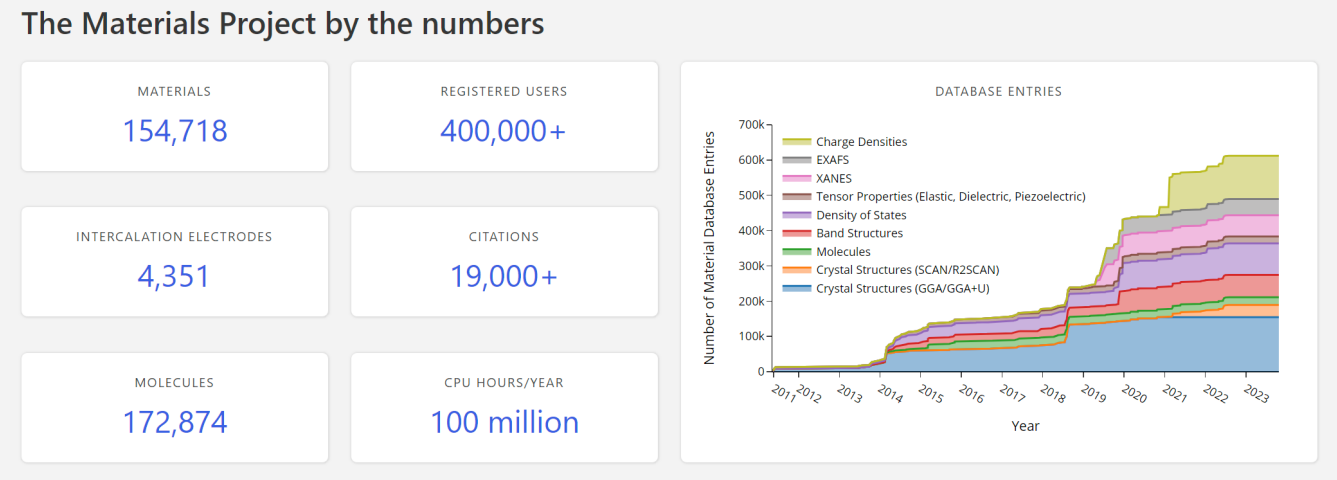
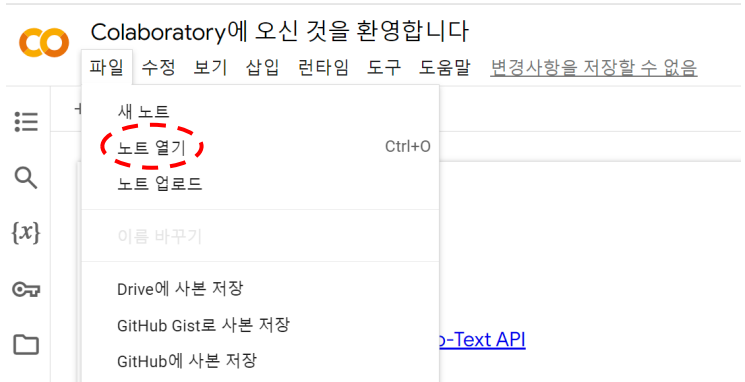
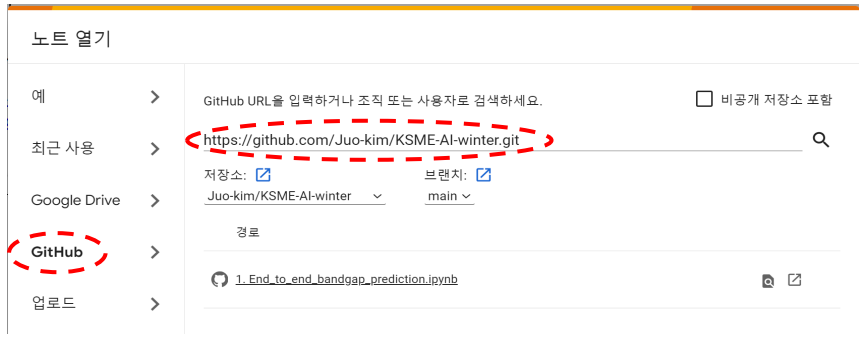
실습 자료 안내



1. Colab 접속 (https://colab.google/)
2. 파일 ➔ 노트 열기 ➔ GitHub ➔ URL 검색





- 15만여개 Inorganic 물질에 대한 DFT 계산 정보를 포함하고 있는 Materials Project 데이터 베이스 활용
- 물질의 전자 상태를 나타내는 값인 Bandgap 예측하는 모델 생성

URL : https://github.com/Juo-kim/KSME-AI-winter.git

KSME-AI-winter

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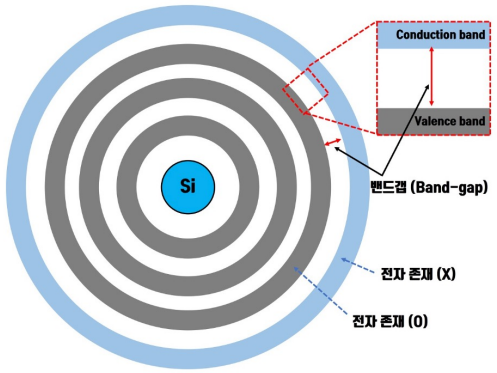
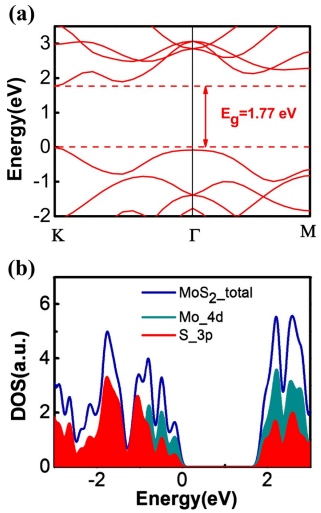
Bandgap?

