pce_prediction

May 17, 2025

[240]:
```
# Machine Learning Analysis: Predicting PCE
# Predicting Power Conversion Efficiency (PCE) of materials based on physical␣
↪and chemical features.
# Goal: Build regression models to estimate PCE from features like thickness,␣
↪band gap,
# electron affinity, doping concentration, and defect density
```

[241]:
```
import pandas as pd
import numpy as np
import seaborn as sns
import matplotlib.pyplot as plt
import numpy as np
from sklearn.linear_model import LinearRegression
from sklearn.ensemble import RandomForestRegressor
from sklearn.model_selection import KFold, cross_val_score, train_test_split
from sklearn.metrics import make_scorer, root_mean_squared_error, r2_score
from functools import partial
from sklearn.inspection import PartialDependenceDisplay
```

[242]:
```
## load the data
df = pd.read_csv("data.csv")
```

[243]:
```
# prepocessing and cleaning
```

[244]:
```
df.head()
```

[244]:
```
   SN thickness          defect band_gap electron_affinity            doping  \
0   1       0.7  10000000000000     1.41              3.555  1000000000000000
1   2       0.7  10000000000000     1.41              3.555            1E+016
2   3       0.7  10000000000000     1.41              3.555            1E+017
3   4       0.7  10000000000000     1.41              3.555            1E+018
4   5       0.7  10000000000000     1.41              3.655  1000000000000000

          pce
0  20.1292728
1  20.2300126
2  20.2786026
```

```
3   20.4586816
4   22.8840414
```

[245]:
```
df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 2163 entries, 0 to 2162
Data columns (total 7 columns):
 #   Column             Non-Null Count  Dtype
---  ------             --------------  -----
 0   SN                 2161 non-null   object
 1   thickness          2161 non-null   object
 2   defect             2161 non-null   object
 3   band_gap           2161 non-null   object
 4   electron_affinity  2161 non-null   object
 5   doping             2161 non-null   object
 6   pce                2161 non-null   object
dtypes: object(7)
memory usage: 118.4+ KB
```

[246]:
```
df = df.apply(pd.to_numeric, errors='coerce')
```

[247]:
```
df.describe()
```

[247]:
```
                SN    thickness        defect     band_gap  electron_affinity  \
count  2160.000000  2160.000000  2.160000e+03  2160.000000        2160.000000
mean    600.500000     0.900000  2.777500e+15     1.510000           3.755000
std     398.087031     0.258259  4.188812e+15     0.081669           0.141454
min       1.000000     0.500000  1.000000e+13     1.410000           3.555000
25%     270.750000     0.700000  7.750000e+13     1.410000           3.655000
50%     540.500000     0.900000  5.500000e+14     1.510000           3.755000
75%     900.250000     1.100000  3.250000e+15     1.610000           3.855000
max    1440.000000     1.300000  1.000000e+16     1.610000           3.955000

             doping          pce
count  2.160000e+03  2160.000000
mean   2.777500e+17    19.194824
std    4.188812e+17     2.438354
min    1.000000e+15    11.703817
25%    7.750000e+15    17.525714
50%    5.500000e+16    19.266821
75%    3.250000e+17    20.908662
max    1.000000e+18    25.317546
```

[248]:
```
df = df.drop(columns=['SN'])
```

[249]:
```
df.thickness
```

[249]:
```
0       0.7
1       0.7
2       0.7
3       0.7
4       0.7
       …
2158    1.3
2159    1.3
2160    1.3
2161    1.3
2162    1.3
Name: thickness, Length: 2163, dtype: float64
```

[250]:
```
df.defect
```

[250]:
```
0       1.000000e+13
1       1.000000e+13
2       1.000000e+13
3       1.000000e+13
4       1.000000e+13
            …
2158    1.000000e+16
2159    1.000000e+16
2160    1.000000e+16
2161    1.000000e+16
2162    1.000000e+16
Name: defect, Length: 2163, dtype: float64
```

[251]:
```
df.band_gap
```

[251]:
```
0       1.41
1       1.41
2       1.41
3       1.41
4       1.41
        …
2158    1.61
2159    1.61
2160    1.61
2161    1.61
2162    1.61
Name: band_gap, Length: 2163, dtype: float64
```

[252]:
```
df.electron_affinity
```

[252]:
```
0       3.555
1       3.555
```

```
2       3.555
3       3.555
4       3.655
        …
2158    3.855
2159    3.955
2160    3.955
2161    3.955
2162    3.955
Name: electron_affinity, Length: 2163, dtype: float64
```

[253]:
```
df.doping
```

[253]:
```
0       1.000000e+15
1       1.000000e+16
2       1.000000e+17
3       1.000000e+18
4       1.000000e+15
            …
2158    1.000000e+18
2159    1.000000e+15
2160    1.000000e+16
2161    1.000000e+17
2162    1.000000e+18
Name: doping, Length: 2163, dtype: float64
```

[254]:
```
df.pce
```

[254]:
```
0       20.129273
1       20.230013
2       20.278603
3       20.458682
4       22.884041
          …
2158    21.293994
2159    18.527718
2160    19.421001
2161    20.305046
2162    21.390849
Name: pce, Length: 2163, dtype: float64
```

[255]:
```
df.isna().sum()
```

[255]:
```
thickness            3
defect               3
band_gap             3
electron_affinity    3
```

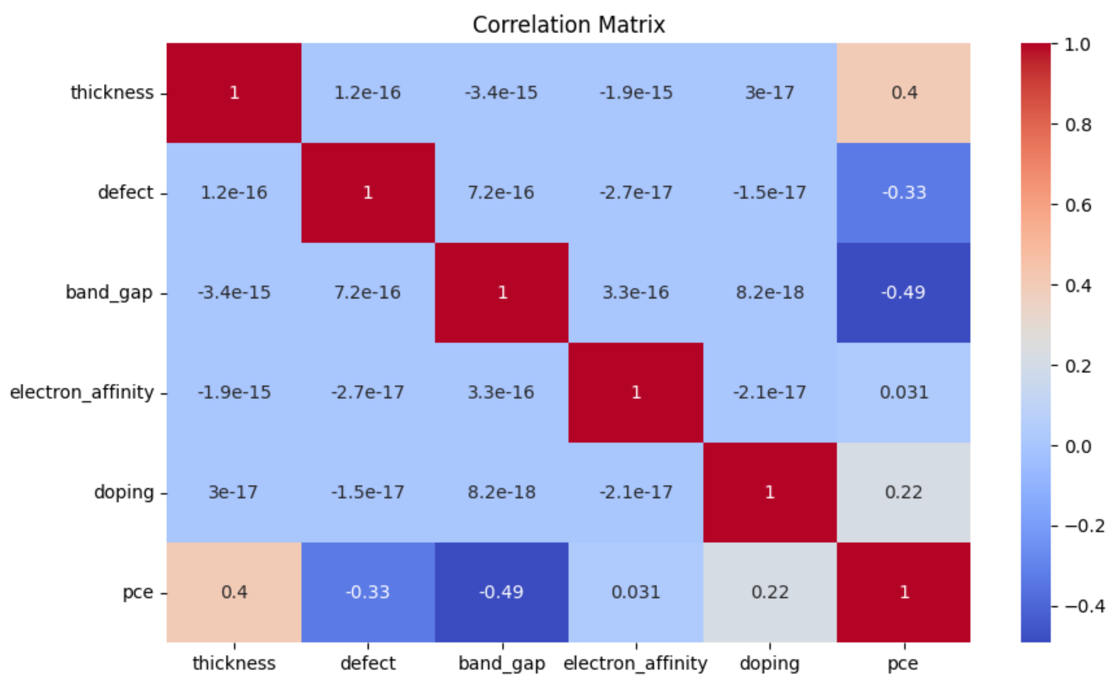
```
doping              3
pce                 3
dtype: int64
```

[256]:
```
df = df.dropna()
df.isna().sum()
```

[256]:
```
thickness           0
defect              0
band_gap            0
electron_affinity   0
doping              0
pce                 0
dtype: int64
```

