

ABX₃ 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 ABO_3 perovskite records
- 13 feature columns

Methodology

Phase 1

- Data management
- Data analysis

Phase 2

- Model building
- various techniques

Phase 3

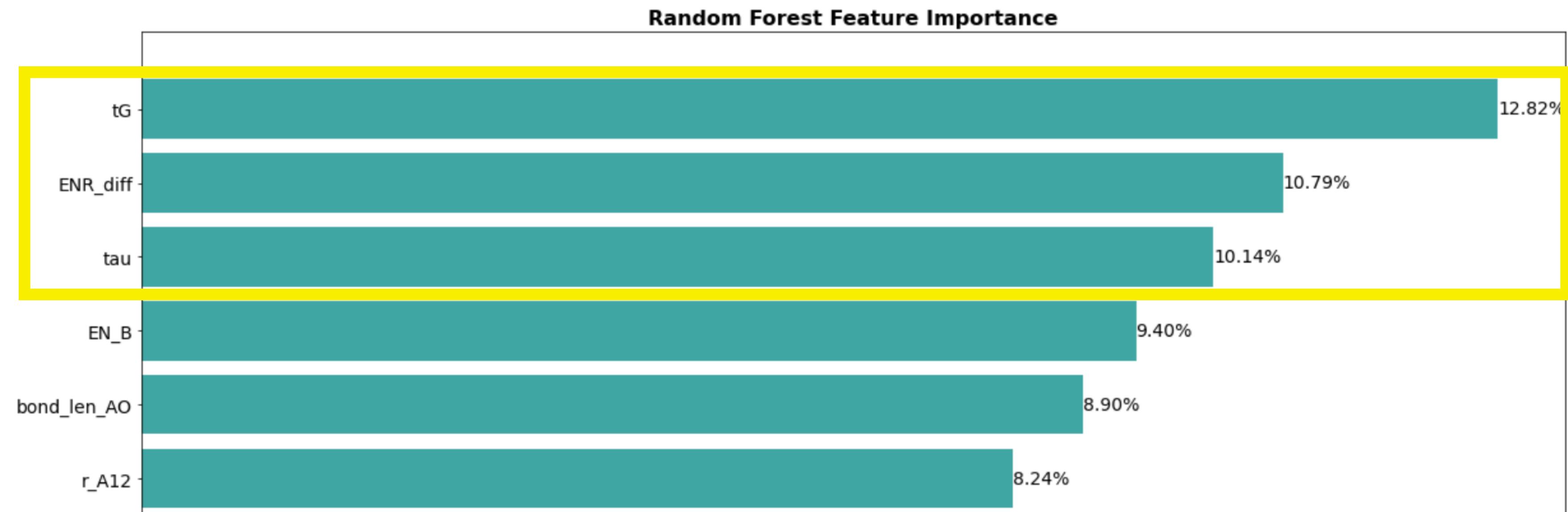
