In [ ]:
```
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
```

In [ ]:
```
data=pd.read_csv('material_data.txt')
data
```

Out[ ]:

	Elements	Atomic_Number	Electronegativity	Atomic_Radius	Thermal_Conductivity	Density	Crystal_System
0	H	1	2.20	0.25	0.1805	0.09	HEX
1	He	2	0.00	1.20	0.1513	0.18	HCP
2	Li	3	0.98	1.45	85.0000	530.00	BCC
3	Be	4	1.57	1.05	190.0000	1850.00	HCP
4	B	5	2.04	0.85	27.0000	2340.00	RHO
...	...	...	...	...	...	...	...
90	U	92	1.38	1.75	27.0000	18950.00	ORTH
91	Np	93	1.36	1.75	6.0000	20200.00	ORTH
92	Pu	94	1.28	1.75	6.0000	19840.00	MON
93	Am	95	1.30	1.75	10.0000	13670.00	HCP
94	Cm	96	1.30	1.76	8.8000	13500.00	HCP

95 rows × 7 columns

In [ ]:
```
for i in data.columns:
    print(i, data[i].dtype)
```

```
Elements object
Atomic_Number int64
Electronegativity float64
Atomic_Radius float64
Thermal_Conductivity float64
Density float64
Crystal_System object
```

Normalizing the data

In [ ]:
```
data = data[['Electronegativity', 'Atomic_Radius', 'Density', 'Thermal_Conductivity']]
```

In [ ]:
```
from sklearn.decomposition import PCA
from sklearn.preprocessing import StandardScaler, MinMaxScaler

# Standardize the features
scaler = StandardScaler()
data_standardized = scaler.fit_transform(data)

# Apply PCA
pca = PCA()
data_pca = pca.fit_transform(data_standardized)

# Normalize the transformed features
scaler_pca = MinMaxScaler()
data_normalized_pca = scaler_pca.fit_transform(data_pca)

data=pd.DataFrame(data_normalized_pca, columns=['Electronegativity', 'Atomic_Radius', 'Density', 'Thermal_Conductivity'])
data
```

Out[ ]:

	Electronegativity	Atomic_Radius	Density	Thermal_Conductivity
0	0.817528	0.080231	0.374366	0.694952
1	0.259807	0.025388	0.543575	0.782250
2	0.344477	0.212992	0.612142	0.443457
3	0.546820	0.393159	0.749450	0.492883
4	0.632594	0.189693	0.379998	0.495577
...	...	...	...	...
90	0.236661	0.552660	0.066426	0.481104
91	0.224927	0.548823	0.000000	0.505274
92	0.215199	0.537514	0.014456	0.518756
93	0.243397	0.414823	0.151665	0.427338
94	0.241212	0.410118	0.152706	0.420631

95 rows × 4 columns

1. Decision Tree

In [ ]:
```
X_1 = data[['Electronegativity']]
X_2 = data[['Atomic_Radius']]
X_3 = data[['Density']]
X_4 = data[['Electronegativity', 'Atomic_Radius', 'Density']]
X = [X_1,X_2,X_3,X_4]
Plot_Name = ['Electronegativity', 'Atomic Radius', 'Density', 'Combined']
Y = data[['Thermal_Conductivity']]
```

In [ ]:
```
from sklearn.model_selection import train_test_split
from sklearn.tree import DecisionTreeRegressor
from sklearn.metrics import r2_score
```

