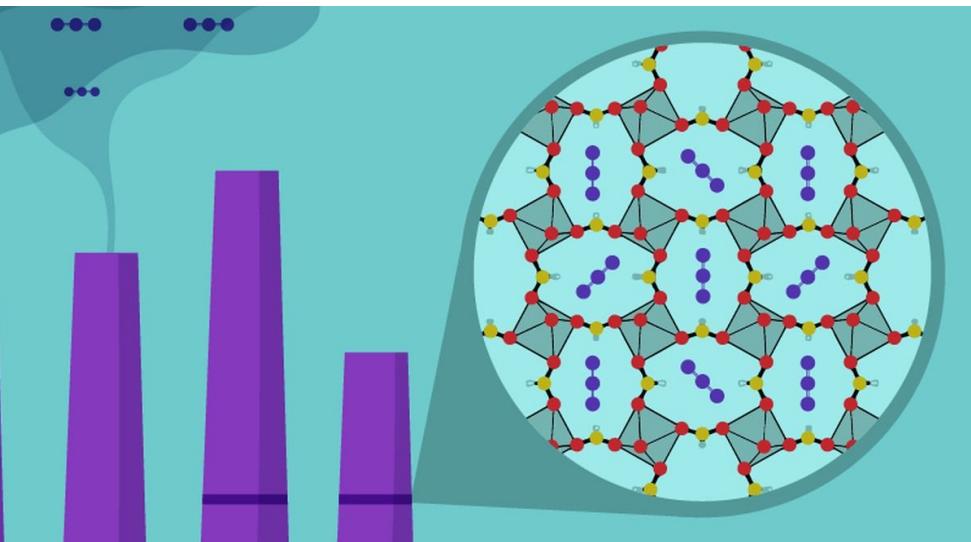


# Carbon Capture Capstone

Designing MOFs to clean power plant exhaust

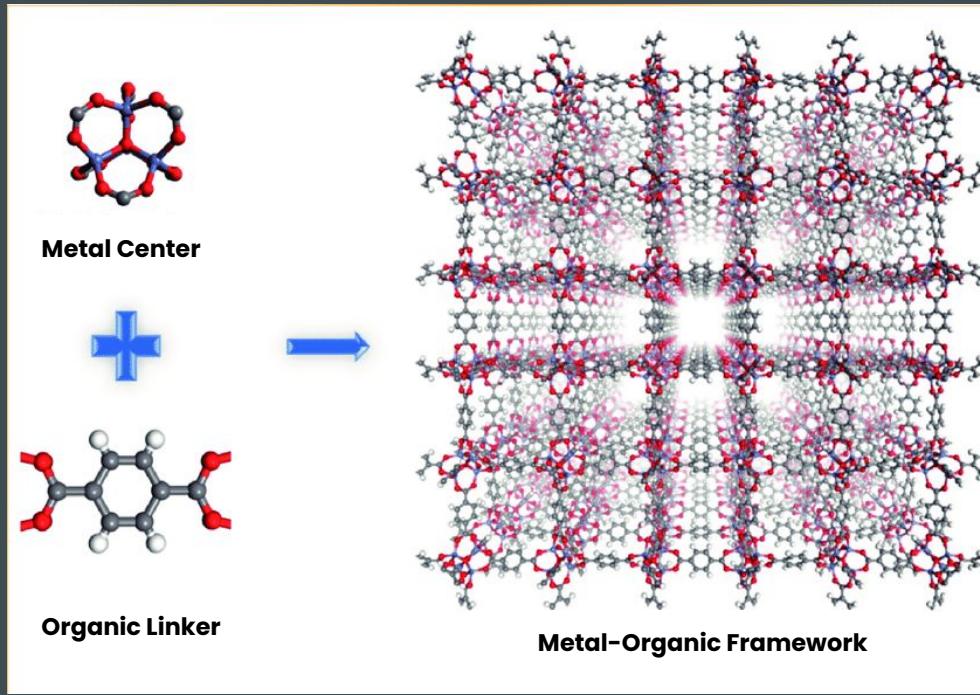
By Zachary Brown

# Carbon Capture and Sequestration



Source: <https://cosmosmagazine.com>

# What is a MOF?



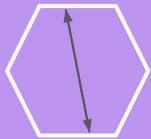
Source:

