Project

April 19, 2025

1 PHYS 310 FINAL PROJECT

1.0.1 Load the Dataset

Dataset is obtained from the paper:
"Prediction and Classification of Formation Energies of Binary Compounds by Machine Learning" https://pubs.acs.org/doi/10.1021/acsomega.1c01517?goto=supporting-info#_i28

[14]:
```
import pandas as pd
file_path = "ao1c01517_si_003.xlsx"
df = pd.read_excel(file_path, skiprows = 51)
df
```

[14]:

	Substance	H(J/mol-atomes)	S0 J/cal/mol)	BDE(kj/mol)	SA(J/cal/deg)	\
0	Li2C2	-14850.0000	5.770000	0.0	29.1	
1	Li3N	-41200.0000	4.681075	0.0	29.1	
2	Li2O	-199300.0000	5.298567	340.5	29.1	
3	Li2O2	-158475.0000	5.770000	340.5	29.1	
4	LiF	-307500.0000	5.770000	577.0	29.1	
..	…	…	…	…	…	
178	BaF2	-402933.3333	5.298567	580.0	62.4	
179	BaS	-231800.0000	5.770000	0.0	62.4	
180	BaCl2	-286200.0000	5.298567	439.3	62.4	
181	BaBr2	-252566.6667	5.298567	359.9	62.4	
182	Ba2Sn	-125533.3333	5.298567	0.0	62.4	

	SB(J/cal/mol)	A_IP(ev)	A_EA(ev)	A_EN(ev)	A_H_ks_level(ev)	…	\
0	5.70	-5.329	-0.698	3.014	-2.874	…	
1	95.75	-5.329	-0.698	3.014	-2.874	…	
2	102.55	-5.329	-0.698	3.014	-2.874	…	
3	102.55	-5.329	-0.698	3.014	-2.874	…	
4	101.35	-5.329	-0.698	3.014	-2.874	…	
..	…	…	…	…	…	…	
178	101.35	-5.516	0.278	2.619	-3.346	…	
179	32.00	-5.516	0.278	2.619	-3.346	…	
180	111.50	-5.516	0.278	2.619	-3.346	…	
181	76.10	-5.516	0.278	2.619	-3.346	…	

```
182          51.20    -5.516     0.278     2.619           -3.346  …

     B4_number  B5_NNN  B5_number  B6_NNN  B6_number  B7_NNN  B7_number  \
0            -       -          -       -          -       -          -
1            -       -          -       -          -       -          -
2            -       -          -       -          -       -          -
3            -       -          -       -          -       -          -
4            -       -          -       -          -       -          -
..         …     …        …     …        …     …       …
178          -       -          -       -          -       -          -
179          -       -          -       -          -       -          -
180          -       -          -       -          -       -          -
181          -       -          -       -          -       -          -
182          -       -          -       -          -       -          -

     B8_NNN  B8_number  Vol(A3)
0         -          -    95.88
1         -          -    45.10
2         -          -    98.15
3         -          -    66.96
4         -          -    68.62
..      …        …      …
178       -          -   245.78
179       -          -   256.05
180       -          -   429.84
181       -          -   407.39
182       -          -   518.86

[183 rows x 93 columns]
```

1.1 Select Features and Clean Data

Choose physical and atomic descriptors as features and `H(J/mol-atomes)` as the target (formation energy).

[15]:
```
target = "H(J/mol-atomes)"
features = [
    'S0 J/cal/mol)', 'BDE(kj/mol)', 'SA(J/cal/deg)', 'SB(J/cal/mol)',
    'A_IP(ev)', 'A_EA(ev)', 'A_EN(ev)', 'B_IP(ev)', 'B_EA(ev)', 'B_EN(ev)',
    'Vol(A3)', 'length_a(A)', 'length_b(A)', 'length_c(A)',
    'A_rs(A)', 'A_rp(A)', 'A_rd(A)', 'B_rs(A)', 'B_rp(A)', 'B_rd(A)',
    'Z', 'SG_Number', 'R_Value'
]
df_clean = df[features + [target]].replace("-", pd.NA)
df_clean = df_clean.dropna()
df_clean = df_clean.astype(float)
```

```
X = df_clean[features]
y = df_clean[target]
X.head(), y.head()
```

