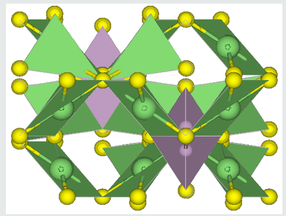
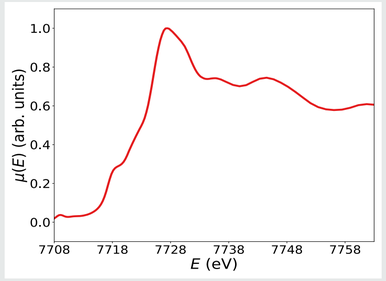
Database

Structure



Spectrum



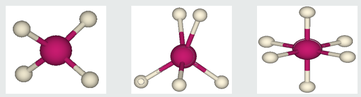
Spectral Feature Vector

$$[x_1, x_2, ..., x_{199}, x_{200}]$$

Absorption Atom Local Environment Features

12 Coord. Num.

CN4 CN5 CN6 ...



Coord. Num. OPs

CN1: 0.023
CN2: 0.214
...
CN12: 0.653

OPs > 0.2

Coord. Num. OPs

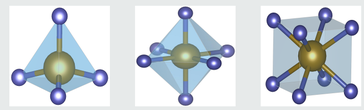
CN2: 0.214
CN12: 0.653

Ranking Labels

CN12 - CN2

25 Coord. Motifs

tet oct cubic ...



CN1
Motif 1: 0.134
Motif 2: 0.527
Motif 3: 0.031
...
CN8
Motif 5: 0.134
Motif 6: 0.527

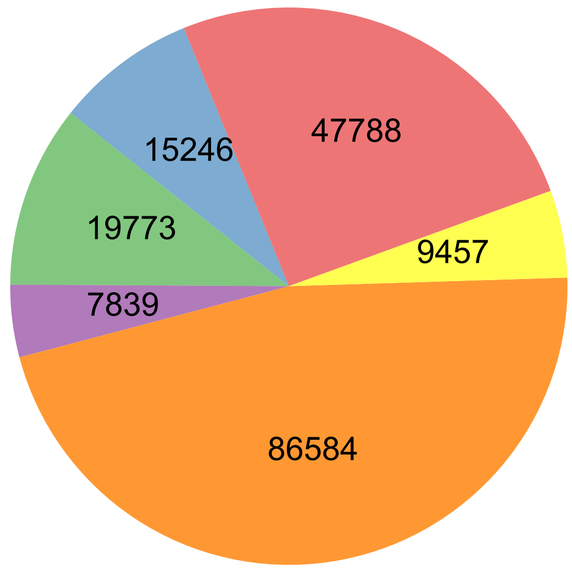
OPs > 0.05

CN1 Motif 1: 0.134, Motif 2: 0.527 ... *CN8* Motif 5: 0.134, Motif 6: 0.527

Ranking Labels

CN1- Motif 2 - Motif 1
CN8- Motif 6 - Motif 5

Distribution of training data



Train the Machine Learning Algorithm

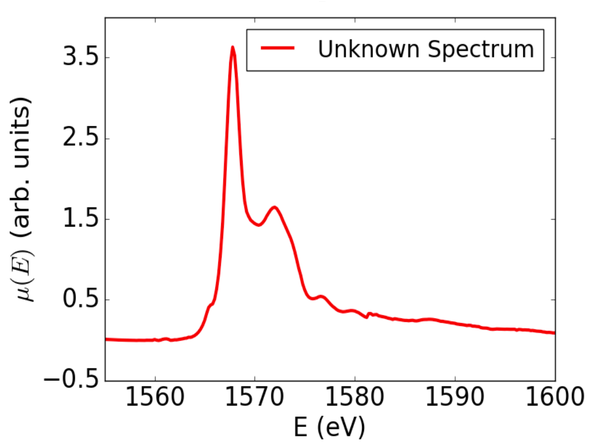
Element-wise classification model

Li	Be											B	C
Na	Mg											Al	Si
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn

- Alkali
- Alkaline earth
- Metalloid
- Carbon
- TM
- Post-TM

Prediction

Input



Predicted Coord. Env

CN4 - Motif 1

CN5 - Motif 2 - Motif 3

CN6 - Motif 4