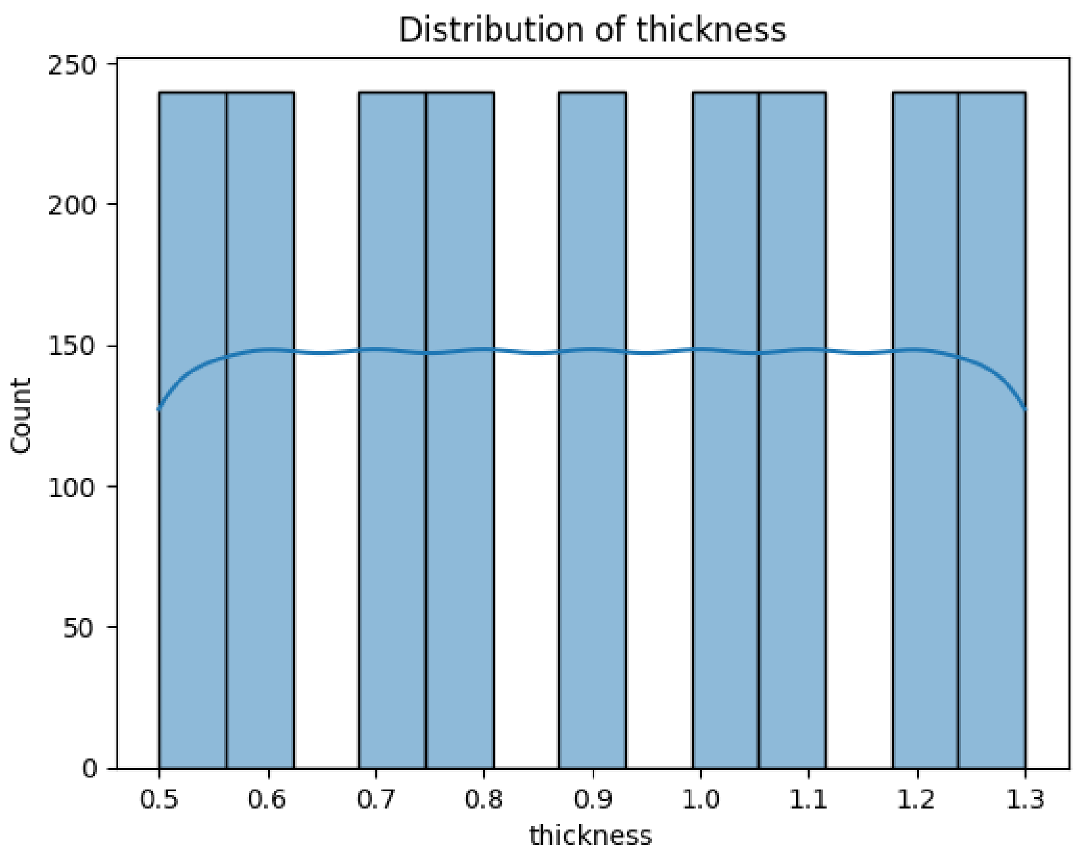
[257]:
```
# EDA - Exploratory Data Analysis
```

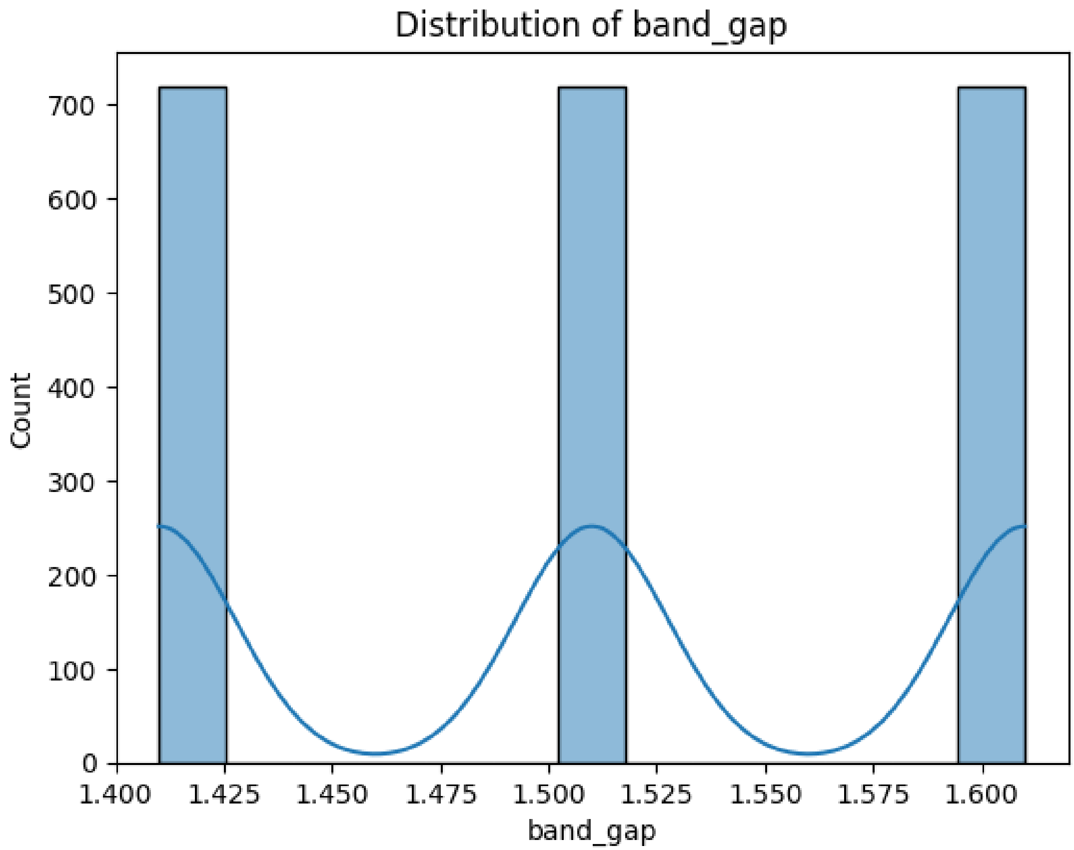
[258]:
```
## show correlation matrix for depicting relation between features
plt.figure(figsize=(10, 6))
sns.heatmap(df.corr(numeric_only=True), annot=True, cmap='coolwarm')
plt.title("Correlation Matrix")
plt.savefig("plots/correlation-matrix-1.png")
plt.show()
```