[15]:
```
(   S0 J/cal/mol)  BDE(kj/mol)  SA(J/cal/deg)  SB(J/cal/mol)  A_IP(ev)  \
 0       5.770000          0.0           29.1           5.70    -5.329
 1       4.681075          0.0           29.1          95.75    -5.329
 2       5.298567        340.5           29.1         102.55    -5.329
 3       5.770000        340.5           29.1         102.55    -5.329
 4       5.770000        577.0           29.1         101.35    -5.329

    A_EA(ev)  A_EN(ev)  B_IP(ev)  B_EA(ev)  B_EN(ev)  …  length_c(A)  \
 0    -0.698     3.014   -10.852    -0.872     5.862  …      5.43440
 1    -0.698     3.014   -13.585    -1.867     7.726  …      3.87932
 2    -0.698     3.014   -16.433    -3.006     9.720  …      4.61280
 3    -0.698     3.014   -16.433    -3.006     9.720  …      7.72400
 4    -0.698     3.014   -19.404    -4.273    11.839  …      4.09400

    A_rs(A)  A_rp(A)  A_rd(A)  B_rs(A)  B_rp(A)  B_rd(A)    Z  SG_Number  \
 0    1.652    1.995     6.93    0.644    0.630    1.631  2.0       71.0
 1    1.652    1.995     6.93    0.539    0.511    1.540  1.0      191.0
 2    1.652    1.995     6.93    0.462    0.427    2.219  4.0      225.0
 3    1.652    1.995     6.93    0.462    0.427    2.219  2.0      194.0
 4    1.652    1.995     6.93    0.406    0.371    1.428  4.0      225.0

    R_Value
 0   0.0210
 1   0.0000
 2   0.0794
 3   0.0000
 4   0.0000

 [5 rows x 23 columns],
 0    -14850.0
 1    -41200.0
 2   -199300.0
 3   -158475.0
 4   -307500.0
 Name: H(J/mol-atomes), dtype: float64)
```

1.2 Train Model

Use **Random Forest Regressor** model

[16]:
```
from sklearn.model_selection import train_test_split
from sklearn.ensemble import RandomForestRegressor
from sklearn.metrics import mean_absolute_error, r2_score
```

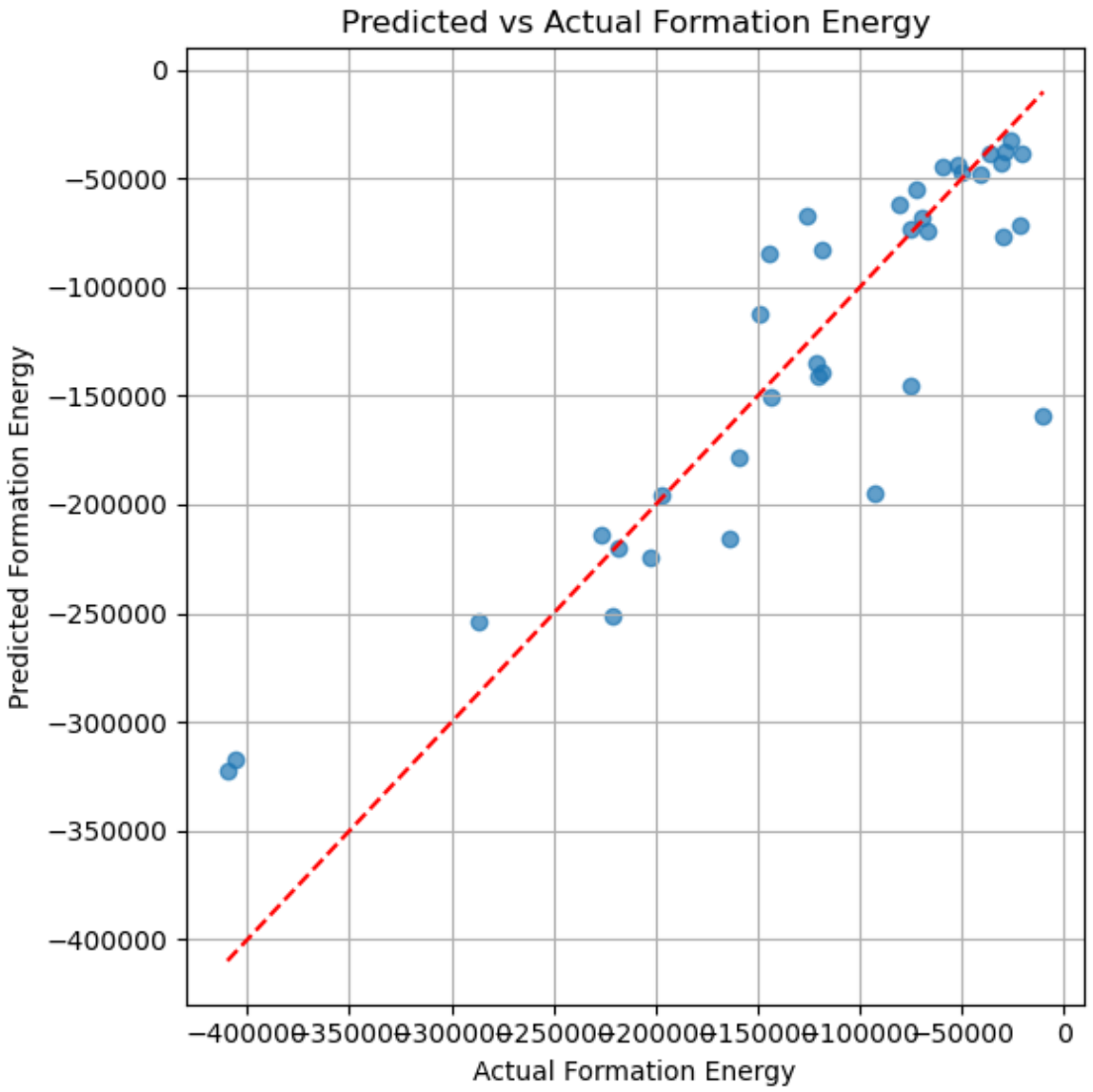
```
# Split the data & initialize & train
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
 ↪random_state=42)
model = RandomForestRegressor(n_estimators=100, random_state=42)
model.fit(X_train, y_train)

# Predict on test data & evaluale
y_pred = model.predict(X_test)
mae = mean_absolute_error(y_test, y_pred)
r2 = r2_score(y_test, y_pred)

print(f"Mean Absolute Error is: {mae:.2f}")
print(f"R² Score is: {r2:.2f}")
```

```
Mean Absolute Error is: 30972.76
R² Score is: 0.78
```

