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Elemental  
Database

Element

{'Si', 'O'}

Organized elements  
w.r.t. electronegativity

{'Si', 'O'}

Elementary data

1. Group
2. Period
3. Mass
4. Electron Negativity
5. Electron Affinity
6. Covalent radius
7. Atomic radius
8. vdw radius
9. Melting point

Add to  
features

Compound  
List  
4100\*1

Fraction

{'Si':1, 'O':2}

Add to  
features

PyMatGen

MaterialsProject  
Database

Most-stable  
polymorph

Add to  
features

1. Atoms/unitcell
2. Density
3. Enerav/atom

Internal  
library

Add to  
features

Num. of  
Symmetries

Compound  
Formula

'SiO2'

Point group



Feature  
Matrix  
4100\*44

Expt.  
bandgap  
4100\*1

Training Set

Train SVM  
Classifier

Choose Kernel  
Function and C

Classifier  
Accuracy Test

Cross-Valid Set

Test Set

**Metal/Nonmetal Classification**

Training Set

Train SVM  
Regression

Choose Kernel  
Function and C

Regression  
Accuracy Test

Cross-Valid Set

Test Set

**Band Gap Prediction**

Eg>0?