- Evaluation
- Comparison

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

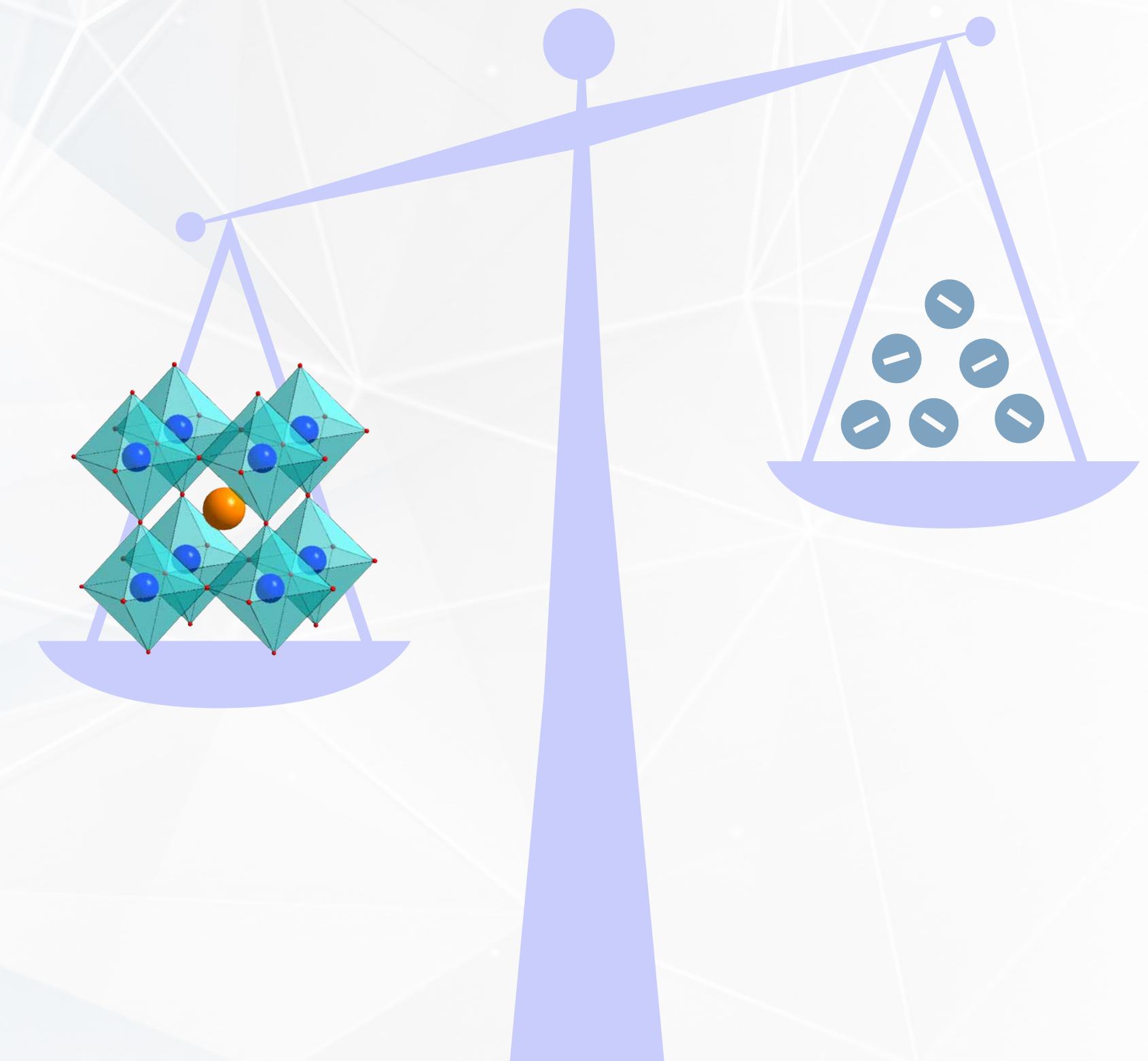
Additional empirical data

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

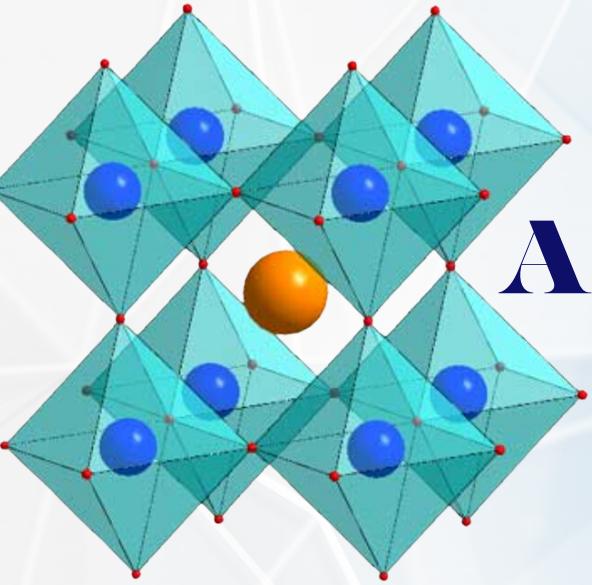