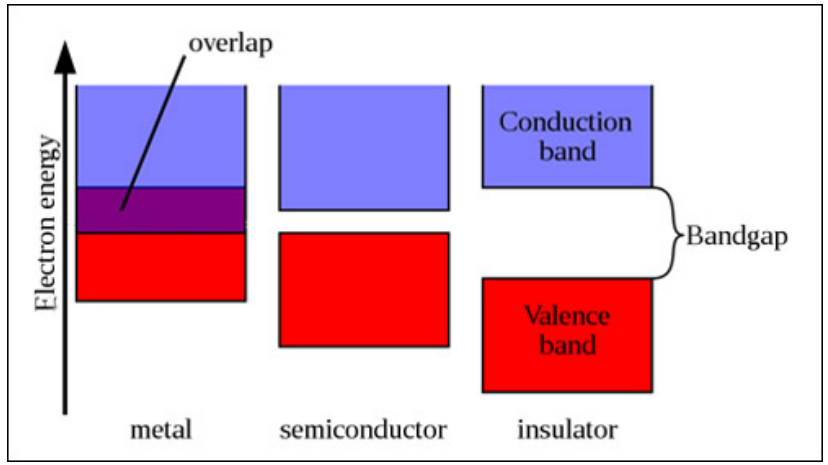
- Energy gap : 전자가 존재하고 있는 가장 높은 에너지 레벨 (Valence Band) 부터 전자가 존재하지 않는 가장 낮은 에너지레벨 (Conduction Band) 사이의 에너지 준위
- 물질이 외부에서 충분한 에너지를 공급받게 된다면, Valence band에 위치한 전자가 Conduction Band로 뛰어넘는 것이 가능함
- Bandgap의 크기에 따라 물질의 전기적 성질을 확인할 수 있음
- Metal = 0 eV, 0 eV < Semiconductor < 4 eV, Insulator ≥ 4 eV
- 전기적 성질을 알아보기 위해서 매우 중요하지만, Bandgap 계산을 위해 필요한 계산적, 실험적 cost가 큼



https://j-science.tistory.com/11



DOI: 10.1186/1556-276X-9-676

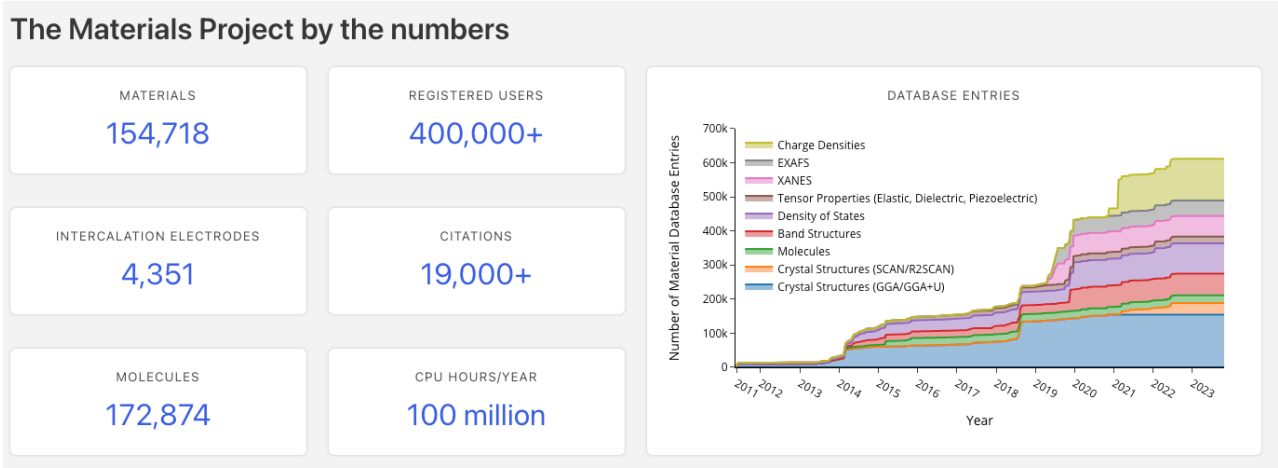


http://solarcellcentral.com/junction_page.html

Materials Project

- Open source Inorganic database 중 하나
- 154,718개의 Inorganic 물질에 대한 DFT 계산 기반의 물성 포함
- Bandgap, Energy above hull, Space group number, Crystal structure 등 많은 계산 결과

➔ Materials Project database로 bandgap을 예측할 수 있는 regression model을 만드는 것이 실습의 목표



Chemical Descriptor

Meaning of chemical descriptors (CDs)	Number of attributes		Attributes
Stoichiometric attributes	6		Ncomp, Comp_L2Norm, Comp_L3Norm, Comp_L5Norm, Comp_L7Norm, Comp_L10Norm
Elemental-property-based attributes	132	Mean (22)	Atomic Number, MendeleevNumber, AtomicWeight, MeltingT, Column, Row, CovalentRadius, Electronegativity, NsValence, NpValence, NdValence, NfValence, NValance, NsUnfilled, NpUnfilled, NdUnfilled, NfUnfilled, NUnfilled, GSvolume_pa, GSbandgap, GSmagmom, SpaceGroupNumber
		Range (22)	
		Dev (22)	
		Max (22)	
		Min (22)	
		Most (22)	
Valance orbital occupation attributes	4		frac_sValence, frac_pValence, frac_dValence, frac_fValence
Ionic compound attributes	3		CanFormIonic, MaxIonicChar, MeanIonicChar

