

# Studying band gaps in Metal Organic Frameworks

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<https://github.com/bmourino/ch359.git>

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## MOFs 101

Metal Organic Frameworks (MOFs) are porous, crystalline materials formed by metal nodes connected by organic linkers.<sup>1</sup>

Explored for optoelectronic properties in, e.g., photocatalysis.<sup>1</sup>

**Goal:** Computationally handle MOFs - visualize, clean and get an overview on basic properties.

## MOF Database & Machine Learning

Database on electronic properties of MOFs.<sup>2</sup>

**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.<sup>3</sup>

**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 and COFs?

@MOF\_papers @COF\_papers



<sup>1</sup>DOI:10.1039/C9TA13506E

<sup>2</sup>DOI:10.1016/j.matt.2021.02.015

<sup>3</sup>DOI:10.1021/acs.jpcllett.1c00543