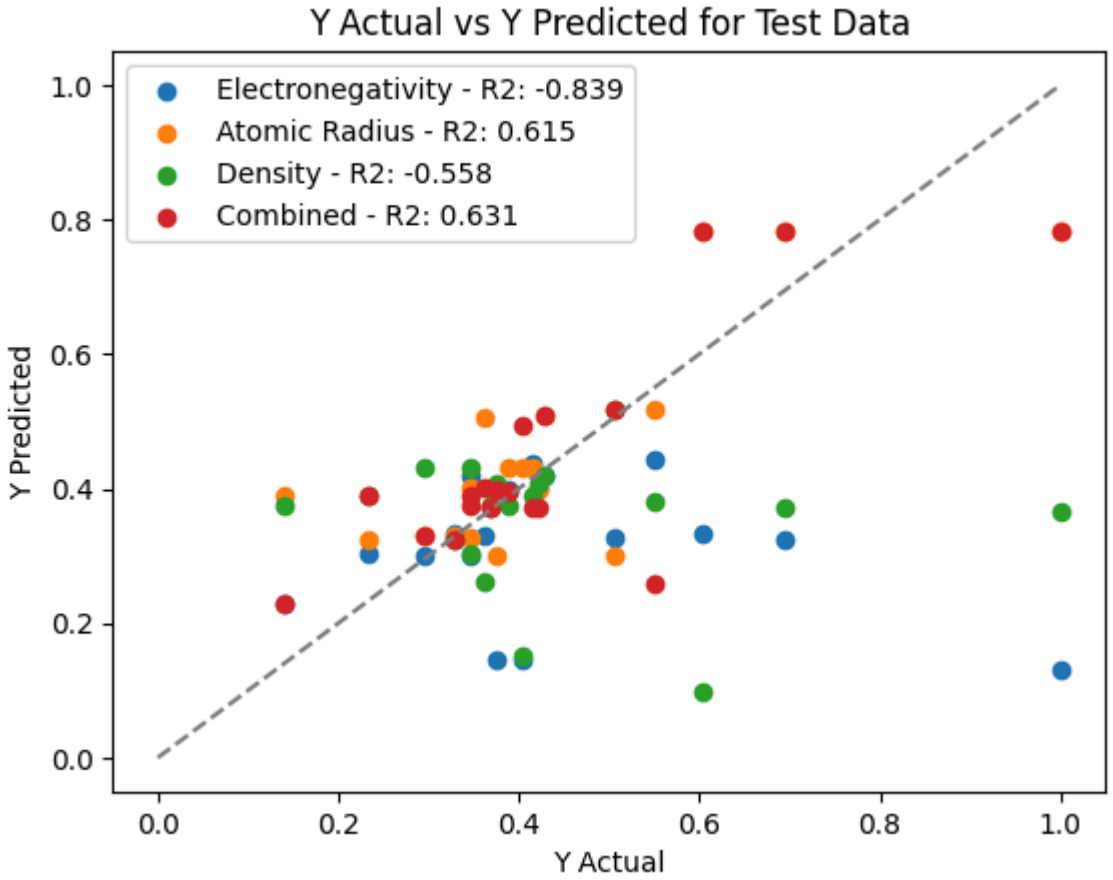
```
model = DecisionTreeRegressor()

for i in range(len(X)):
    X_train, X_test, Y_train, Y_test = train_test_split(
        X[i], Y, test_size=0.20, random_state=96)

    model.fit(X_train,Y_train)

    Y_test_predicted = model.predict(X_test)
    plt.scatter(Y_test,Y_test_predicted, label=(f'{(Plot_Name[i])} - R2: {r2_score(Y_test,Y_test_predicted):.3f}'))
    plt.legend()

plt.plot([Y.min(), Y.max()], [Y.min(), Y.max()], '--', color='gray')
plt.xlabel('Y Actual')
plt.ylabel('Y Predicted')
plt.title('Y Actual vs Y Predicted for Test Data')
plt.show()
```



Random Forest

In [ ]:
```
from sklearn.ensemble import RandomForestRegressor
model = RandomForestRegressor()

for i in range(len(X)):
    X_train, X_test, Y_train, Y_test = train_test_split(
        X[i], Y, test_size=0.20, random_state=96)

    model.fit(X_train,Y_train)
```

```python
    Y_test_predicted = model.predict(X_test)
    plt.scatter(Y_test,Y_test_predicted, label=(f'{(Plot_Name[i])} - R2: {r2_score(Y_test,Y_test_predicted):.3f}'))
    plt.legend()

plt.plot([Y.min(), Y.max()], [Y.min(), Y.max()], '--', color='gray')
plt.xlabel('Y Actual')
plt.ylabel('Y Predicted')
plt.title('Y Actual vs Y Predicted for Test Data')
plt.show()
```

```
c:\Users\manda\AppData\Local\Programs\Python\Python311\Lib\site-packages\sklearn\base.py:1351: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
  return fit_method(estimator, *args, **kwargs)
c:\Users\manda\AppData\Local\Programs\Python\Python311\Lib\site-packages\sklearn\base.py:1351: DataConversionWarning: A column-vector y was passed when a 1d array was expected. Please change the shape of y to (n_samples,), for example using ravel().
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  return fit_method(estimator, *args, **kwargs)
```

