

**ABX<sub>3</sub> Laboratories**

# Perovskite Crystal Structure Predictor

A Machine Learning Algorithm

## Business Problem

1. Determine features with structural predictive accuracy.
2. Increase production of desired perovskite structure.

# Data Understanding

- Source: Kaggle (open commons)
- 4,165  $\text{ABO}_3$  perovskite records
- 13 feature columns

# Methodology

## Phase 1

- Data management
- Data analysis

## Phase 2

- Model building
- various techniques

## Phase 3

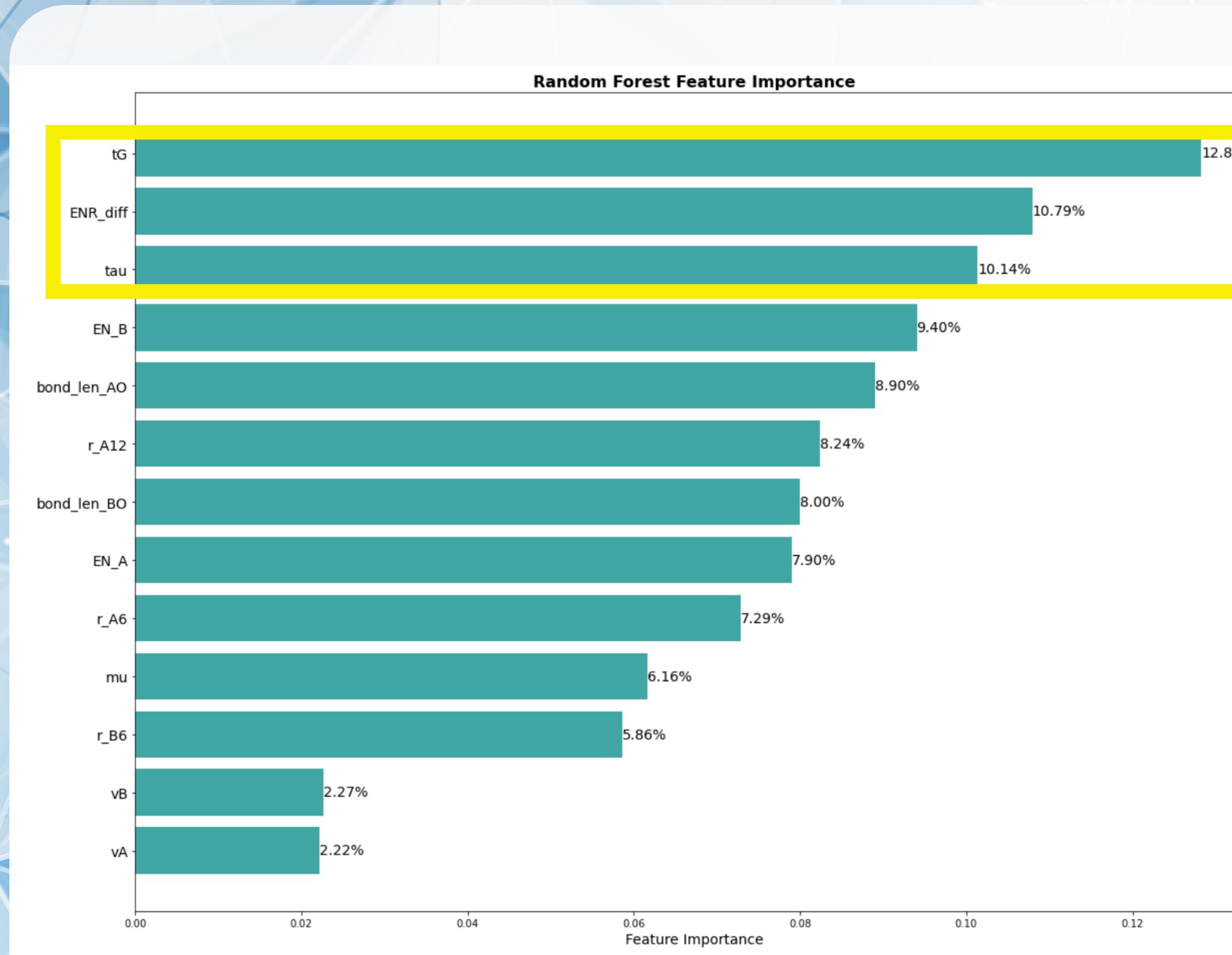
- Evaluation
- Comparison

# Results

## Model Comparison Table

Model	Precision	Recall	Accuracy	F1-Score
Decision Tree	81%	81%	81%	81%
Random Forest	85%	86%	86%	85%
RBF Support Vector Machine	83%	83%	83%	82%