Feature Segmentation

Deep Learning

Improve Electronegativity/
Ionic Radius Estimates

Analyze Halides for
Big Data Processing





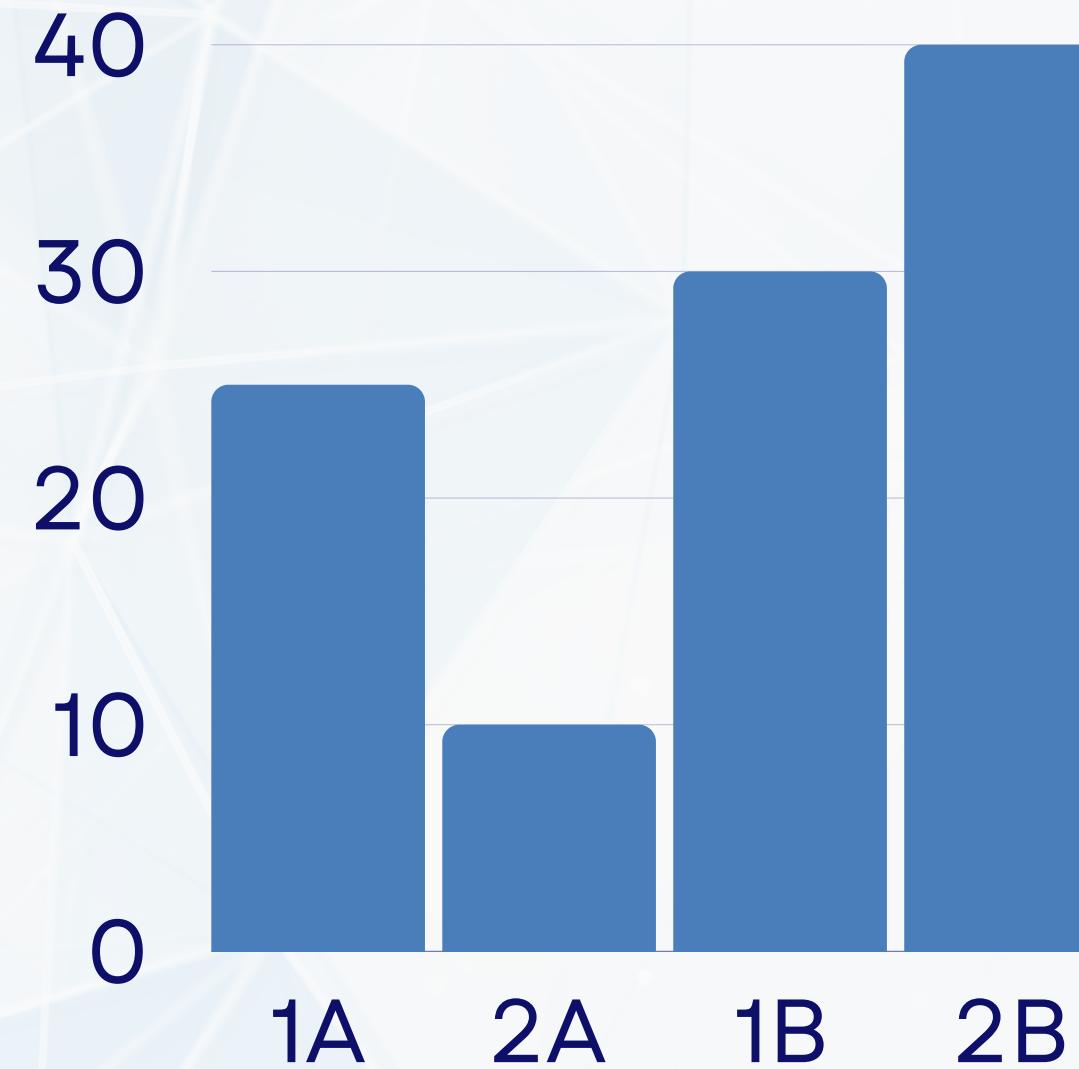
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Thank You

Question and Answer...