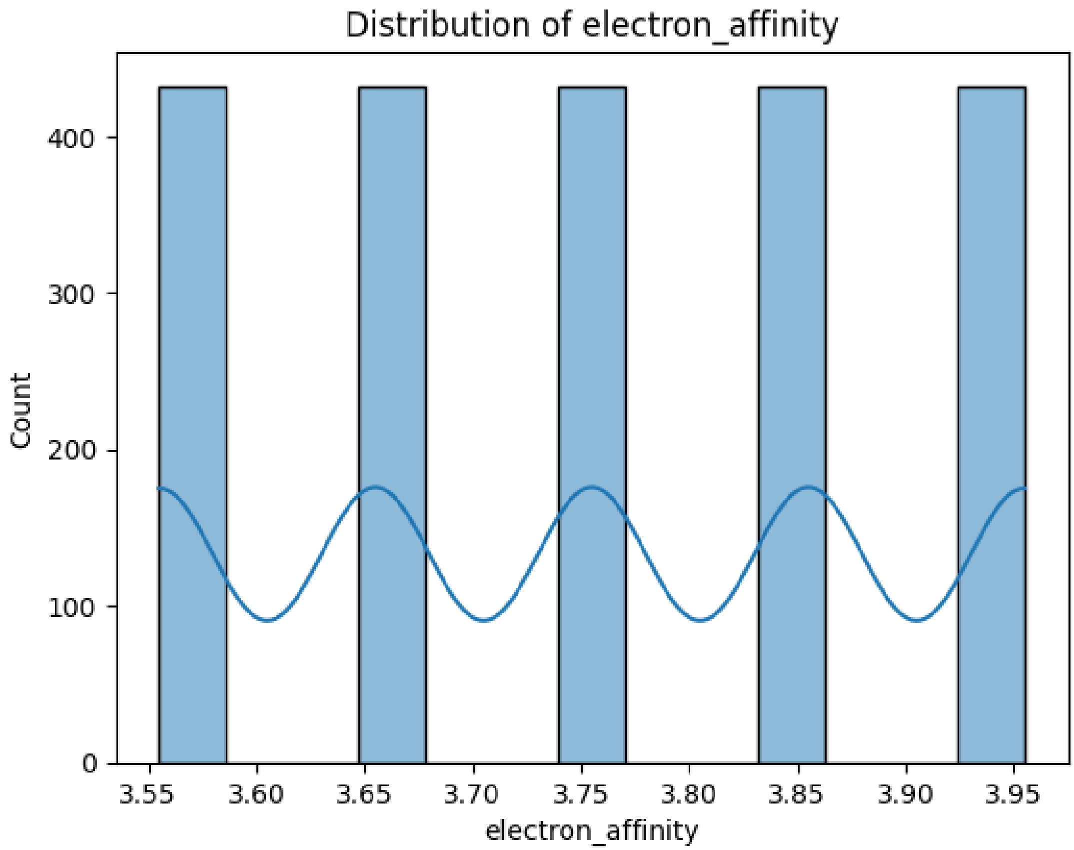


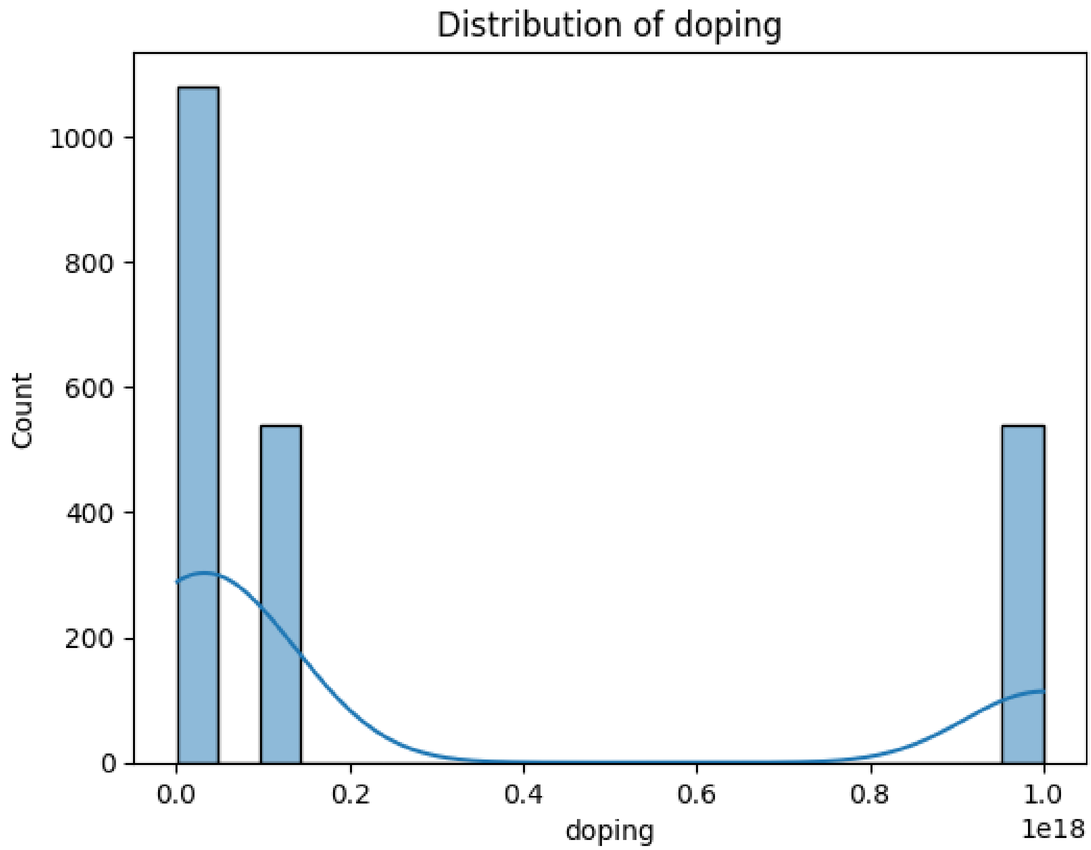
[259]:

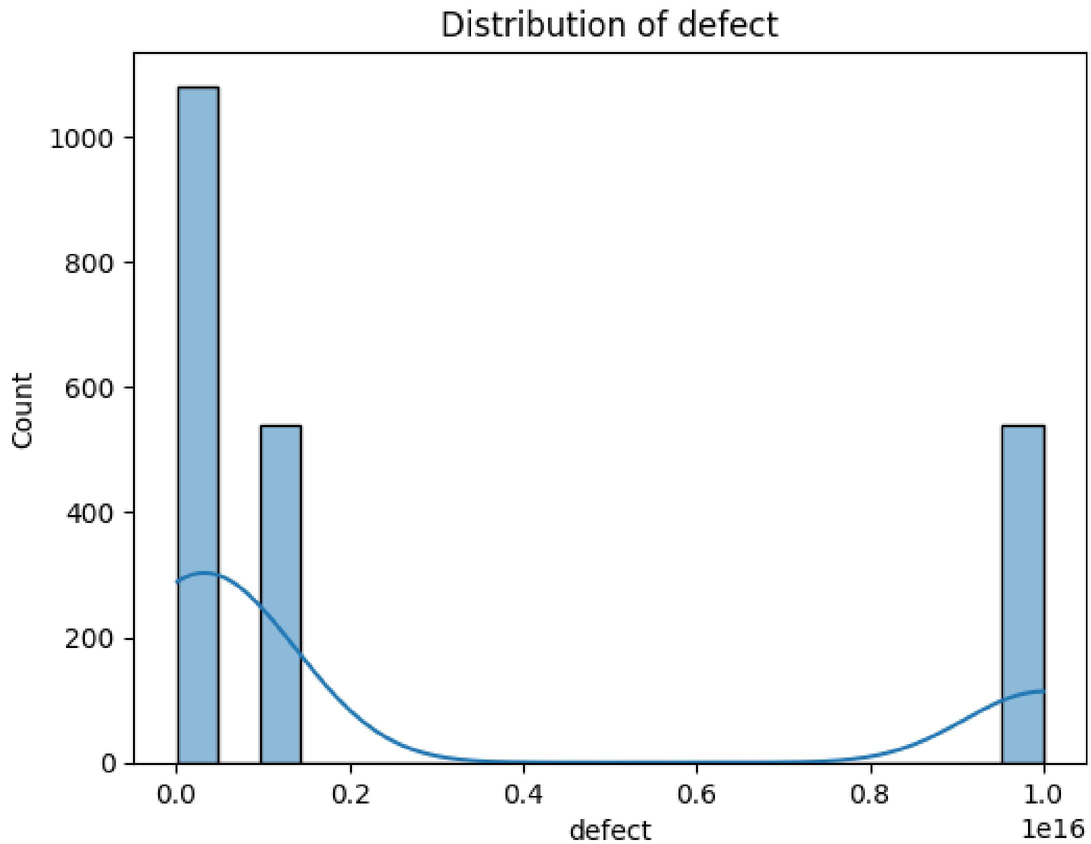
```python
## depicts distribution of the features
for col in ['thickness', 'band_gap','electron_affinity', 'doping', 'defect',␣
↪'pce']:
    sns.histplot(df[col], kde=True)
    plt.title(f'Distribution of {col}')
    plt.savefig("plots/distribution-" + col + ".png")
    plt.show()
```

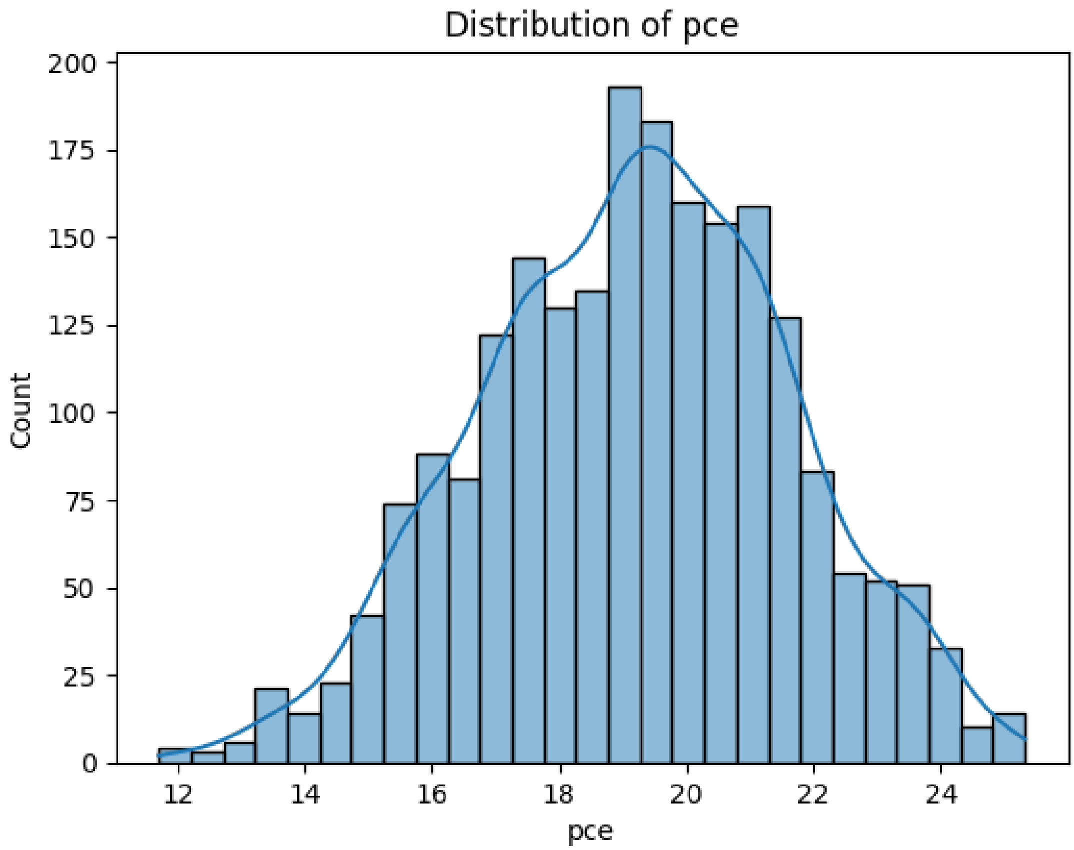



Distribution of band_gap
Count
band_gap
0
100
200
300
400
500
600
700
1.400
1.425
1.450
1.475
1.500
1.525
1.550
1.575
1.600