1.3 Visualization

Plot the predicted vs. actual formation energies and examine features.

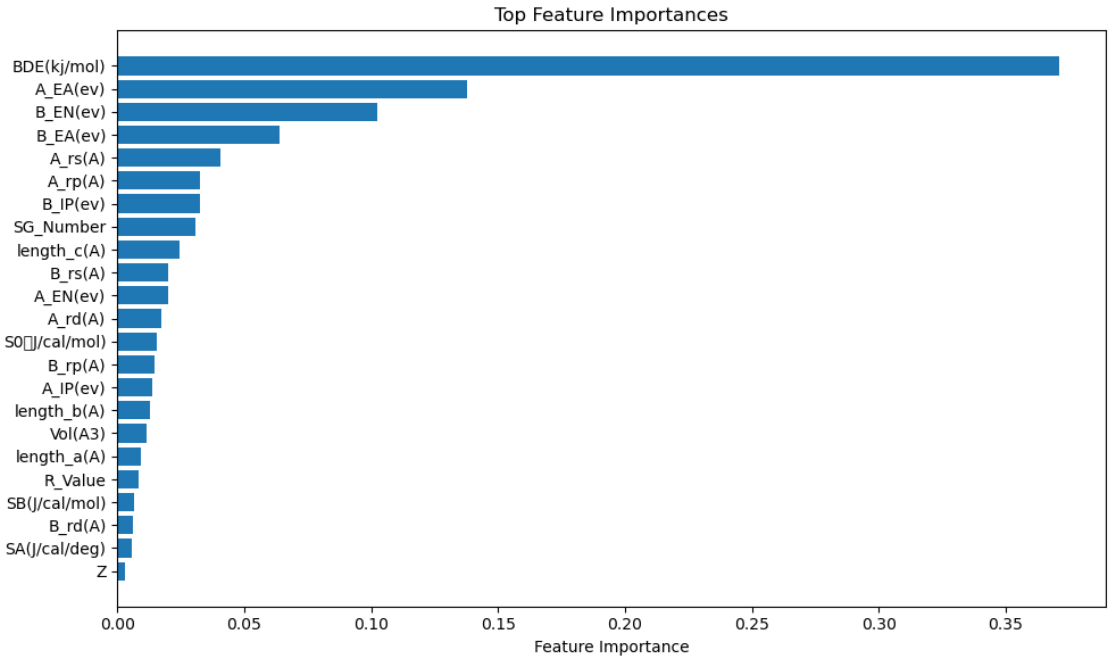
[17]:
```
import matplotlib.pyplot as plt
plt.figure(figsize=(6, 6))
plt.scatter(y_test, y_pred, alpha=0.7)
plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')
plt.xlabel("Actual Formation Energy")
plt.ylabel("Predicted Formation Energy")
plt.title("Predicted vs Actual Formation Energy")
plt.grid(True)
plt.tight_layout()
plt.show()
```