Take a quick look at the Data structure

```
MP_bandgap.head()
```

	Index	Formula	mp-id	bandgap	nsites	spacegroup_number	NComp	Comp_L2Norm	Comp_L3Norm	Comp_L5Norm	...	max_SpaceGroupNumber	min_SpaceGroupNumber	most_SpaceGroupNumber	frac_sValence	frac_pValence	frac_dValence	frac_fValence	CanFormIonic	MaxIonicChar	MeanIonicChar
0	0	LiCaPb	mp-20998	0.0000	9	187	3	0.577350	0.480750	0.415244	...	229	225	226.333333	0.161290	0.064516	0.322581	0.451613	0	0.365948	0.160765
1	1	Li7Mn4CoO12	mp-1175256	0.7477	24	1	4	0.603807	0.536606	0.506969	...	229	12	12.000000	0.353448	0.413793	0.232759	0.000000	0	0.779730	0.357256
2	2	K2CuF4	mp-2865	0.0000	28	142	3	0.654654	0.597048	0.575065	...	229	15	15.000000	0.268293	0.487805	0.243902	0.000000	1	0.917619	0.428188
3	3	Li2Mn3Cr3O12	mp-850956	0.0927	20	10	4	0.644205	0.607092	0.600250	...	229	12	12.000000	0.309735	0.424779	0.265487	0.000000	0	0.779730	0.304103
4	4	Fe1B4	mp-1079437	0.0000	10	58	2	0.824621	0.804145	0.800156	...	229	166	166.000000	0.500000	0.200000	0.300000	0.000000	0	0.010964	0.003509