# Feature Importance



# Recommendations

## 1. MODEL CHOICE

Random Forest Machine Learning Model

## 2. DATA QUANTITY

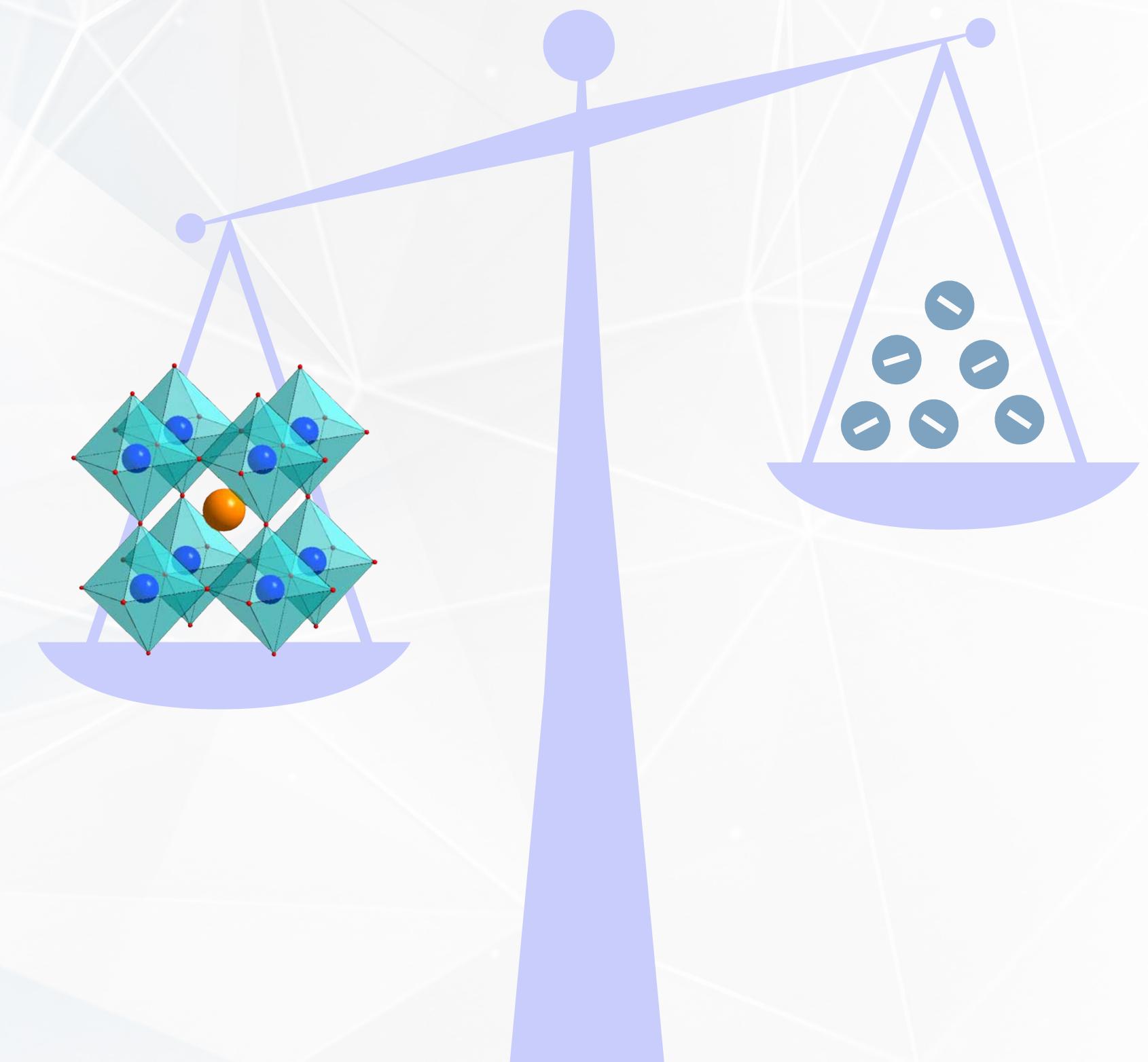
Additional empirical data

## 3. DATA QUALITY

Use feature importance analysis

## 4. DATA TARGET

Target discrete values



# Limitations

1. More detailed explanation of the feature variables would have maximized the data cleaning.
2. An accuracy of 100% was not achieved.

