Material Property Prediction Based on Structure

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01

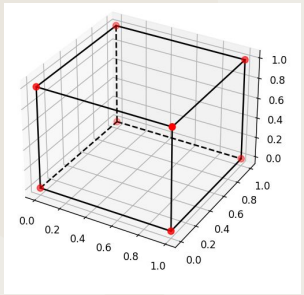
Introduction

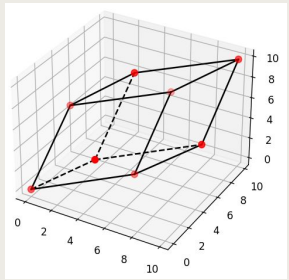
Literature Review

Review

Crystalline Structure

- Arranged in a lattice
- Lattice composed of unit cells
- Elements defined in a unit cell





Density Functional Theory (DFT)

- Common method used for calculating material properties.
  - Bandgap
  - Formation Energy
- Accurate but high computation.

Machine Learning

- Simulations
- Property Prediction

[1-6]

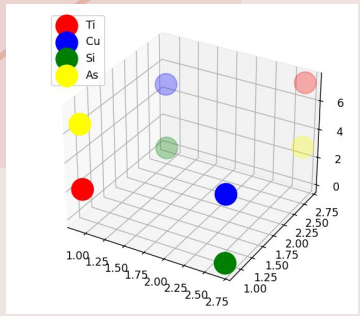
Hypothesis

Descriptive features can be used to represent the crystalline structure and predict properties such as formation energy and bandgap.

02

Methodology

Process



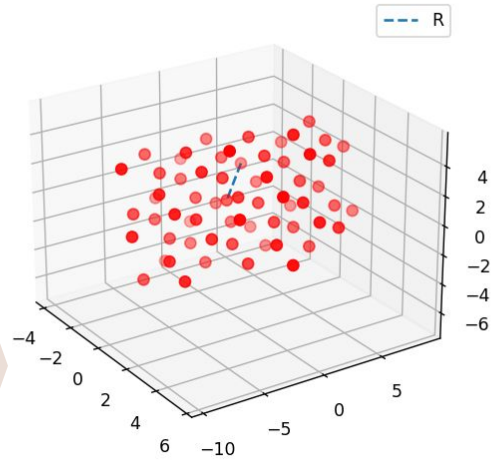
Crystalline Structure

Features

Regression Model

Property Prediction
(Bandgap & Formation Energy)

Features



Material Structure Defined:

- Coordinates of all elements
- Unit Cell

Descriptive Features:

$$G_i^{\text{atom,rad}} = \sum_{j=1}^{N_{\text{atom}}} e^{-\eta\left(R_{ij}-R_s\right)^2} \cdot f_c\left(R_{ij}\right),$$

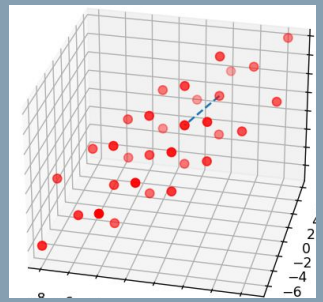
$$f_c\left(R_{ij}\right) = \begin{cases} 0.5 \cdot \left[\cos\left(\frac{\pi R_{ij}}{R_c}\right) + 1\right], & \text{for} \quad R_{ij} \le R_c \\ 0.0, & \text{for} \quad R_{ij} > R_c \end{cases}.$$

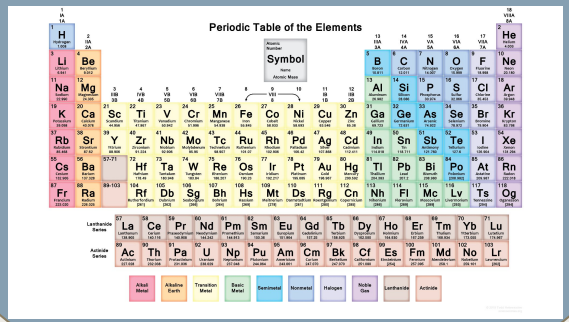
Number of each element in unit cell

[7] Behler

Regression Model

Feature based on atom positions





Random Forest Regression Model (Bandgap)

BandGap

Random Forest Regression Model (Formation Energy)