5 rows × 151 columns

Properties from Materials Project

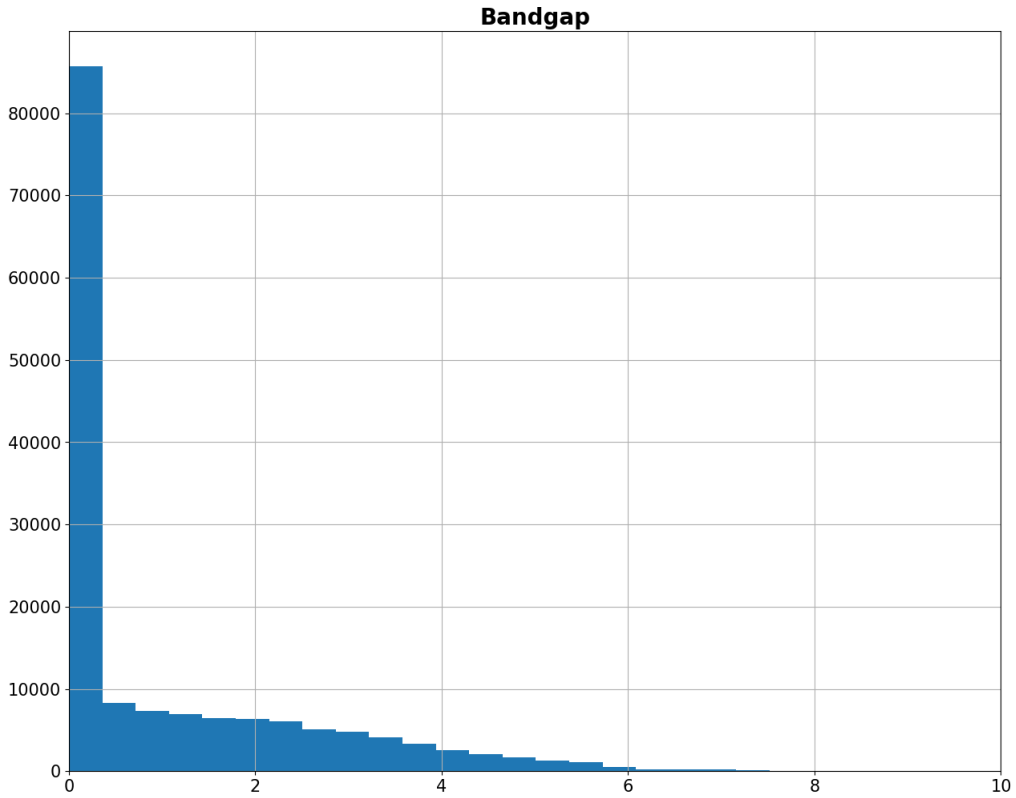
features created by Chemical Descriptor

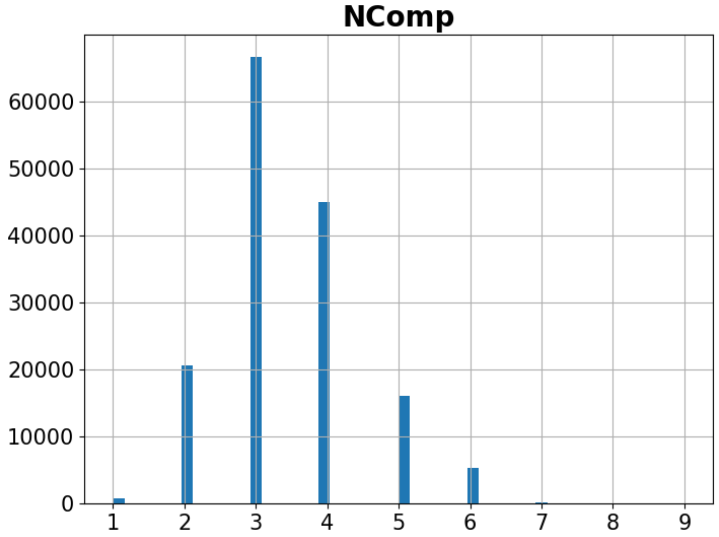
```
MP_bandgap.describe()
```

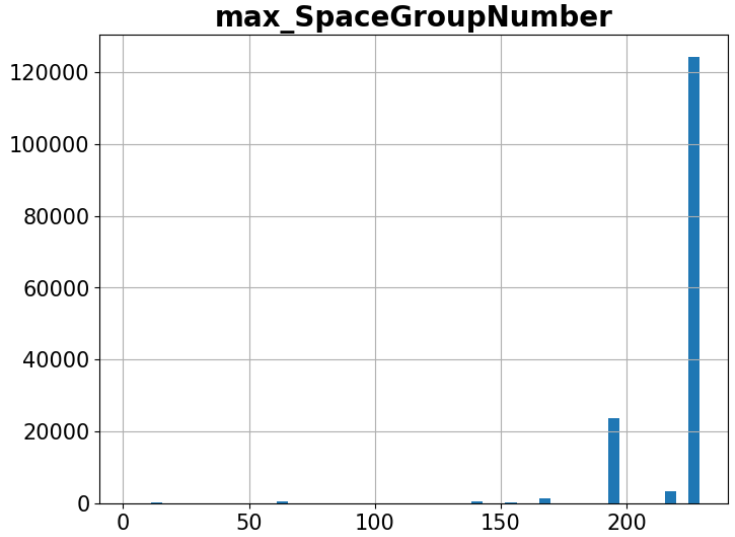
	Index	bandgap	nsites	spacegroup_number	NComp	Comp_L2Norm	Comp_L3Norm	Comp_L5Norm	Comp_L7Norm	Comp_L10Norm	...	max_SpaceGroupNumber	min_SpaceGroupNumber	most_SpaceGroupNumber	frac_sValence	frac_pValence	frac_dValence	frac_fValence	CanFormIonic	MaxIonicChar	MeanIonicChar
count	154718.000000	154718.000000	154718.000000	154718.00000	154718.000000	154718.000000	154718.000000	154718.000000	154718.000000	154718.000000	...	154718.000000	154718.000000	154718.000000	154718.000000	154718.000000	154718.000000	154718.000000	154718.000000	154707.000000	154707.000000
mean	77358.500000	1.055169	31.447233	84.22307	3.464917	0.660476	0.607652	0.584982	0.579643	0.576853	...	220.048895	62.287213	85.186206	0.299354	0.326219	0.269383	0.105043	0.508810	0.514710	0.190607
std	44663.383812	1.503758	34.878837	80.85012	0.990121	0.076313	0.093366	0.105881	0.110447	0.113427	...	20.643270	75.850992	87.614826	0.136632	0.194612	0.218096	0.171638	0.499924	0.289850	0.118522
min	0.000000	0.000000	1.000000	1.00000	1.000000	0.395285	0.297370	0.238495	0.215285	0.199372	...	2.000000	2.000000	2.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
25%	38679.250000	0.000000	10.000000	11.00000	3.000000	0.612372	0.538609	0.506099	0.501109	0.500098	...	225.000000	12.000000	12.000000	0.208333	0.156863	0.094340	0.000000	0.000000	0.229026	0.074326
50%	77358.500000	0.083000	20.000000	62.00000	3.000000	0.648074	0.603681	0.579020	0.572069	0.571484	...	229.000000	12.000000	15.000000	0.297297	0.371163	0.226667	0.000000	1.000000	0.590585	0.203420
75%	116037.750000	1.858600	40.000000	160.00000	4.000000	0.707107	0.658522	0.647881	0.646555	0.645706	...	229.000000	139.000000	194.000000	0.358974	0.487310	0.400000	0.179487	1.000000	0.779730	0.294785
max	154717.000000	17.891400	444.000000	230.00000	9.000000	1.000000	1.000000	1.000000	1.000000	1.000000	...	229.000000	229.000000	229.000000	1.000000	0.750000	1.000000	0.875000	1.000000	0.921450	0.460725