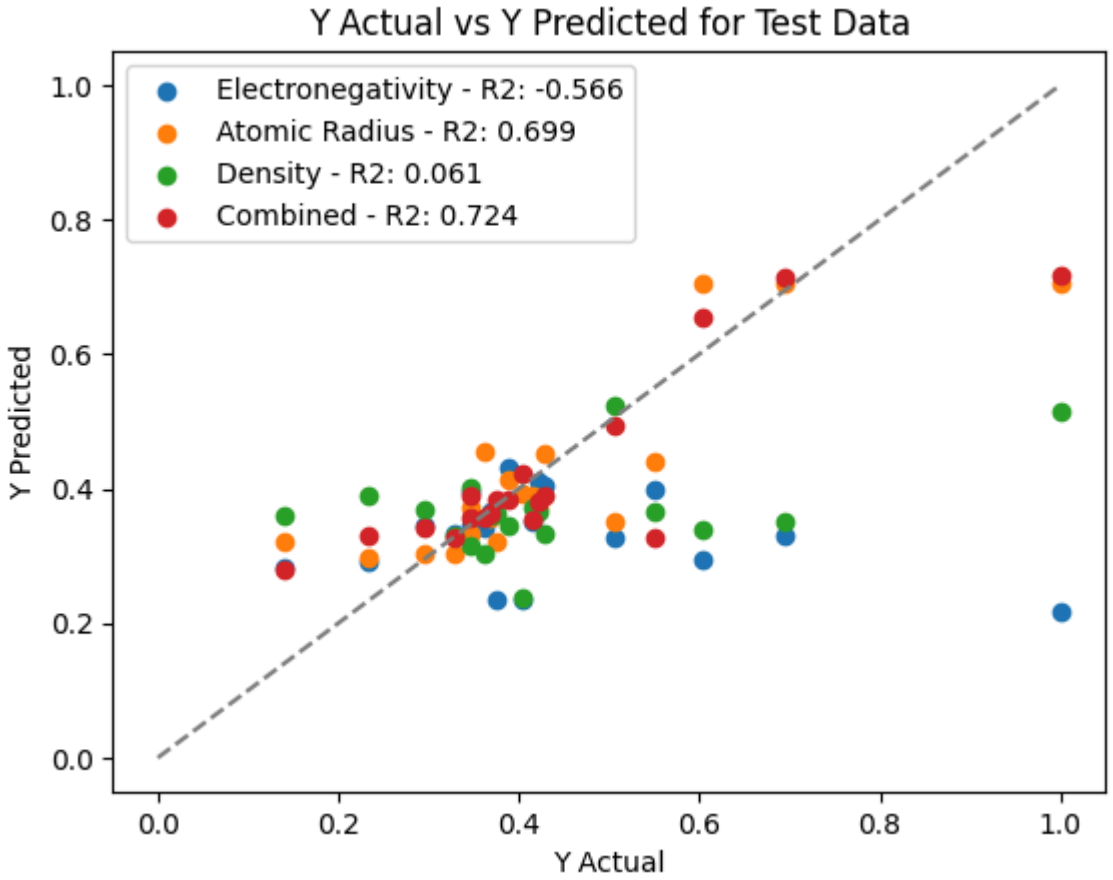
Y Actual vs Y Predicted for Test Data
Electronegativity - R2: -0.566
Atomic Radius - R2: 0.699
Density - R2: 0.061
Combined - R2: 0.724
Y Predicted
Y Actual
0.0
0.2
0.4
0.6
0.8
1.0