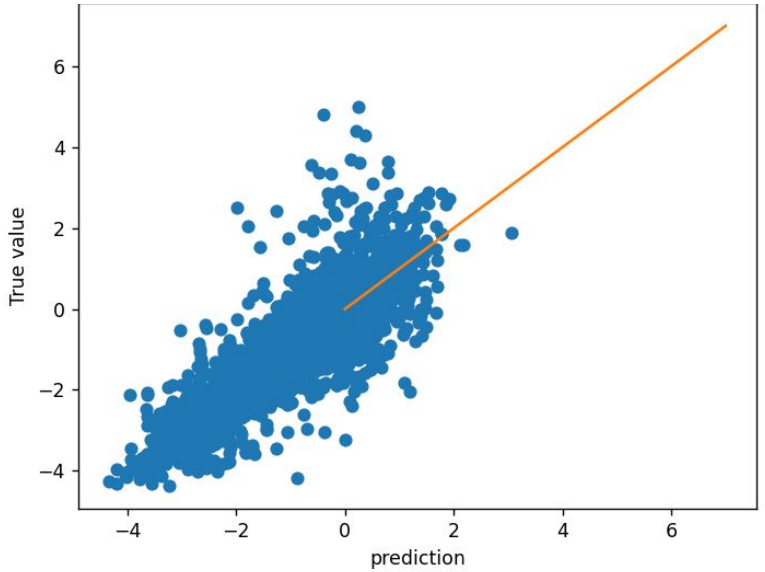
Formation Energy per Atom

03

Results

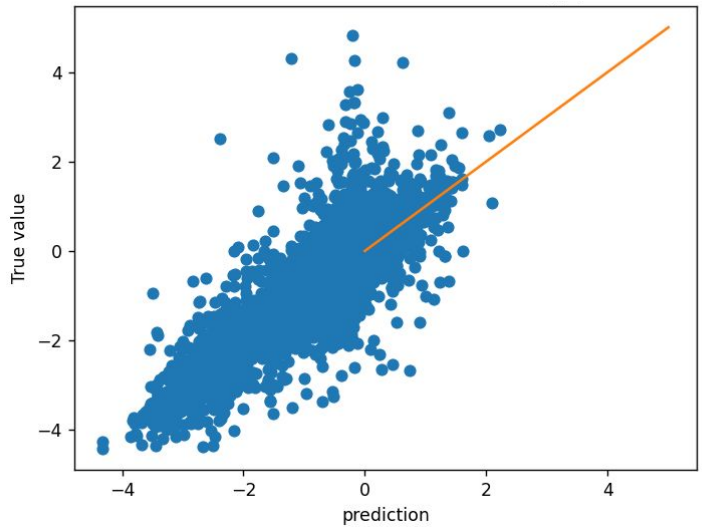
Random Forest Regression for Formation Energy Prediction

Bandgap Prediction Using only Elements



R2: 0.8422261973343066
Variance: 0.8423713682632842

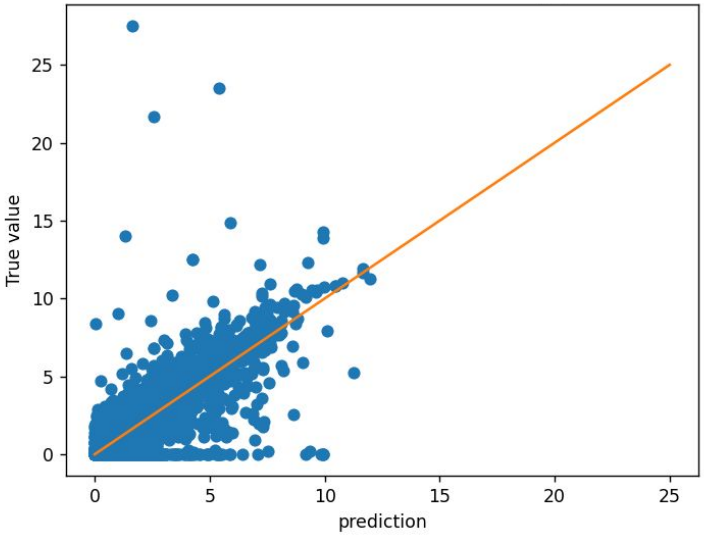
Bandgap Prediction Using Calculated Feature and Elements