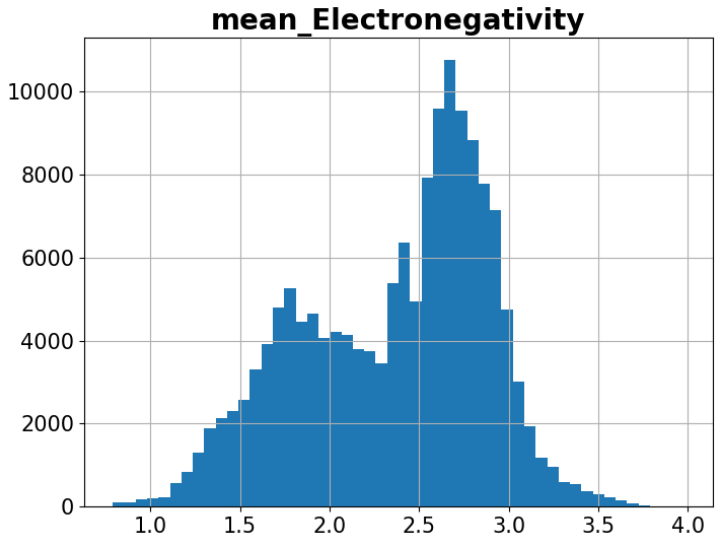
8 rows × 149 columns

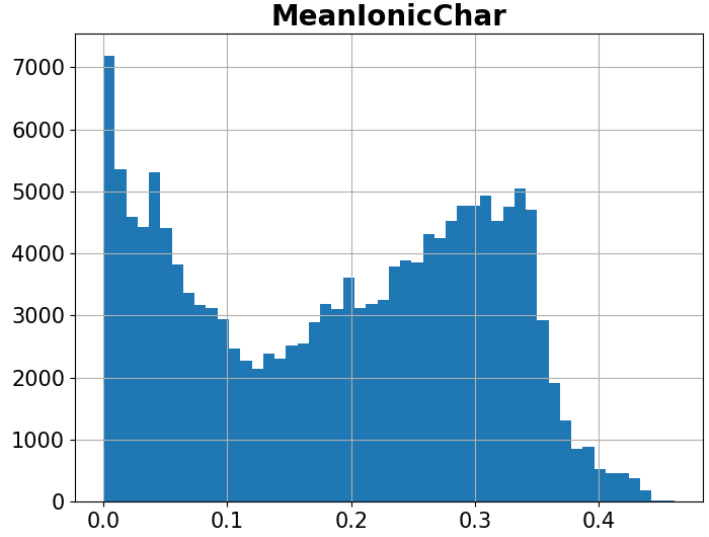
Take a quick look at the Data structure







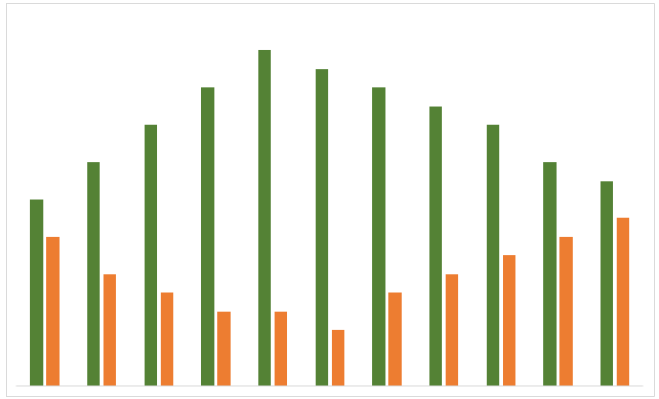


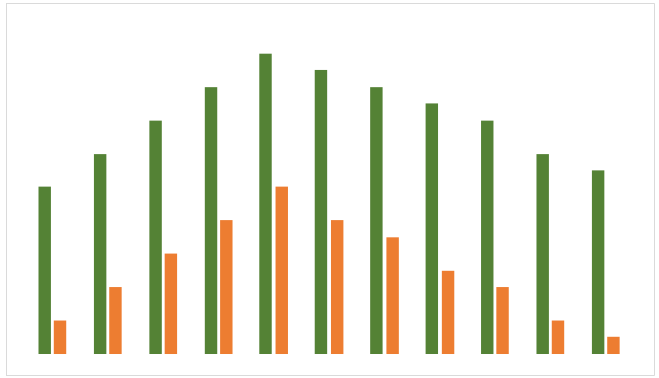


Create a Test set

Database

Sampling



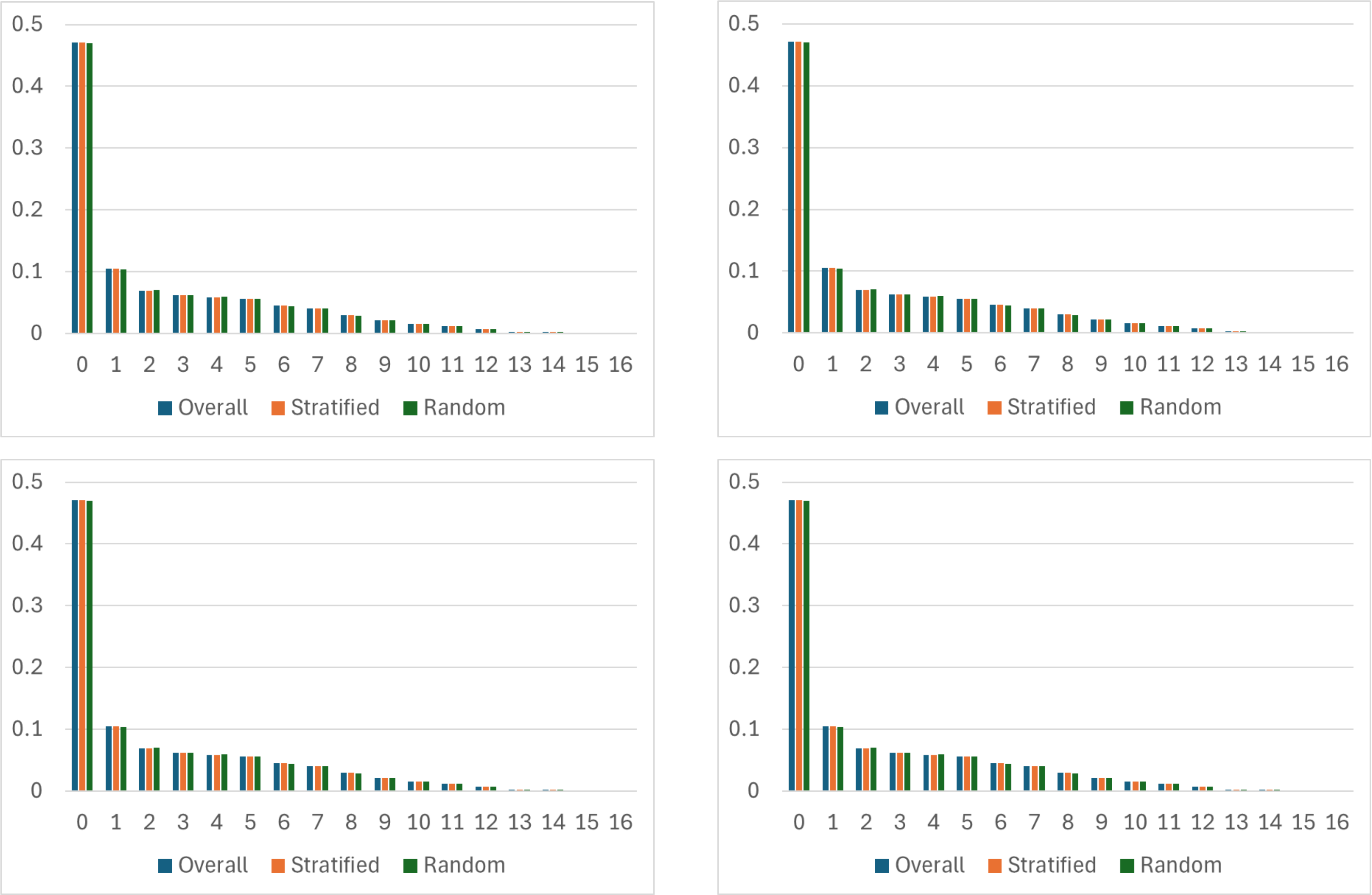


```
[75] from sklearn.model_selection import train_test_split

     random_train_set, random_test_set = train_test_split(MP_bandgap, test_size=0.2, random_state=0)
```

```
[82] from sklearn.model_selection import StratifiedShuffleSplit

     split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=42)
     for train_index, test_index in split.split(MP_bandgap, MP_bandgap["bandgap_cat"]):
         strat_train_set = MP_bandgap.iloc[train_index]
         strat_test_set = MP_bandgap.iloc[test_index]
```