Result



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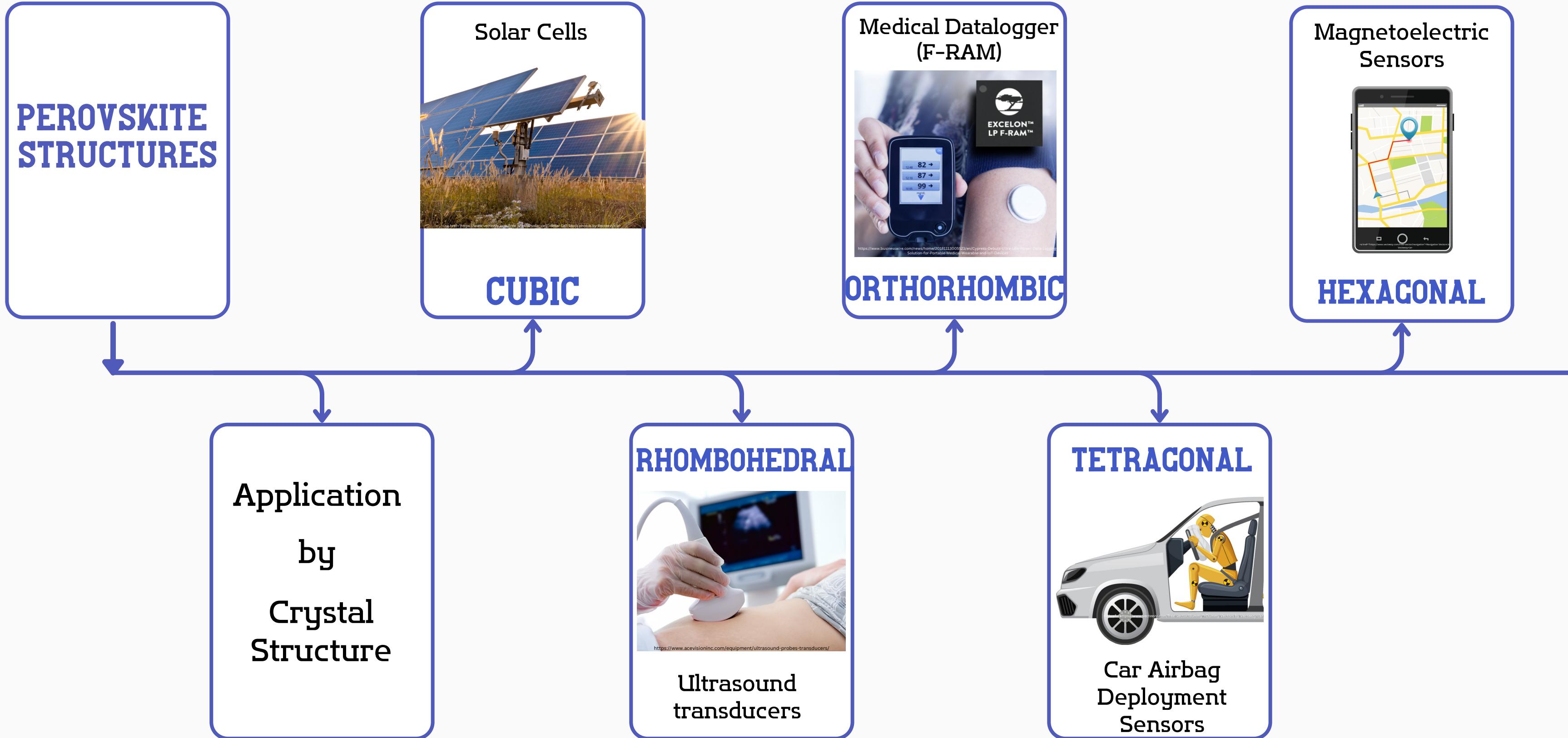
Implementation

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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