Relative Structural Analysis on Molecular Perovskite

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Skills 4 Scientists

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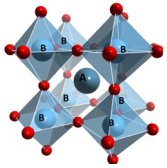
1

What are Perovskite compounds?

Compounds with ABX_3, have small cation B-site, large cation A-site and a bridging ligand anion X-site.



How can we compare from one another?

One way is to use Descriptors: transforms a structure into a multi-dimensional constant sized vector. Smooth Overlap of Atomic Positions (SOAP) is one example from Dscribe.

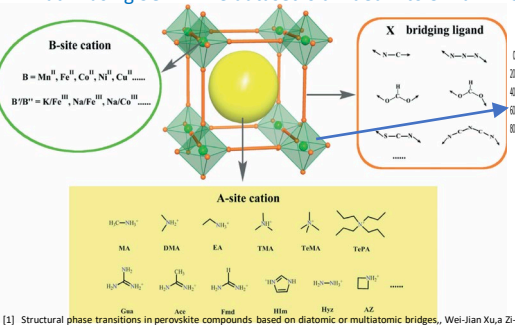
How can you use ML to analyse perovskite compounds?

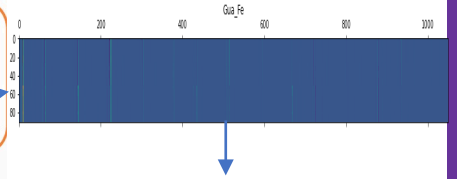
You can use unsupervised learning. Through the use of clustering algorithms, we can find hidden clusters/structure between different crystal structures of the same type.

2

Dataset

Gathered various structures from a perovskite compound paper [1] and turned each structure into a matrix using SOAP. The dataset is divided into 3 main X-site ligands: Formate, Cyano and Azido – Bridges.





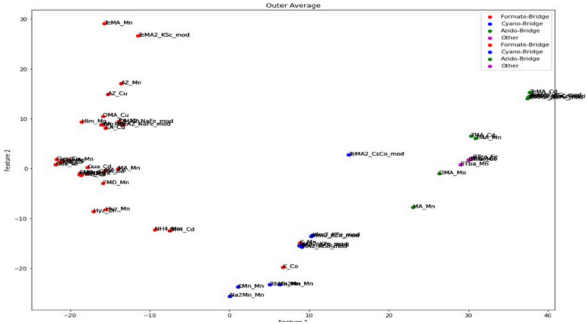
To compare one structure to another, I used 3 different averaging methods: First-Entry, Inner and Outer average.

[1] Structural phase transitions in perovskite compounds based on diatomic or multiatomic bridges,, Wei-Jian Xu,a Zi-Yi Du,b Wei-Xiong Zhang*a and Xiao-Ming Chena , https://doi.org/10.1039/C6CE01485B

3

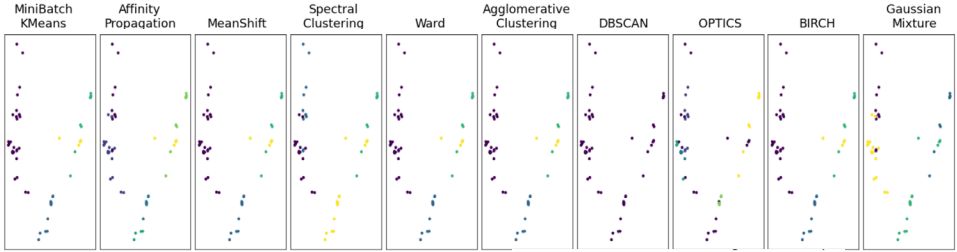
Graphical Representation

Using PCA and Standard Scalar from scikit, I could plot my dataset.



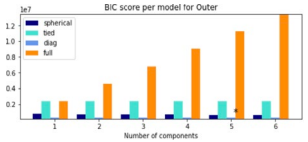
Clustering Algorithm

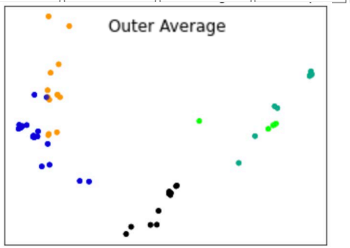
Clustering algorithm can handle multi-dimensional vector datasets.



Optimisation

There are certain ways to measure performance of cluster models.





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