- ✓ Stratified sampling
- 모집단을 여러 층으로 분류하고 각 층에서 n개씩 랜덤하게 추출하는 방법
- 데이터 편향을 예방할 수 있음

Random vs Stratified sampling



Correlation Coefficient

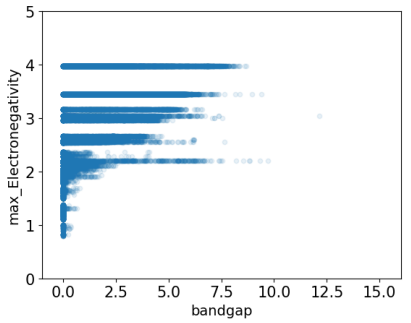
```
[94] corr_matrix = train_set.corr()
```

```
[95] corr_matrix['bandgap'].sort_values(ascending=False)
```

```
bandgap                     1.000000
CanFormIonic                0.512913
frac_pValence               0.494154
max_Electronegativity       0.420207
maxdiff_Electronegativity   0.400274
                              ...
frac_dValence              -0.403884
most_CovalentRadius        -0.408413
mean_Row                   -0.413997
mean_CovalentRadius        -0.420306
min_CovalentRadius         -0.421281
Name: bandgap, Length: 146, dtype: float64
```

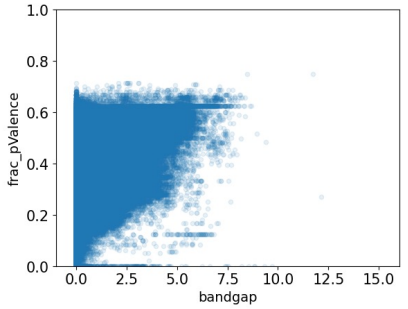
```
train_set.plot(kind="scatter", x="bandgap", y="max_Electronegativity",
               alpha=0.1)
plt.axis([-1, 16, 0, 5])
```

```
(-1.0, 16.0, 0.0, 5.0)
```



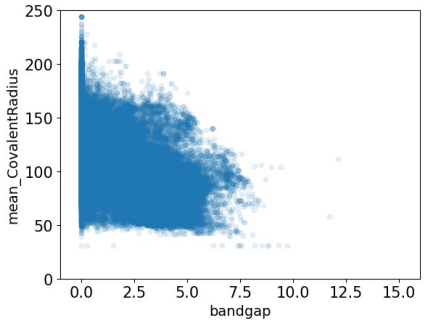

```
train_set.plot(kind="scatter", x="bandgap", y="frac_pValence",
               alpha=0.1)
plt.axis([-1.0, 16, 0, 1.0])
```

```
(-1.0, 16.0, 0.0, 1.0)
```



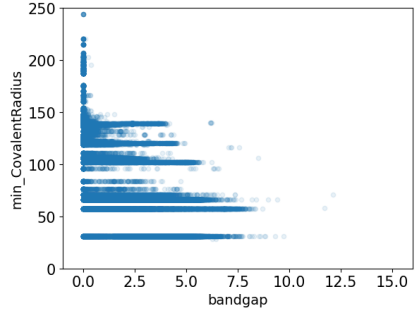

```
[101] train_set.plot(kind="scatter", x="bandgap", y="mean_CovalentRadius",
                     alpha=0.1)
      plt.axis([-1, 16, 0, 250])
```

```
(-1.0, 16.0, 0.0, 250.0)
```

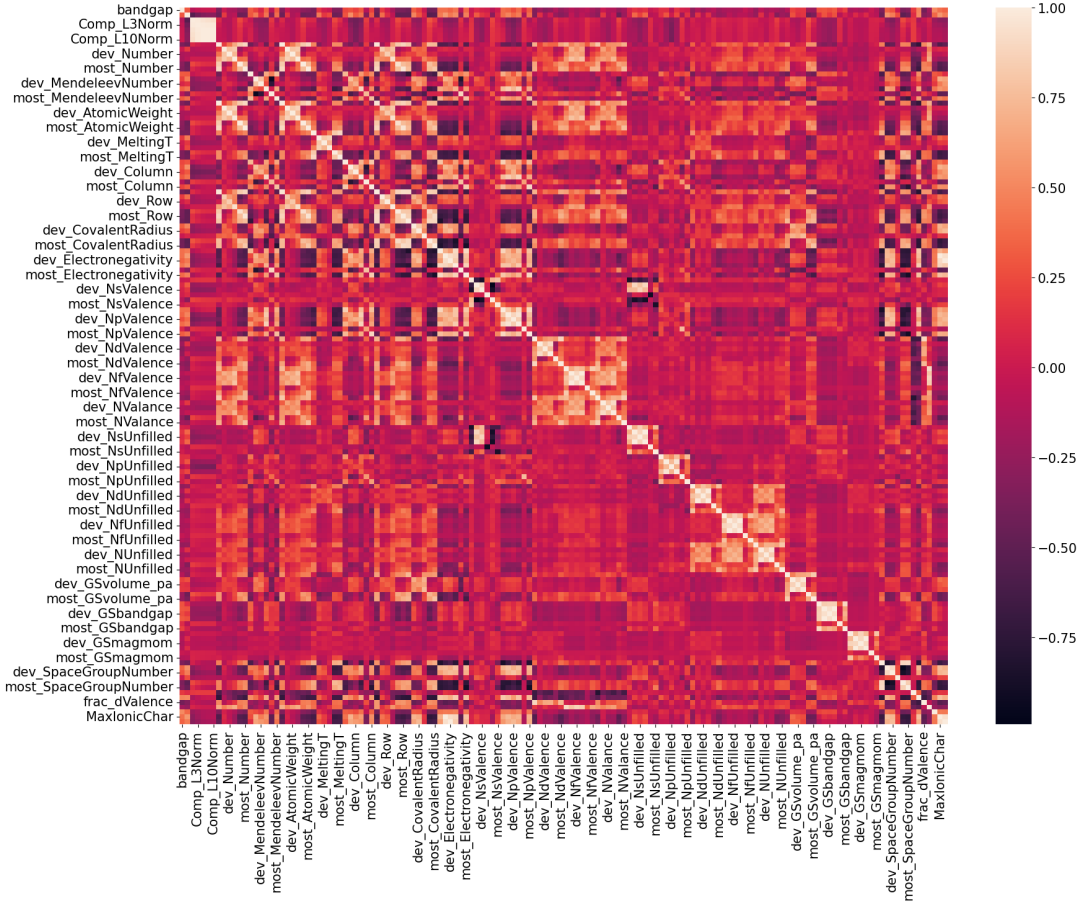



```
train_set.plot(kind="scatter", x="bandgap", y="min_CovalentRadius",
               alpha=0.1)
plt.axis([-1, 16, 0, 250])
```

```
(-1.0, 16.0, 0.0, 250.0)
```




```
import seaborn as sns

plt.figure(figsize = (20,15))
sns.heatmap(corr_matrix)
```



