Studying band gaps in Metal Organic Frameworks

CH-359 Projects in Computational Chemistry, prof. Berend Smit
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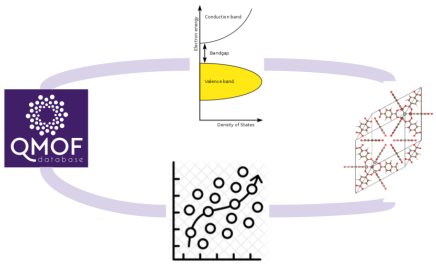
MOFs 101

Metal Organic Frameworks (MOFs) are porous, crystalline materials formed by metal nodes connected by organic linkers.[1]
Explored for optoelectronic properties in, e.g., photocatalysis.[1]
Goal: Computationally handle MOFs - visualize, clean and get an overview on basic properties.

MOF Database & Machine Learning



Database on electronic properties of MOFs.[2]
Goal: Quantitative structure property relationship modelling of MOF band gaps.
How: Build ML models step by step, *i.e.*, data preparation, model training, and model evaluation. Compare different featurization methods and analyze their effects on models.

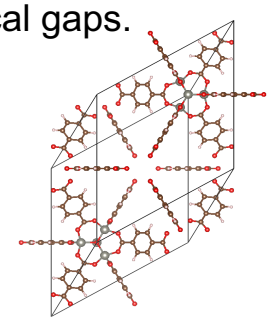
MOFs & DFT: Digging deeper

MOF-5: Explored extensively for its electronic properties.[3]
Goal: Take a deeper, critical look into DFT band gaps.
How: Find ground state and perform calculations with different functionals. Compare with literature, and with values predicted from your ML model.

Learning outcomes

Understand advantages and limitations of ML and DFT to obtain band gaps.
Understand the difference between fundamental and optical gaps.

Want to know more about MOFs?
@MOF_papers



[1]DOI:10.1039/C9TA13506E
[2]DOI:10.1016/j.matt.2021.02.015
[3]DOI:10.1021/acs.jpclett.1c00543

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