Distribution of electron_affinity
Count
400
300
200
100
0
3.55
3.60
3.65
3.70
3.75
3.80
3.85
3.90
3.95
electron_affinity

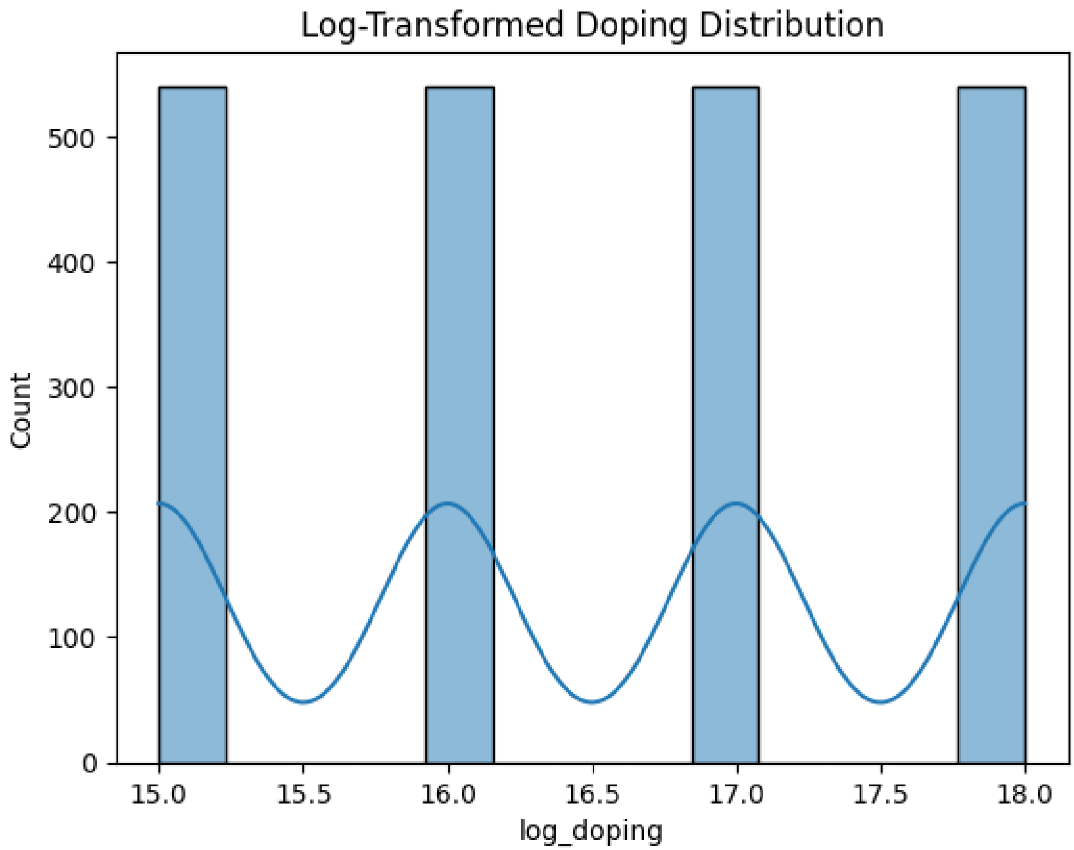

Distribution of doping
Count
1000
800
600
400
200
0
0.0
0.2
0.4
0.6
0.8
1.0
1e18
doping

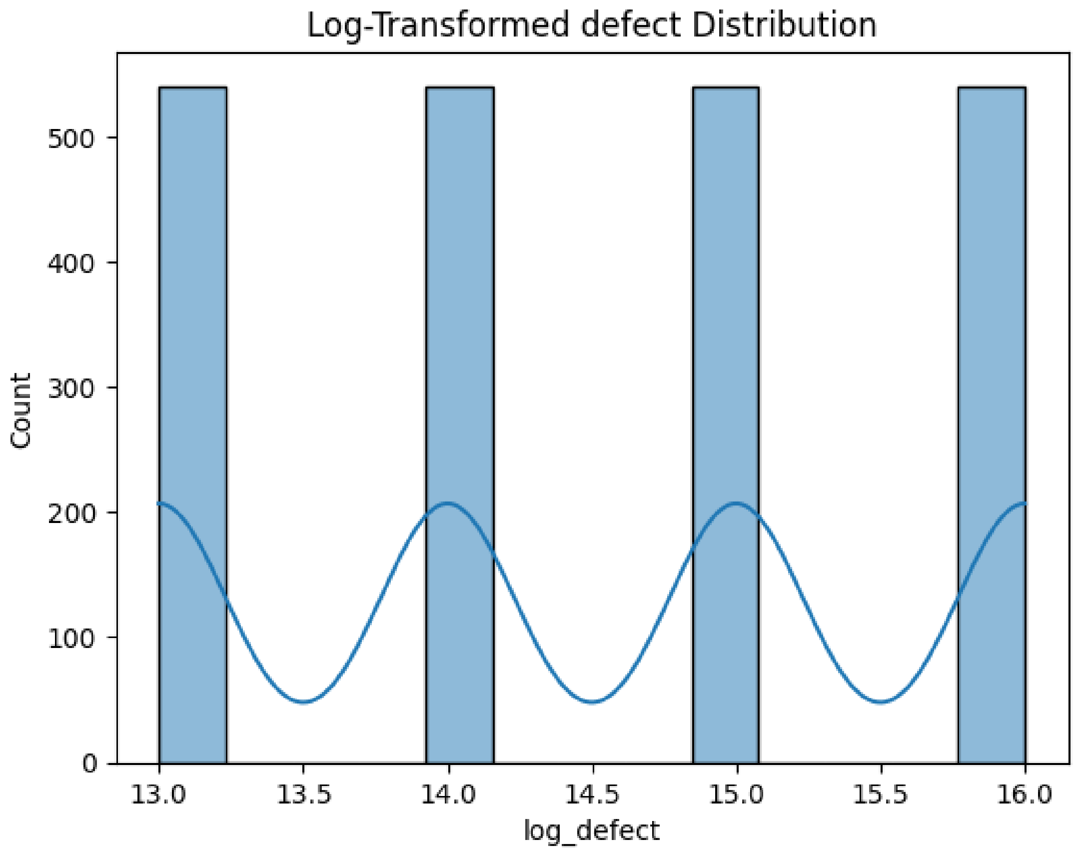

Distribution of defect
Count
1000
800
600
400
200
0
0.0
0.2
0.4
0.6
0.8
1.0
1e16
defect



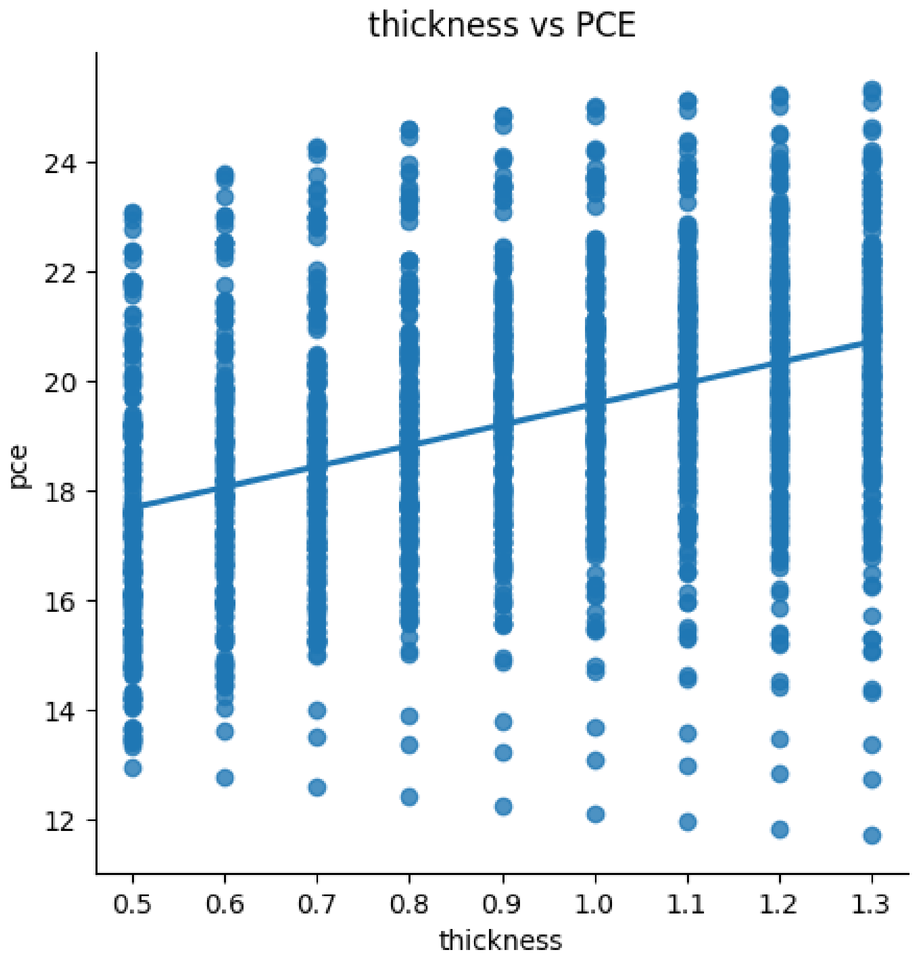
[260]:
```
## create new features log_doping and log_defect to search for more normalize␣
↪features
df['log_doping'] = np.log10(df['doping'])
df['log_defect'] = np.log10(df['defect'])
```