# Next Steps

Use Structural Parameters  
for Prediction

Gather Additional  
Empirical Data

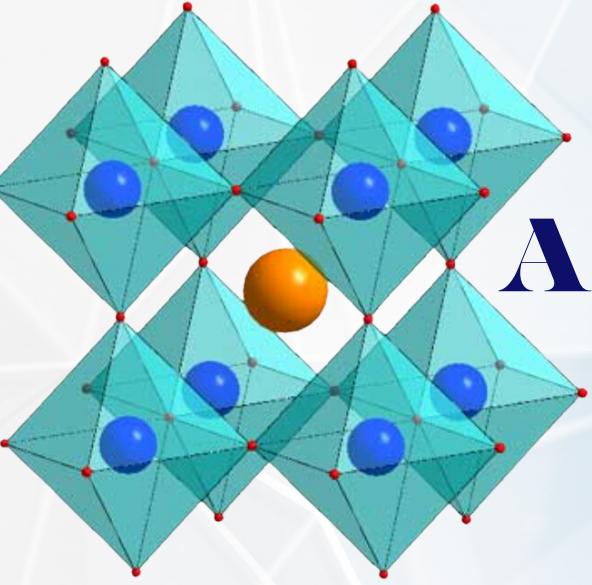
Feature Segmentation

Deep Learning

Improve Electronegativity/  
Ionic Radius Estimates

Analyze Halides for  
Big Data Processing





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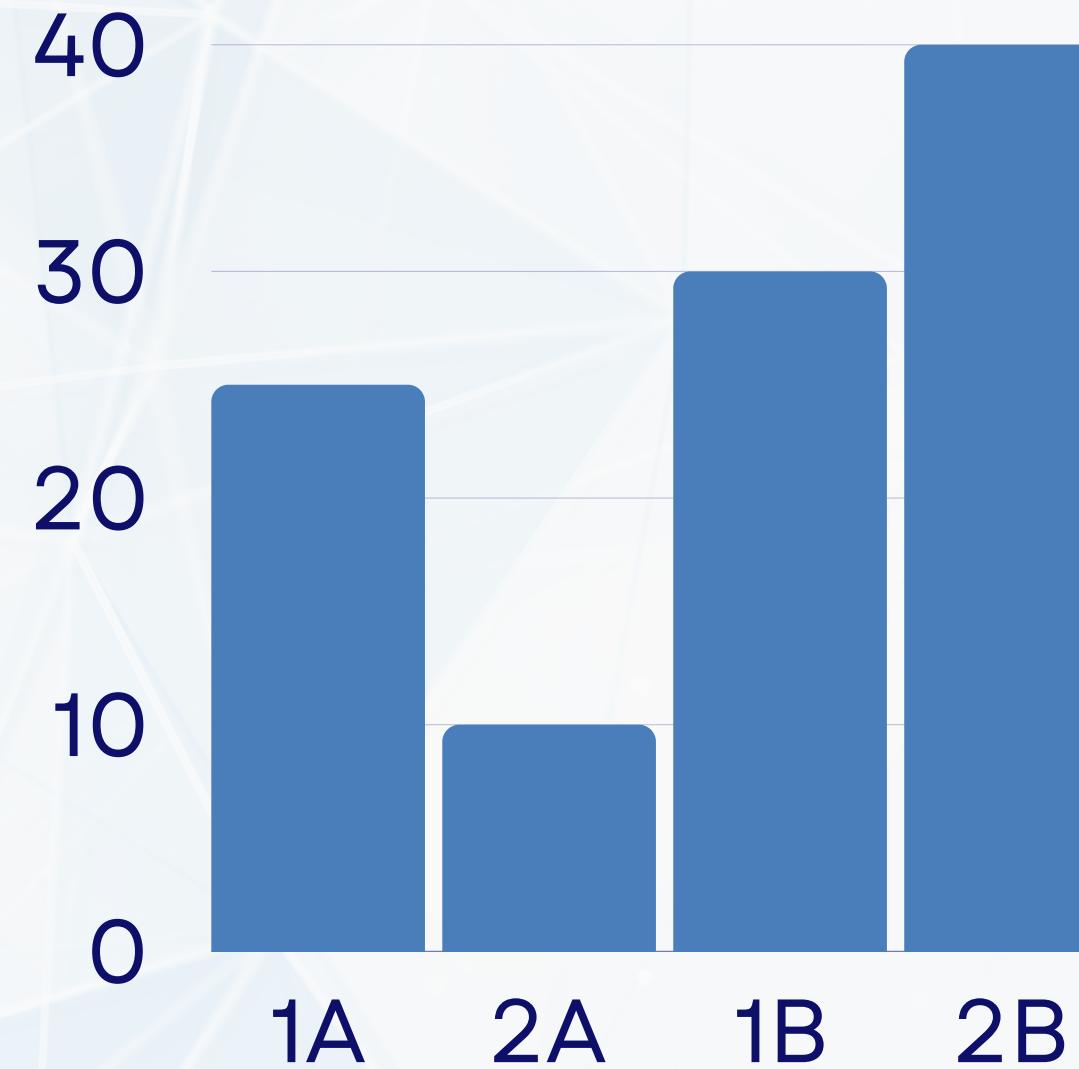
**Thank You**