<https://www.researchgate.net/>

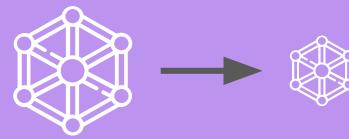
## Project Goal

To develop recommendations to help chemists create metal-organic frameworks with high volumetric carbon dioxide working capacity for use as a carbon dioxide adsorbent

# Design Principles



**Target 0-10 angstrom pore limiting and largest cavity diameters**



Minimize unit cell volume



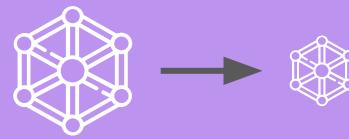
Target probe accessible volume fraction of 0.4–0.5



# Design Principles



Target 0-10 angstrom pore limiting and largest cavity diameters



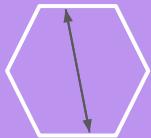
Minimize unit cell volume



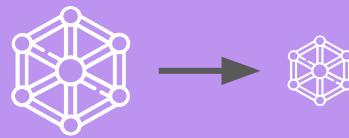
Target probe accessible volume fraction of 0.4-0.5



# Design Principles



Target 0-10 angstrom pore limiting and largest cavity diameters



Minimize unit cell volume



Target probe accessible volume fraction of 0.4-0.5



# The Data

## ARC-MOF: A Diverse Database of Metal-Organic Frameworks with DFT-Derived Partial Atomic Charges and Descriptors for Machine Learning

Jake Burner, Jun Luo, Andrew White, Adam Mirmiran, Ohmin Kwon, Peter G. Boyd, Stephen Maley, Marco Gibaldi, Scott Simrod, Victoria Ogden, and Tom K. Woo\*

**Cite this:** *Chem. Mater.* 2023, 35, 3, 900–916

Publication Date: January 20, 2023 ▾

<https://doi.org/10.1021/acs.chemmater.2c02485>

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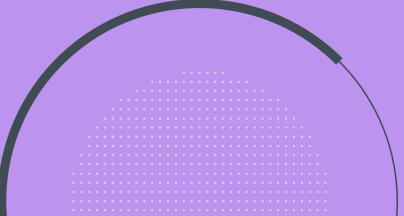


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# The Data



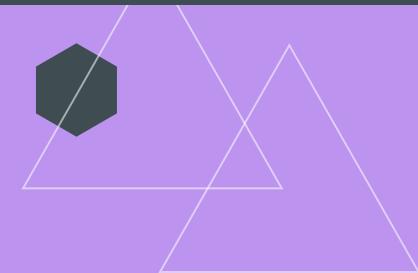
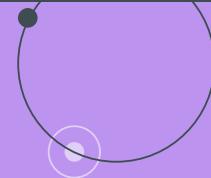
Topology