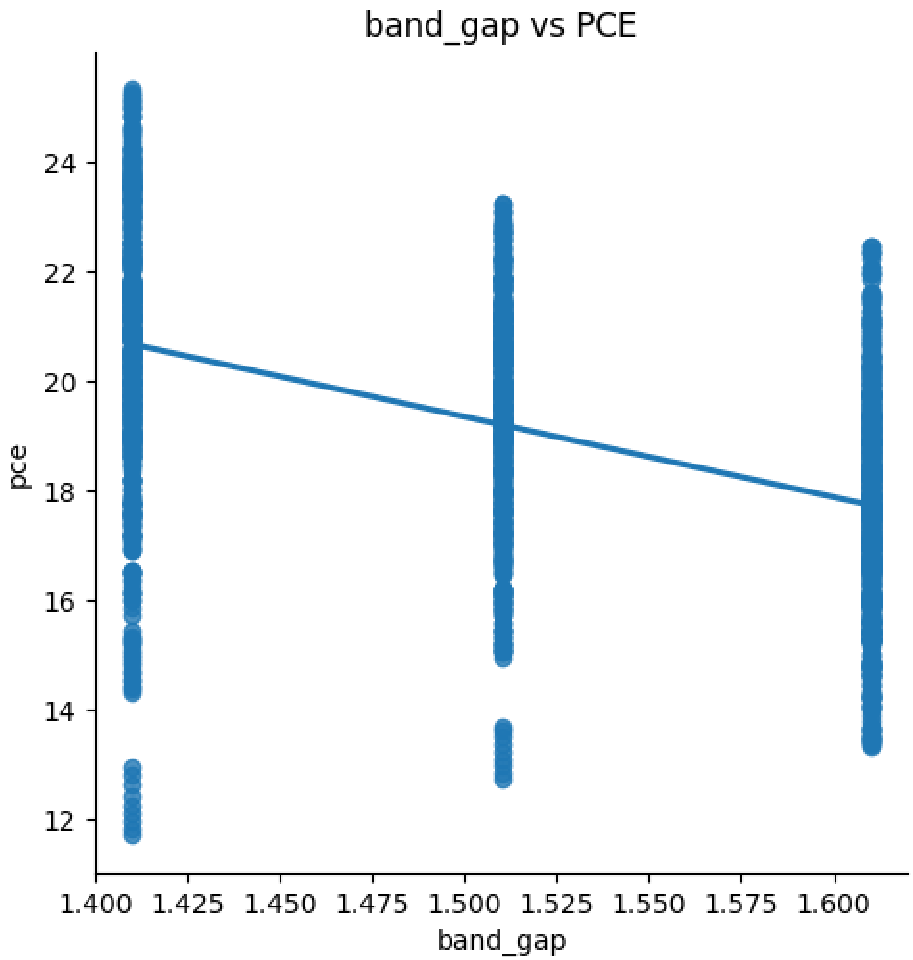
[261]:
```
## depicts distribution of log_doping, log_defect
sns.histplot(df['log_doping'], kde=True)
plt.title("Log-Transformed Doping Distribution")
plt.savefig("plots/distribution-log-doping.png")
plt.show()

sns.histplot(df['log_defect'], kde=True)
plt.title("Log-Transformed defect Distribution")
plt.savefig("plots/distribution-log-defect.png")
plt.show()
```

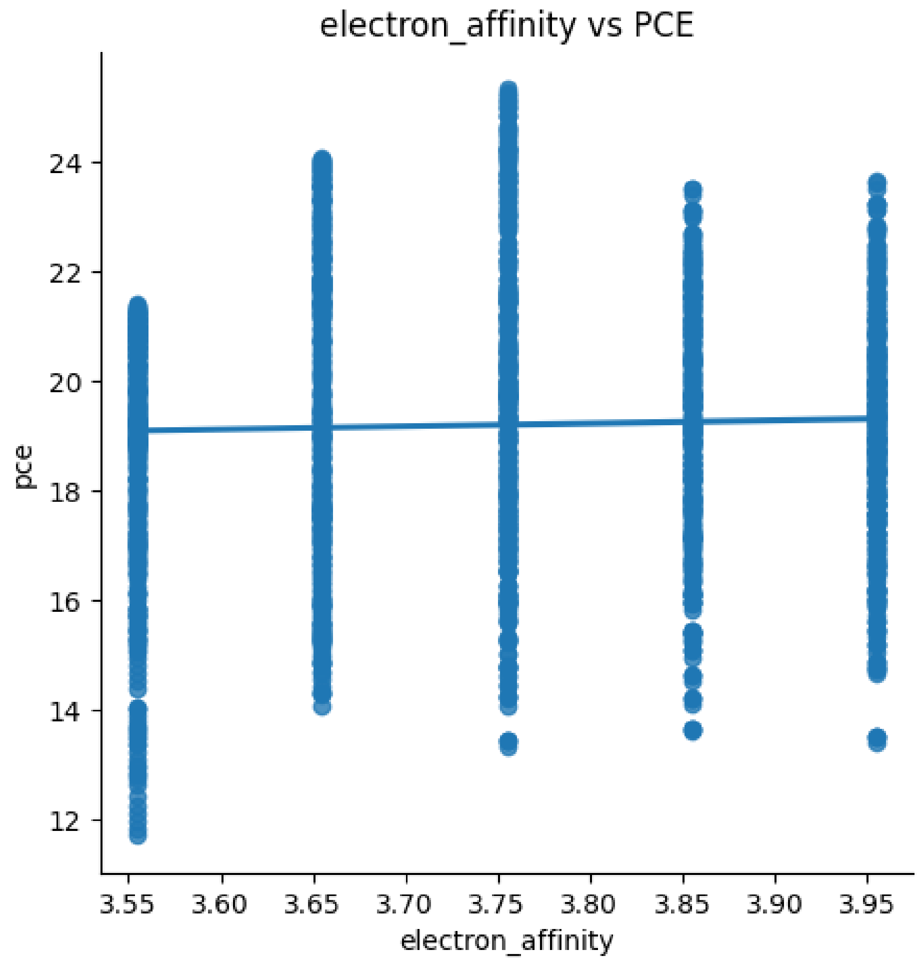

Log-Transformed Doping Distribution
Count
0
100
200
300
400
500
15.0
15.5
16.0
16.5
17.0
17.5
18.0
log_doping