[18]:
```
importances = model.feature_importances_
feature_importance_df = pd.DataFrame({
    'Feature': X.columns,
    'Importance': importances
}).sort_values(by='Importance', ascending=False)

# Bar plot of top features
plt.figure(figsize=(10, 6))
plt.barh(feature_importance_df['Feature'], feature_importance_df['Importance'])
plt.xlabel("Feature Importance")
plt.title("Top Feature Importances")
plt.gca().invert_yaxis()
plt.tight_layout()
```

```
plt.show()
```

```
/tmp/ipykernel_686/1796090255.py:13: UserWarning: Glyph 65288 (\N{FULLWIDTH LEFT
PARENTHESIS}) missing from current font.
  plt.tight_layout()
/opt/conda/lib/python3.12/site-packages/IPython/core/pylabtools.py:170:
UserWarning: Glyph 65288 (\N{FULLWIDTH LEFT PARENTHESIS}) missing from current
font.
  fig.canvas.print_figure(bytes_io, **kw)
```



1.4 Model Comparison

Compare our Random Forest model to a Gradient Boosting Regressor.

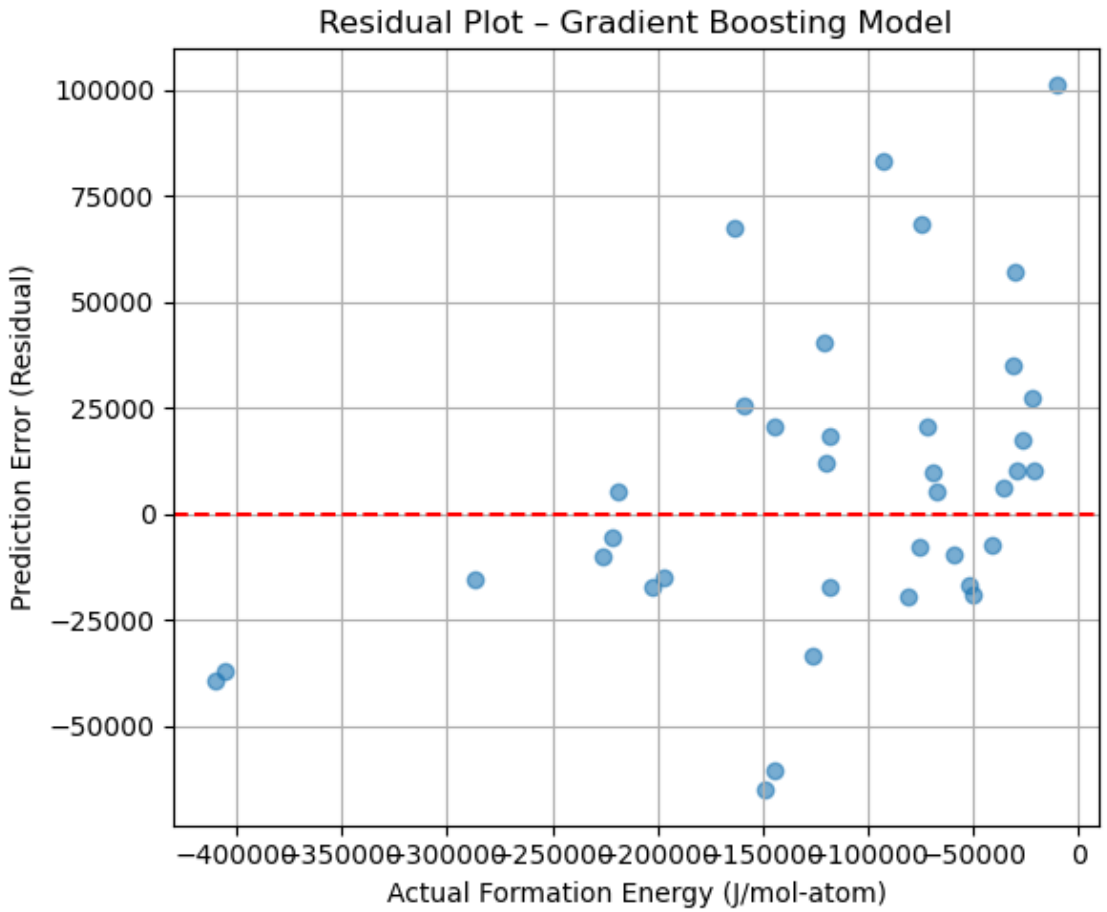
[19]:
```
from sklearn.ensemble import GradientBoostingRegressor
gbr = GradientBoostingRegressor(n_estimators=100, random_state=42)
gbr.fit(X_train, y_train)
y_pred_gbr = gbr.predict(X_test)
mae_gbr = mean_absolute_error(y_test, y_pred_gbr)
r2_gbr = r2_score(y_test, y_pred_gbr)
print(f"MAE: {mae_gbr:.2f}")
print(f"R² Score: {r2_gbr:.2f}")
```

```
MAE: 28059.17
R² Score: 0.86
```

