Exploring Quantum Property-Data Correlations in Metal Organic Frameworks using Unsupervised Learning

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In this study, we explore the correlations between quantum properties and experimental data of Metal Organic Frameworks (MOFs) through the analysis of the QMOF database. To reveal these connections, we utilize unsupervised learning techniques, offering valuable insights for researchers engaged in the synthesis of MOFs. The methodology is based on clustering techniques to identify emerging patterns in the quantum properties of MOFs. Furthermore, exploring feature combinations through brute force testing expands our understanding of the complex relationships between properties and behaviour of MOFs. The primary contribution of this study lies in the systematic exploration of feature combinations. Here, the clusterization of the MOFs will unveil a classification of electronic/structural characteristics between different MOFs. The potential practical impact of the project lies in the future creation of algorithms based on the results obtained, which could assist experimental researchers in defining more efficient routes for the synthesis of MOFs with desired characteristics, significantly reducing dependence on empirical methods.

References

[1] Rosen, A.S., Fung, V., Huck, P., *et al. npj Comput Mater* **8**, 112 (2022).
[2] Andrew S. Rosen, Shaelyn M. Iyer, *et al.* Matter **4**, 5 (2021) 1578-1597

Figures

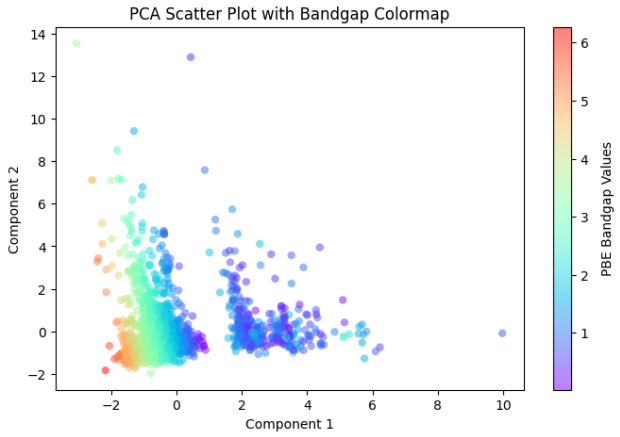

Figure 1: Clusters identified through PCA and K-means analysis, color-coded by bandgap values, offering insight into the data pattern