R2: 0.8002507610815063
Variance: 0.8003173143298815

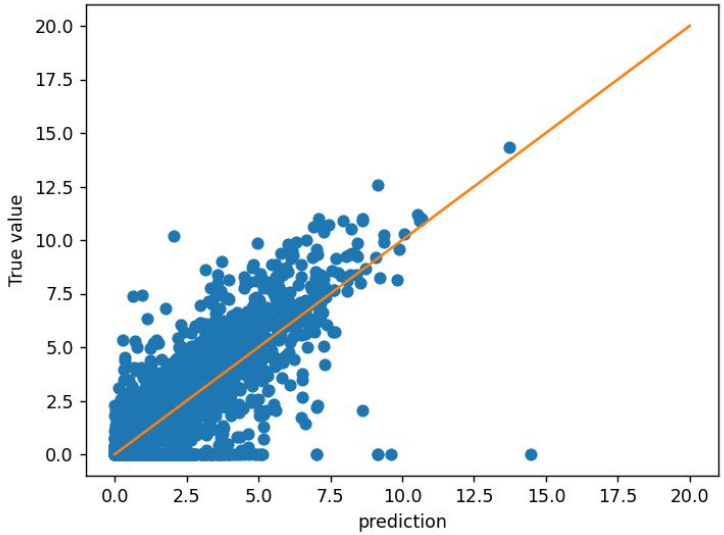
Random Forest Regression for Bandgap Prediction

Bandgap Prediction Using only Elements



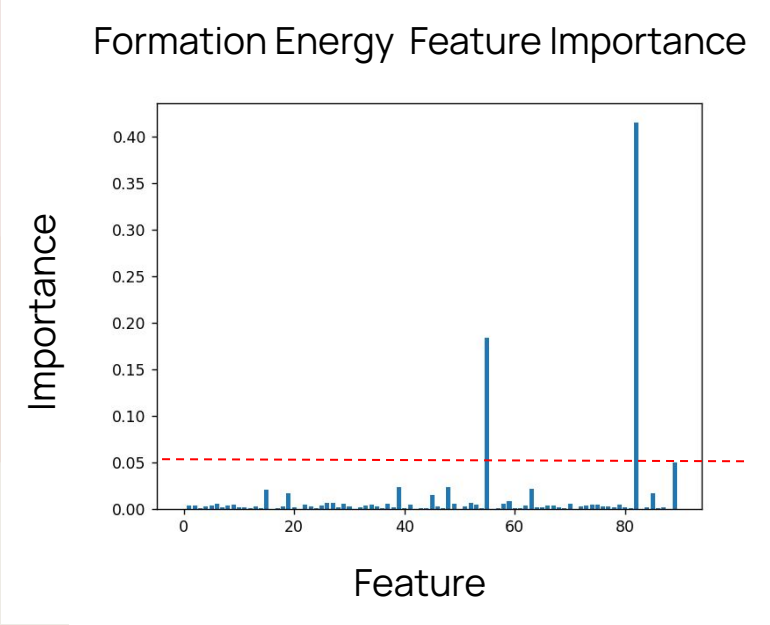
R2: 0.584878101702888
Variance: 0.5855821960922392

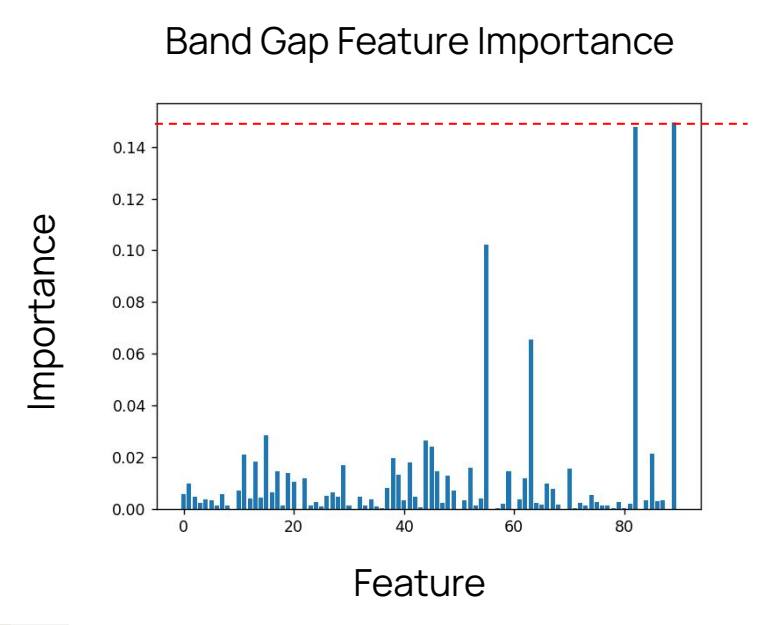
Bandgap Prediction Using Calculated Features and Elements



R2: 0.6416132047560574
Variance: 0.6416381704153014

Feature Importance for Formation Energy & Bandgap Models





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Conclusions

Conclusion

Summary		
Model	**Highest R2 Value**	**Features Used**
Formation Energy	0.84	# of each element
Bandgap	0.64	# of each element & structure feature

- Crystalline Structure is more relevant in predicting the bandgap than the formation energy
- The number of each element in the unit cell is related to the formation energy

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THANKS!

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