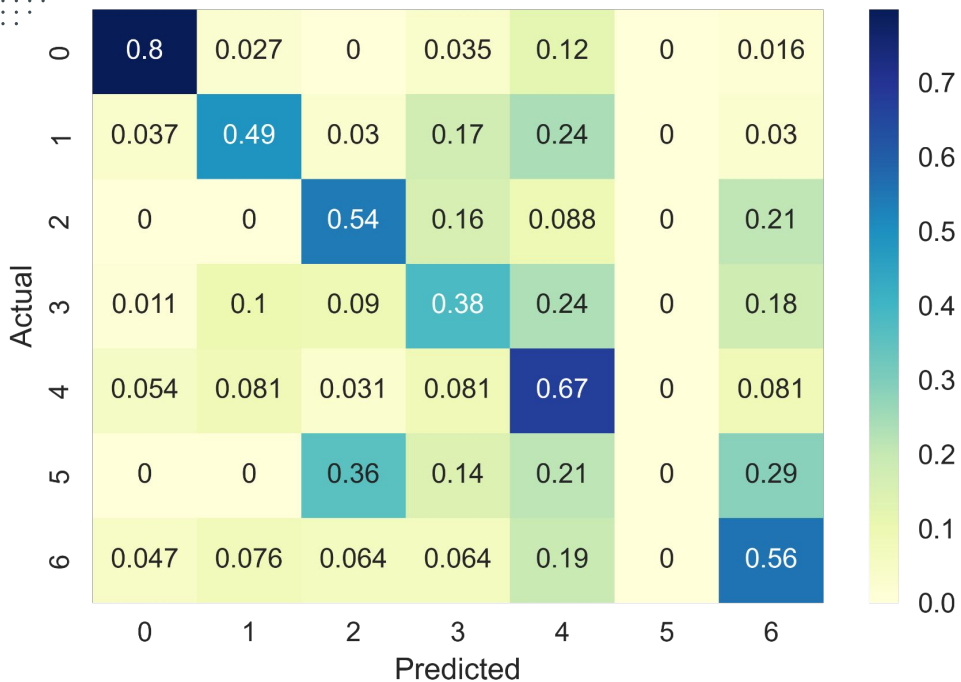
# Neural Network

-  Layer 1 – 100 Neurons  
ReLU activation Layer
-  Layer 2 – 50 Neurons  
ReLU activation Layer
-  Layer 3 – 20 Neurons  
ReLU activation Layer
-  Output Layer – 7 Neurons  
Softmax activation Layer



## Method 3 Neural Network

Confusion Matrix



**Testing Accuracy: 62.0%**

0 - cubic

1 - hexagonal

2 - monoclinic

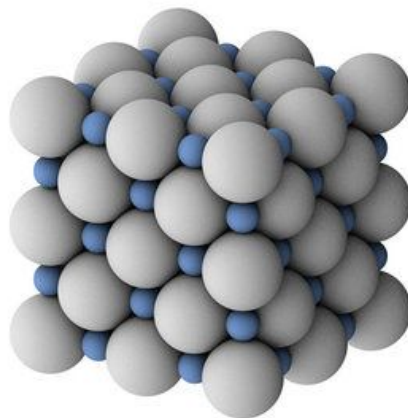
3 - orthorhombic

4 - tetragonal

5 - triclinic

6 - trigonal

## Conclusions



ML can be used to class the crystalline structure of a compound given DFT material properties, however Deep Learning should be further investigated to improve accuracy

# Thanks!

Do you have any questions?

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[https://scholar.google.com/citations?user=Fw-qo9sAAAAJ  
&hl=en](https://scholar.google.com/citations?user=Fw-qo9sAAAAJ&hl=en)