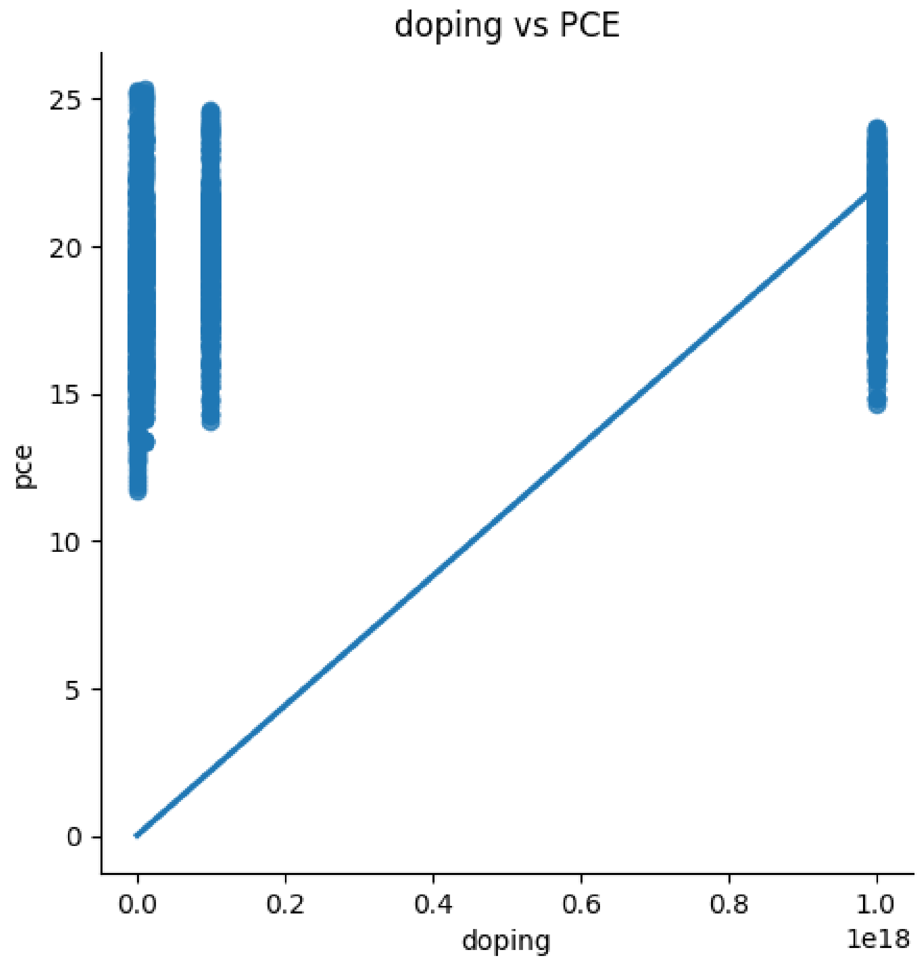


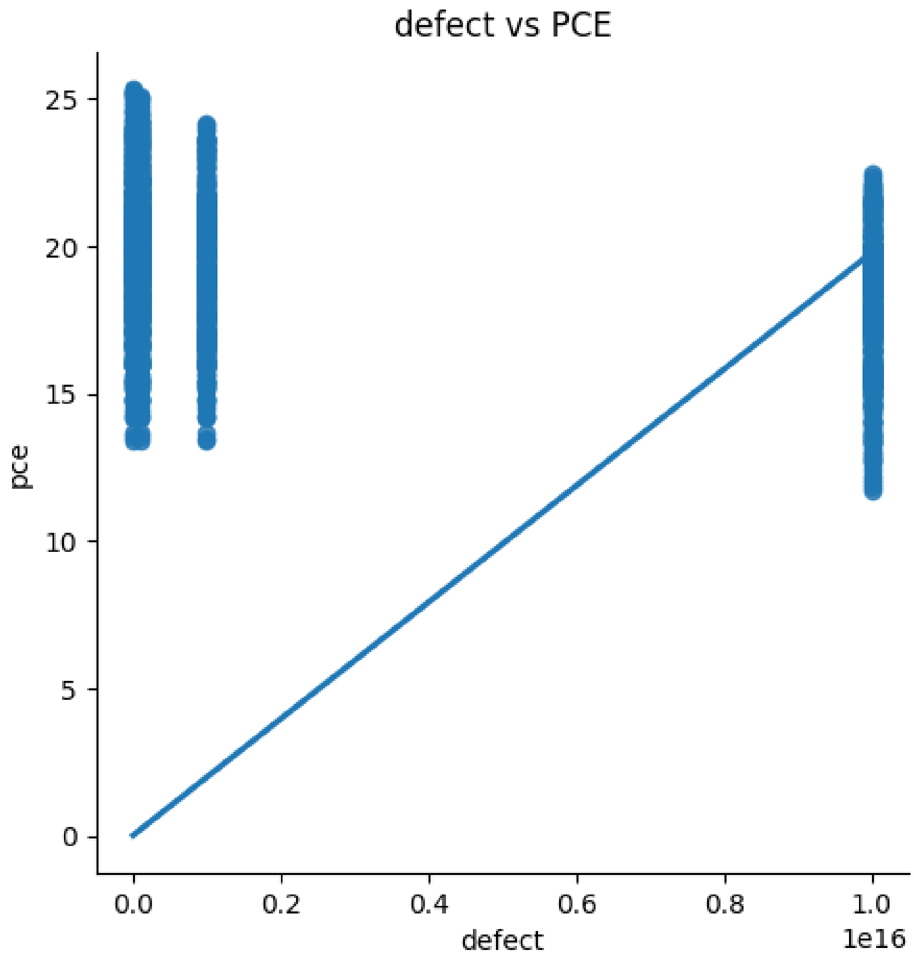
[262]:
```
## depicts relation of each features with pce
for feature in ['thickness', 'band_gap', 'electron_affinity', 'doping',␣
↪'defect', 'log_doping', 'log_defect']:
    sns.lmplot(x=feature, y='pce', data=df, ci=None)
    plt.title(f'{feature} vs PCE')
    plt.savefig("plots/pce-vs" + feature + ".png")
    plt.show()
```

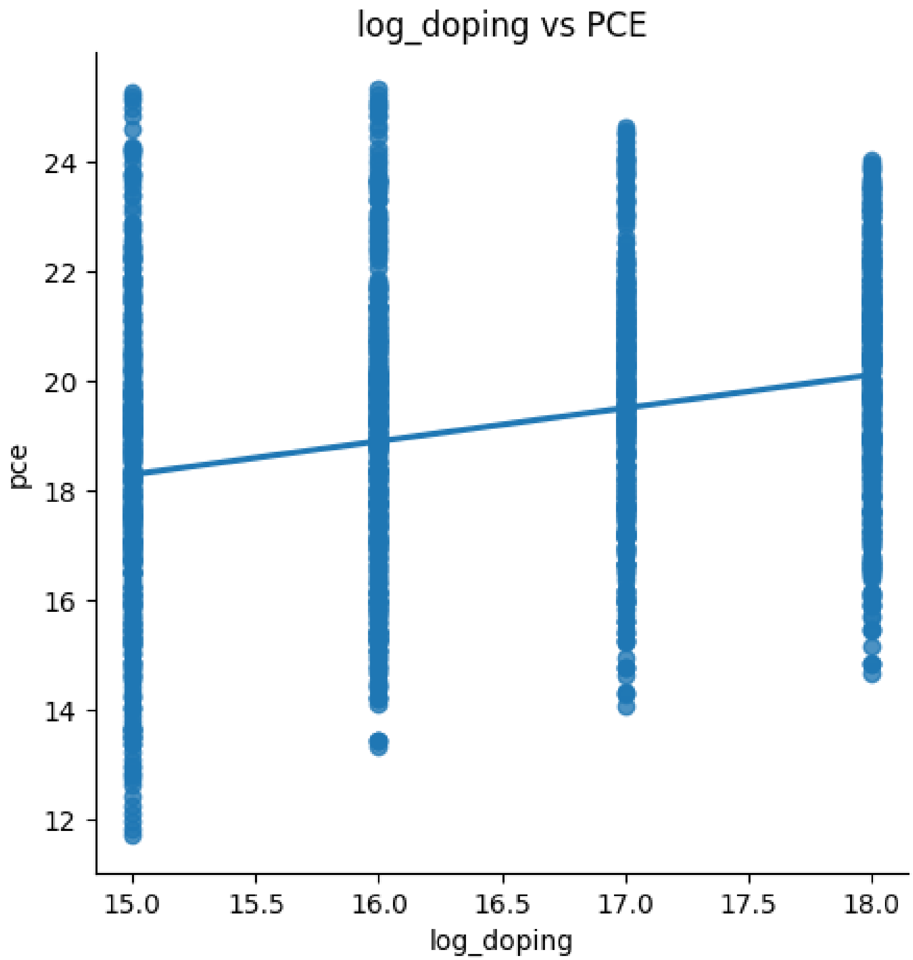

thickness vs PCE
pce
thickness
24
22
20
18
16
14
12
0.5
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3