Geometry

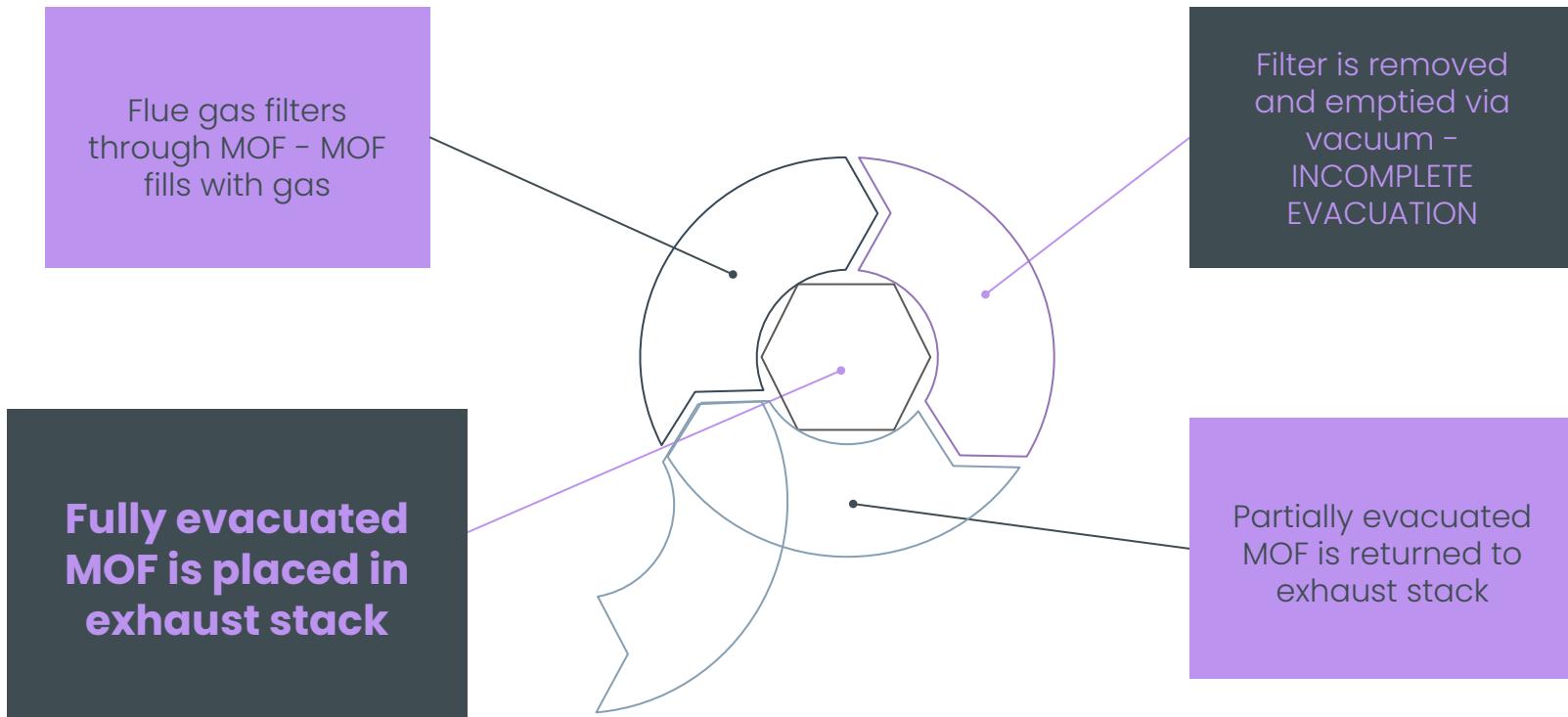
Radial  
Distribution  
Functions  
(RDFs)

Process

Revised  
Autocorrelations  
(RACs)