[20]:
```
from sklearn.model_selection import cross_val_score, cross_val_predict
from sklearn.metrics import mean_absolute_error, make_scorer

# Cross Validation
mae_scorer = make_scorer(mean_absolute_error)
rf_cv_r2 = cross_val_score(model, X, y, cv=5, scoring='r2')
rf_cv_mae = cross_val_score(model, X, y, cv=5, scoring=mae_scorer)

gbr_cv_r2 = cross_val_score(gbr, X, y, cv=5, scoring='r2')
gbr_cv_mae = cross_val_score(gbr, X, y, cv=5, scoring=mae_scorer)

print("Random Forest - CV R²:", rf_cv_r2.mean(), "CV MAE:", rf_cv_mae.mean())
print("Gradient Boosting - CV R²:", gbr_cv_r2.mean(), "CV MAE:", gbr_cv_mae.
  ↪mean())
```

```
Random Forest - CV R²: 0.7618753893096278 CV MAE: 31896.04232084183
Gradient Boosting - CV R²: 0.7855547850181079 CV MAE: 29402.273959916365
```

[21]:
```
# Residual plot for best model
residuals = y_test - y_pred_gbr

plt.figure(figsize=(6, 5))
plt.scatter(y_test, residuals, alpha=0.6)
plt.axhline(0, color='red', linestyle='--')
plt.xlabel("Actual Formation Energy (J/mol-atom)")
plt.ylabel("Prediction Error (Residual)")
plt.title("Residual Plot - Gradient Boosting Model")
plt.grid(True)
plt.tight_layout()
plt.show()
```



1.5 Model with Top 5 features

Smaller model with top 5 features and PCA

[22]:
```
top_features = feature_importance_df.sort_values(by='Importance',␣
↪ascending=False)['Feature'].head(5).tolist()
print("Top 5 features:", top_features)
```

```
Top 5 features: ['BDE(kj/mol)', 'A_EA(ev)', 'B_EN(ev)', 'B_EA(ev)', 'A_rs(A)']
```

[23]:
```
X_small = X[top_features]
X_train_small, X_test_small, y_train_small, y_test_small =␣
↪train_test_split(X_small, y, test_size=0.2, random_state=42)
gbr_small = GradientBoostingRegressor(n_estimators=100, random_state=42)
gbr_small.fit(X_train_small, y_train_small)
y_pred_small = gbr_small.predict(X_test_small)
mae_small = mean_absolute_error(y_test_small, y_pred_small)
r2_small = r2_score(y_test_small, y_pred_small)
print("Small GBR model - MAE:", mae_small)
```

```
print("Small GBR model - R²:", r2_small)
```

```
Small GBR model - MAE: 29182.571420915418
Small GBR model - R²: 0.8291392845150648
```

[24]:
```
from sklearn.decomposition import PCA
from sklearn.pipeline import make_pipeline
from sklearn.preprocessing import StandardScaler
pca_pipeline = make_pipeline(StandardScaler(), PCA(n_components=5),␣
 ↪GradientBoostingRegressor(n_estimators=100, random_state=42))
pca_pipeline.fit(X_train, y_train)
y_pred_pca = pca_pipeline.predict(X_test)
mae_pca = mean_absolute_error(y_test, y_pred_pca)
r2_pca = r2_score(y_test, y_pred_pca)

print("PCA + GBR model - MAE:", mae_pca)
print("PCA + GBR model - R²:", r2_pca)
```

```
PCA + GBR model - MAE: 42237.20621168072
PCA + GBR model - R²: 0.652603372243924
```

1.5.1 Summary

The goal of this project was to develop a machine learning model that could accurately predict the formation energy of binary compounds using only atomic and compositional features to support faster screening of materials.

The Gradient Boosting model showed superior performance compared to Random Forest model, achieving an R^2 score of 0.86 and a mean absolute error (MAE) of 28,000 J/mol-atom, which suggests that the model is able to make fairly accurate predictions. To further evaluate model reliability, I applied 5-fold cross-validation in which Gradient Boosting remained the best performer with a cross-validated R^2 of 0.79 and MAE of 29,400 J/mol-atom.