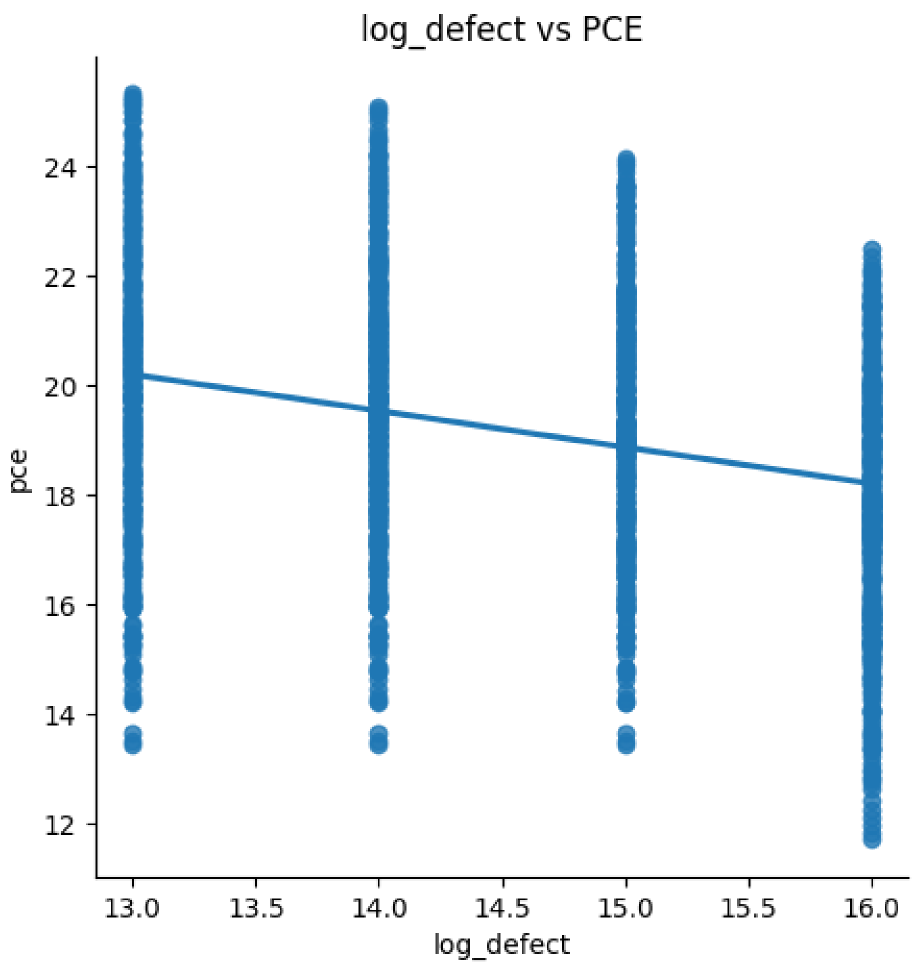

band_gap vs PCE
pce
band_gap
24
22
20
18
16
14
12
1.400
1.425
1.450
1.475
1.500
1.525
1.550
1.575
1.600


electron_affinity vs PCE
pce
24
22
20
18
16
14
12
3.55
3.60
3.65
3.70
3.75
3.80
3.85
3.90
3.95
electron_affinity

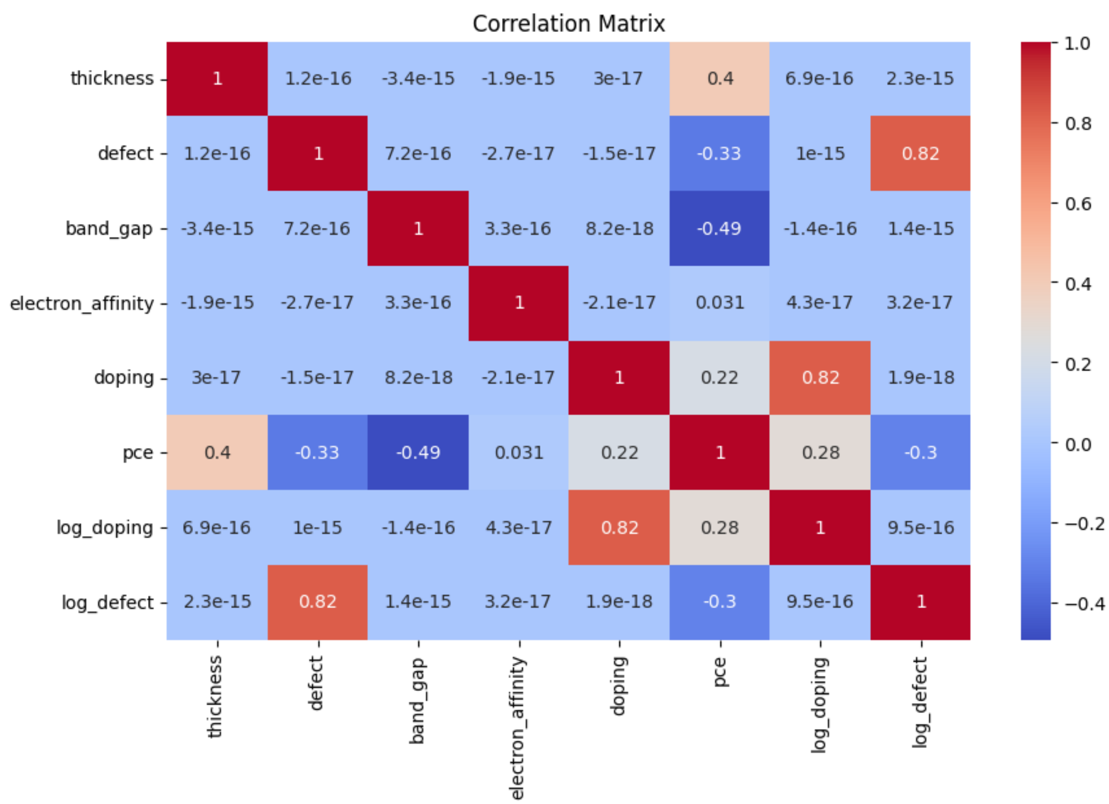

doping vs PCE
pce
doping
1e18
25
20
15
10
5
0
0.0
0.2
0.4
0.6
0.8
1.0


defect vs PCE
pce
25
20
15
10
5
0
0.0
0.2
0.4
0.6
0.8
1.0
1e16
defect


log_doping vs PCE
24
22
20
18
16
14
12
pce
15.0
15.5
16.0
16.5
17.0
17.5
18.0
log_doping



[263]:
```
## corelation matrix with log_doping and log_defect
plt.figure(figsize=(10, 6))
sns.heatmap(df.corr(numeric_only=True), annot=True, cmap='coolwarm')
plt.title("Correlation Matrix")
plt.savefig("plots/correlation-matrix-2.png")
plt.show()
```



[264]:
```
# Modelling
```

[265]:
```
### define Features and target
X = df[['thickness', 'band_gap', 'electron_affinity', 'doping', 'defect']]
y = df['pce']
```

[266]:
```
### test train split
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2,␣
↪random_state=42, shuffle=True)
```

[267]:
```
### define regression model
random_forest_model = RandomForestRegressor(n_estimators=200, random_state=42)
```

[268]:
```
## K-Fold cross-validator
kf = KFold(n_splits=5, shuffle=True, random_state=42)

# Scorers
rmse_scorer = make_scorer(root_mean_squared_error)  # RMSE

random_forest_model_rmse = cross_val_score(random_forest_model, X_train,␣
↪y_train, cv=kf, scoring=rmse_scorer)
```

```
random_forest_model_r2 = cross_val_score(random_forest_model, X_train, y_train,␣
↪cv=kf, scoring='r2')


print("\nRandom Forest Regression:")
print("  RMSE (per fold):", random_forest_model_rmse)
print("  Mean RMSE:", np.mean(random_forest_model_rmse))
print("  R2 (per fold):", random_forest_model_r2)
print("  Mean R2:", np.mean(random_forest_model_r2))
```

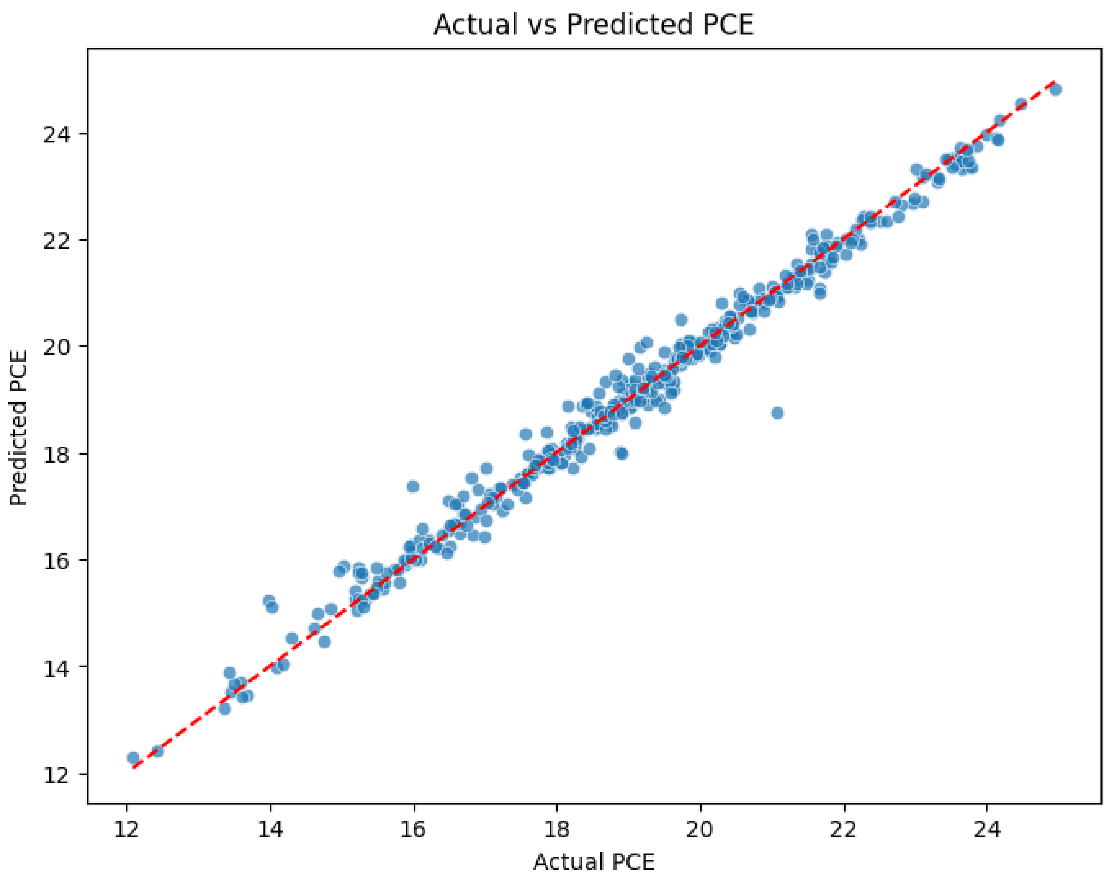
```
Random Forest Regression:
  RMSE (per fold): [0.28283345 0.32007955 0.35847553 0.32847316 0.27780387]
  Mean RMSE: 0.3135331128806485
  R2 (per fold): [0.98603596 0.98222863 0.98047921 0.97990717 0.98775423]
  Mean R2: 0.9832810406863851
```