Prepare the Data for Machine Learning Algorithms

✓ MaxIonicChar, MeanIonicChar의 feature 값들이 없는 부분 존재

- Option 1 : 해당 data 삭제

```
[104] sample_incomplete_rows.dropna(subset=["MaxIonicChar", "MeanIonicChar"])  # option 1
```

bandgap	NComp	Comp_L2Norm	Comp_L3Norm	Comp_L5Norm	Comp_L7Norm	Comp_L10Norm	mean_Number	maxdiff_Number	dev_Number	...	max_SpaceGroupNumber	min_SpaceGroupNumber	most_SpaceGroupNumber	frac_sValence	frac_pValence	frac_dValence	frac_fValence	CanFormIonic	MaxIonicChar	MeanIonicChar

0 rows × 146 columns

- Option 2 : 해당 feature 삭제

```
sample_incomplete_rows.drop(["MaxIonicChar", "MeanIonicChar"], axis=1)       # option 2
```

	bandgap	NComp	Comp_L2Norm	Comp_L3Norm	Comp_L5Norm	Comp_L7Norm	Comp_L10Norm	mean_Number	maxdiff_Number	dev_Number	...	maxdiff_SpaceGroupNumber	dev_SpaceGroupNumber	max_SpaceGroupNumber	min_SpaceGroupNumber	most_SpaceGroupNumber	frac_sValence	frac_pValence	frac_dValence	frac_fValence	CanFormIonic
780	11.7274	1	1.0	1.0	1.0	1.0	1.0	10.0	0	0.0	...	0	0.0	225	225	225.0	0.25	0.75	0.0	0.0	0
12013	16.5864	1	1.0	1.0	1.0	1.0	1.0	2.0	0	0.0	...	0	0.0	225	225	225.0	1.00	0.00	0.0	0.0	0
8509	17.8914	1	1.0	1.0	1.0	1.0	1.0	2.0	0	0.0	...	0	0.0	225	225	225.0	1.00	0.00	0.0	0.0	0
7806	8.4898	1	1.0	1.0	1.0	1.0	1.0	18.0	0	0.0	...	0	0.0	225	225	225.0	0.25	0.75	0.0	0.0	0
272	17.7675	1	1.0	1.0	1.0	1.0	1.0	2.0	0	0.0	...	0	0.0	225	225	225.0	1.00	0.00	0.0	0.0	0

5 rows × 144 columns

- Option 3 : mean, average 등 대표값을 취함

```
DataFrame with shape (5, 146)
onicChar"].median()
sample_incomplete_rows["MaxIonicChar"].fillna(maxioncchar_median, inplace=True) # option 3

meanioncchar_median = train_set["MeanIonicChar"].median()
sample_incomplete_rows["MeanIonicChar"].fillna(meanioncchar_median, inplace=True)
```

```
[107] sample_incomplete_rows
```

	bandgap	NComp	Comp_L2Norm	Comp_L3Norm	Comp_L5Norm	Comp_L7Norm	Comp_L10Norm	mean_Number	maxdiff_Number	dev_Number	...	max_SpaceGroupNumber	min_SpaceGroupNumber	most_SpaceGroupNumber	frac_sValence	frac_pValence	frac_dValence	frac_fValence	CanFormIonic	MaxIonicChar	MeanIonicChar
780	11.7274	1	1.0	1.0	1.0	1.0	1.0	10.0	0	0.0	...	225	225	225.0	0.25	0.75	0.0	0.0	0	0.590585	0.203416
12013	16.5864	1	1.0	1.0	1.0	1.0	1.0	2.0	0	0.0	...	225	225	225.0	1.00	0.00	0.0	0.0	0	0.590585	0.203416
8509	17.8914	1	1.0	1.0	1.0	1.0	1.0	2.0	0	0.0	...	225	225	225.0	1.00	0.00	0.0	0.0	0	0.590585	0.203416
7806	8.4898	1	1.0	1.0	1.0	1.0	1.0	18.0	0	0.0	...	225	225	225.0	0.25	0.75	0.0	0.0	0	0.590585	0.203416
272	17.7675	1	1.0	1.0	1.0	1.0	1.0	2.0	0	0.0	...	225	225	225.0	1.00	0.00	0.0	0.0	0	0.590585	0.203416

5 rows × 146 columns

Training and Evaluation

LinearRegression

```
from sklearn.linear_model import LinearRegression

lin_reg = LinearRegression()
lin_reg.fit(train_x, train_y)
```

```
LinearRegression()
```