# Working Capacity



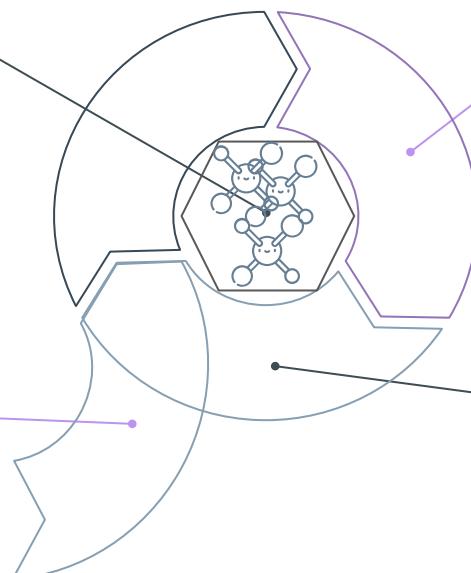
# Working Capacity

**Flue gas filters  
through MOF –  
MOF fills with gas**

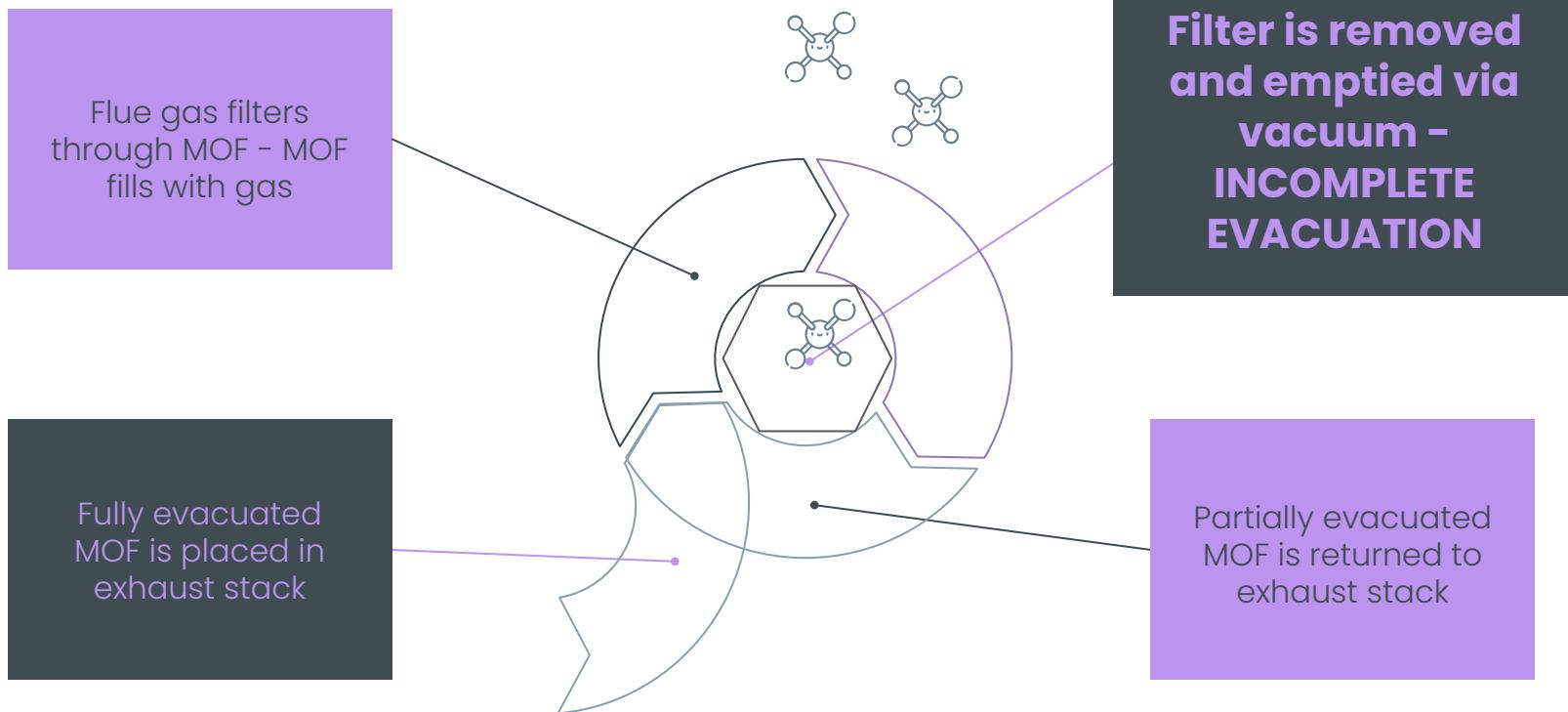
Filter is removed  
and emptied via  
vacuum –  
**INCOMPLETE  
EVACUATION**