[269]:
```
### Fit on full training data and evaluate on test set
random_forest_model.fit(X_train, y_train)
test_score = random_forest_model.score(X_test, y_test)
print("R2 score (on holdout test set):", test_score)
```

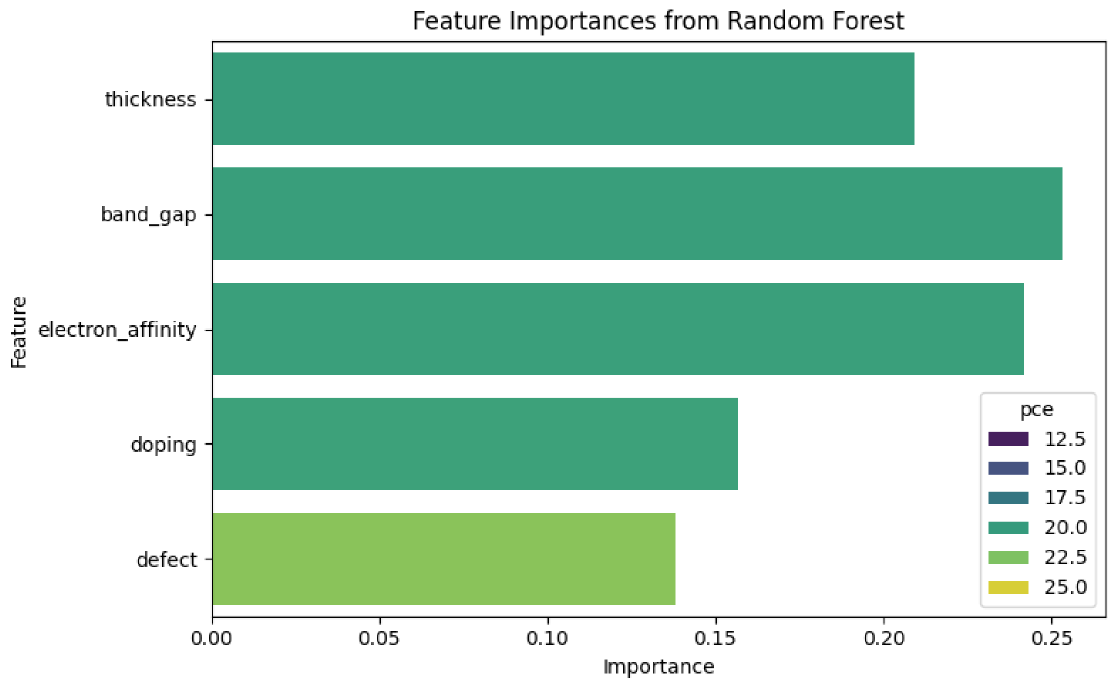
```
R2 score (on holdout test set): 0.9852542718016152
```

[270]:
```
## plot how the model works on unseen data
### predict on the holded test data
y_pred = random_forest_model.predict(X_test)
```

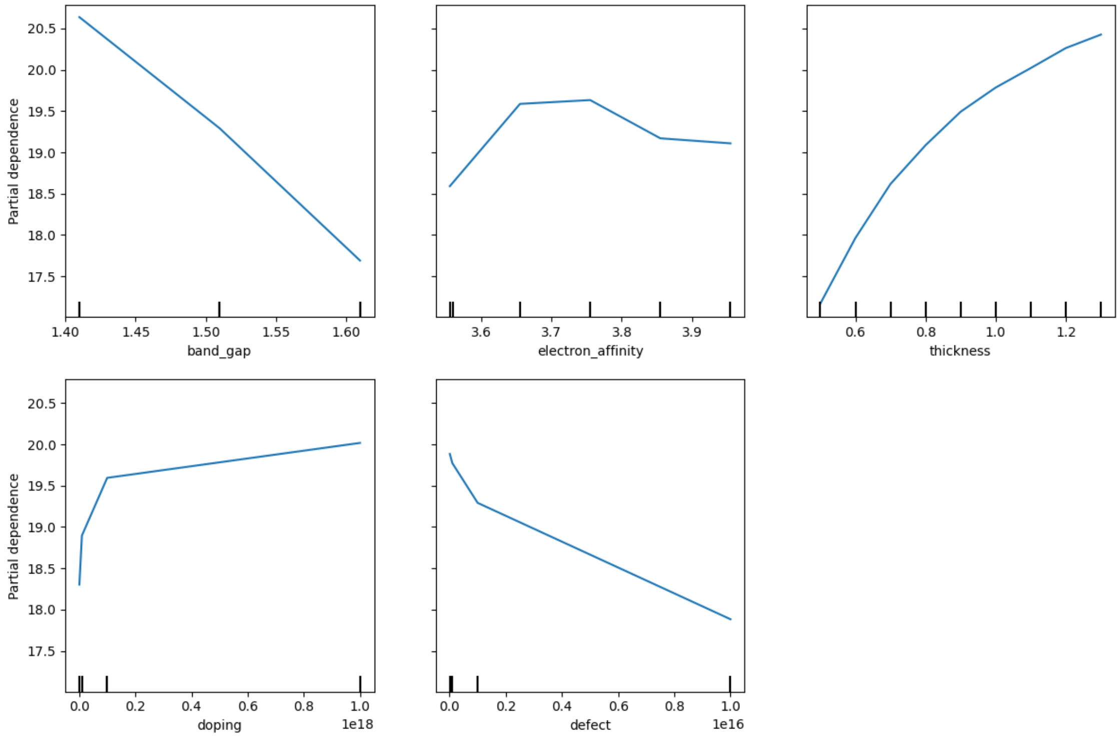
[271]:
```
### plot actual value vs predicted value
plt.figure(figsize=(8, 6))
sns.scatterplot(x=y_test, y=y_pred, alpha=0.7)
plt.plot([y_test.min(), y_test.max()], [y_test.min(), y_test.max()], 'r--')  #␣
↪Diagonal line

plt.xlabel('Actual PCE')
plt.ylabel('Predicted PCE')
plt.title('Actual vs Predicted PCE')
plt.savefig("plots/actual-vs-predicted.png")
plt.show()
```



[272]:
```
## inspection
### feature imortance - the effect of the features on the predicted value
importances = random_forest_model.feature_importances_
features = X_train.columns
importance_df = pd.DataFrame({'Feature': features, 'Importance': importances})
importance_df = importance_df.sort_values(by='Importance', ascending=False)

plt.figure(figsize=(8, 5))
sns.barplot(x='Importance', y='Feature', data=importance_df, palette='viridis',␣
 ↪hue=y)
plt.title('Feature Importances from Random Forest')
plt.tight_layout()
plt.savefig("plots/feature-importance.png")
plt.show()
```



[273]:
```
## partial dependece of the fetaures
### other features are kept constant
top_features = importance_df['Feature']
fig, ax = plt.subplots(figsize=(12, 8))  # Bigger figure size

PartialDependenceDisplay.from_estimator(random_forest_model, X_train,␣
↪top_features, kind="average", grid_resolution=50, ax=ax)
plt.tight_layout()
plt.savefig("plots/partial-dependence.png")
plt.show()
```



[274]:
```python
## train model on full data for the final model
random_forest_model.fit(X,y)

### predict on new data
new_data = pd.DataFrame([{
    'thickness': 0.7,
    'band_gap': 1.41,
    'electron_affinity': 3.555,
    'defect': 1e13,
    'doping': 1e16,
}])
new_data = new_data[X.columns]

predicted_value = random_forest_model.predict(new_data)
print("The predicted PCE: ", predicted_value)
```

```
The predicted PCE:  [20.16633281]
```

[275]:
```python
# Summarize findings:
# Random Forest effectively models nonlinear relationships in data
# Log transform optional depending on model choice
```