Calculate RMSE, MAE, R2

```
[111] from sklearn.metrics import mean_squared_error

LR_bandgap_predictions = lin_reg.predict(test_x)
LR_mse = mean_squared_error(test_y, LR_bandgap_predictions)
LR_rmse = np.sqrt(LR_mse)
LR_rmse
```

```
1.0754600014055637
```

```
[112] from sklearn.metrics import mean_absolute_error

LR_mae = mean_absolute_error(test_y, LR_bandgap_predictions)
LR_mae
```

```
0.8117386380297497
```

```
[113] from sklearn.metrics import r2_score
LR_r2 = r2_score(test_y, LR_bandgap_predictions)
LR_r2
```

```
0.48476581910545014
```

DecisionTreeRegressor

```
[115] from sklearn.tree import DecisionTreeRegressor

DT_reg = DecisionTreeRegressor(random_state=42)
DT_reg.fit(train_x, train_y)
```

```
DecisionTreeRegressor(random_state=42)
```

Calculate RMSE, MAE, R2

```
[116] from sklearn.metrics import mean_squared_error

DT_bandgap_predictions = DT_reg.predict(test_x)
DT_mse = mean_squared_error(test_y, DT_bandgap_predictions)
DT_rmse = np.sqrt(DT_mse)
DT_rmse
```

```
0.8329822526612584
```

```
[117] from sklearn.metrics import mean_absolute_error

DT_mae = mean_absolute_error(test_y, DT_bandgap_predictions)
DT_mae
```

```
0.4128481275736755
```

```
[118] from sklearn.metrics import r2_score
DT_r2 = r2_score(test_y, DT_bandgap_predictions)
DT_r2
```

```
0.6909080899872387
```

RandomForestRegressor

```
[120] from sklearn.ensemble import RandomForestRegressor

RF_reg = RandomForestRegressor(n_estimators=100, random_state=42)
RF_reg.fit(train_x, train_y)
```

```
RandomForestRegressor(random_state=42)
```

Calculate the RMSE, MAE, R2

```
[121] from sklearn.metrics import mean_squared_error

RF_bandgap_predictions = RF_reg.predict(test_x)
RF_mse = mean_squared_error(test_y, RF_bandgap_predictions)
RF_rmse = np.sqrt(RF_mse)
RF_rmse
```

```
0.6598511264068248
```

```
[136] from sklearn.metrics import mean_absolute_error

RF_mae = mean_absolute_error(test_y, RF_bandgap_predictions)
RF_mae
```

```
0.3646210316593357
```

```
[137] from sklearn.metrics import r2_score
RF_r2 = r2_score(test_y, RF_bandgap_predictions)
RF_r2
```

```
0.8060418353047923
```

Training and Evaluation

	LR	DT	RF
R^2	0.485	0.691	0.806
MAE	0.812	0.413	0.365
RMSE	1.075	0.833	0.650

GdPO4	mp-1103324	3.2911	12	141	3	0.70710678	0.67354	0.66692688	0.66667829	0.66666679	18.5	56	15.1666667	64	8
GdPO4	mp-3735	2.613	24	14	3	0.70710678	0.67354	0.66692688	0.66667829	0.66666679	18.5	56	15.1666667	64	8

H2	mp-632291	8.8499	2	139	1	1	1	1	1	1	1	0	0	1	1
H2	mp-24504	8.0699	4	194	1	1	1	1	1	1	1	0	0	1	1
H2	mp-1066989	6.2332	4	65	1	1	1	1	1	1	1	0	0	1	1
H2	mp-730101	9.7197	8	19	1	1	1	1	1	1	1	0	0	1	1
H2	mp-1096977	0.2567	1	123	1	1	1	1	1	1	1	0	0	1	1
H2	mp-632250	7.4222	1	229	1	1	1	1	1	1	1	0	0	1	1
H2	mp-23907	7.4848	2	194	1	1	1	1	1	1	1	0	0	1	1
H2	mp-754417	0	1	191	1	1	1	1	1	1	1	0	0	1	1
H2	mp-634659	7.5517	1	225	1	1	1	1	1	1	1	0	0	1	1
H2	mp-850274	8.5338	2	139	1	1	1	1	1	1	1	0	0	1	1
H2	mp-1188177	7.3865	16	62	1	1	1	1	1	1	1	0	0	1	1
H2	mp-738409	8.1865	32	4	1	1	1	1	1	1	1	0	0	1	1
H2	mp-731827	8.1932	16	62	1	1	1	1	1	1	1	0	0	1	1
H2	mp-973783	8.8022	4	64	1	1	1	1	1	1	1	0	0	1	1
H2	mp-570752	6.6359	2	194	1	1	1	1	1	1	1	0	0	1	1
H2	mp-1181265	1.5178	16	62	1	1	1	1	1	1	1	0	0	1	1
H2	mp-632172	9.3289	2	139	1	1	1	1	1	1	1	0	0	1	1

algorithm	mean mae	std mae	mean rmse	max max_error
coGN	**0.1559**	0.0017	0.3956	7.3352
coNGN	**0.1697**	0.0035	0.4271	7.9674
ALIGNN	**0.1861**	0.0030	0.4635	7.4756
MegNet (kgcnn v2.1.0)	**0.1934**	0.0087	0.4715	7.8821
DimeNet++ (kgcnn v2.1.0)	**0.1993**	0.0058	0.4720	14.0169
Finder_v1.2 structure-based version	**0.2193**	0.0012	0.4989	7.6676
MODNet (v0.1.12)	**0.2199**	0.0059	0.4525	7.5685

https://matbench.materialsproject.org/

- Chemical Composition만을 가지고 물질을 대표하는 feature 생성할 수 없음
- 새로운 ML Model, Hyperparameter optimization 등 정확한 예측을 하기 위한 방법이 존재
- AutoML 사용하여 low code로도 더 많은 비교 가능

Thank you