# Question and Answer...





## Result



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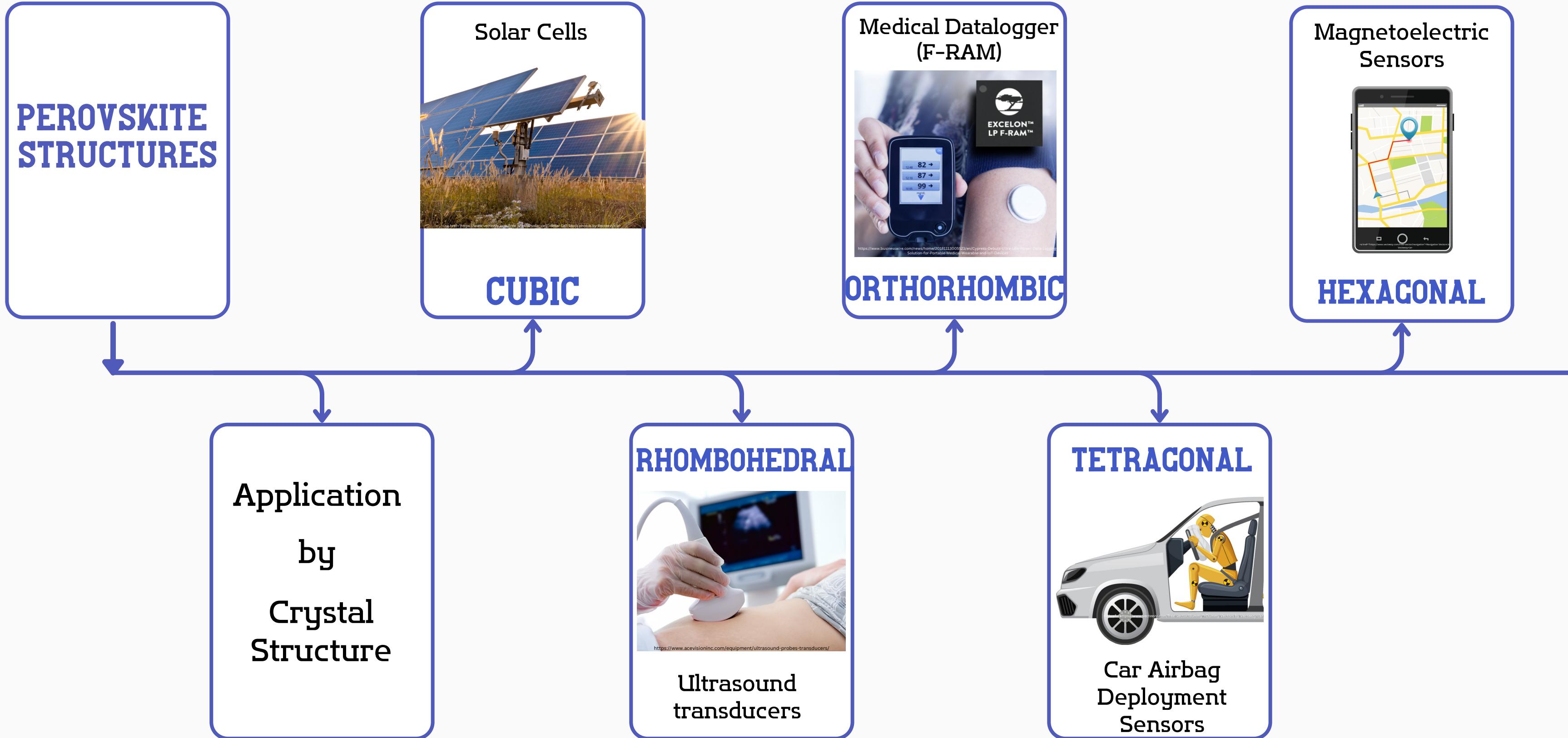
# Implementation

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# EXTRA SLIDES

how can I  
summarize this  
better???

# Introduction



# Introduction

## Background

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How do bond lengths relate to the  
'lowest distortion' classification?

Are certain atoms susceptible to false  
positives within the parameters of the  
different models?

Are the model's predictions  
interpretable based on chemical and  
structural properties?

What insights does analyzing feature  
relationships offer for perovskite  
crystal structures?

## Next Steps

**01** Increase production  
of desired materials

**03** Research Methods

**05** Conclusion

**02** Literary Review

**04** Discussion