Fully evacuated  
MOF is placed in  
exhaust stack

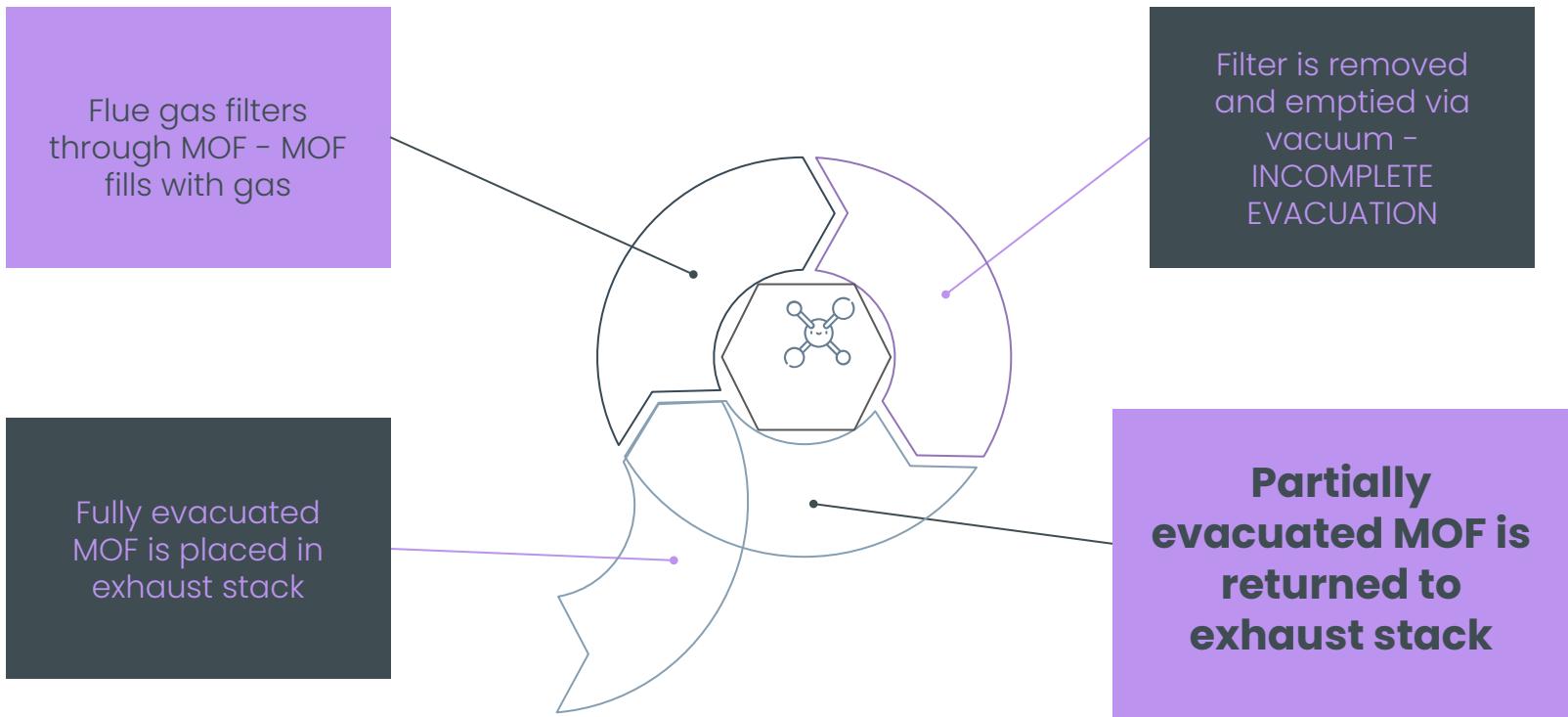
Partially evacuated  
MOF is returned to  
exhaust stack



# Working Capacity

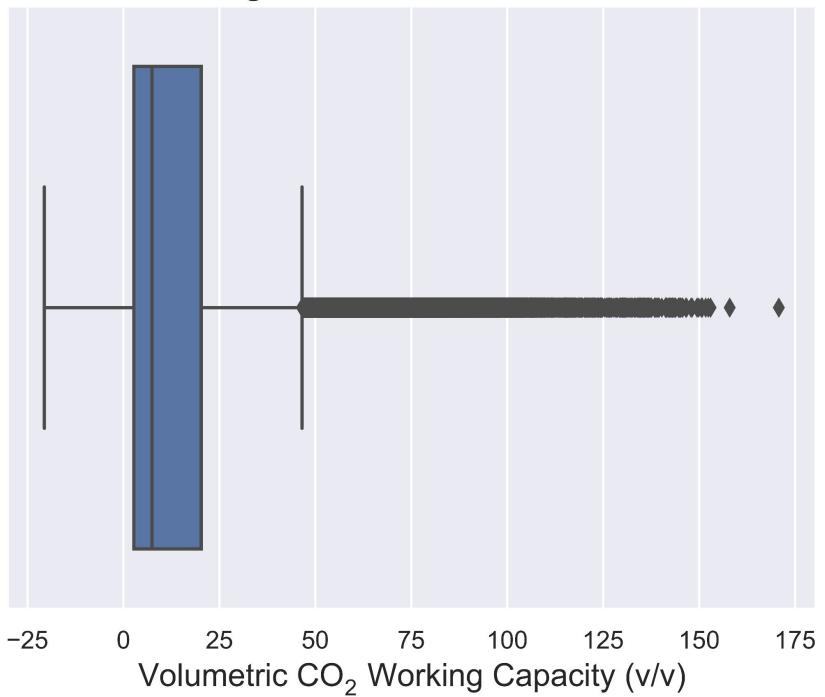


# Working Capacity

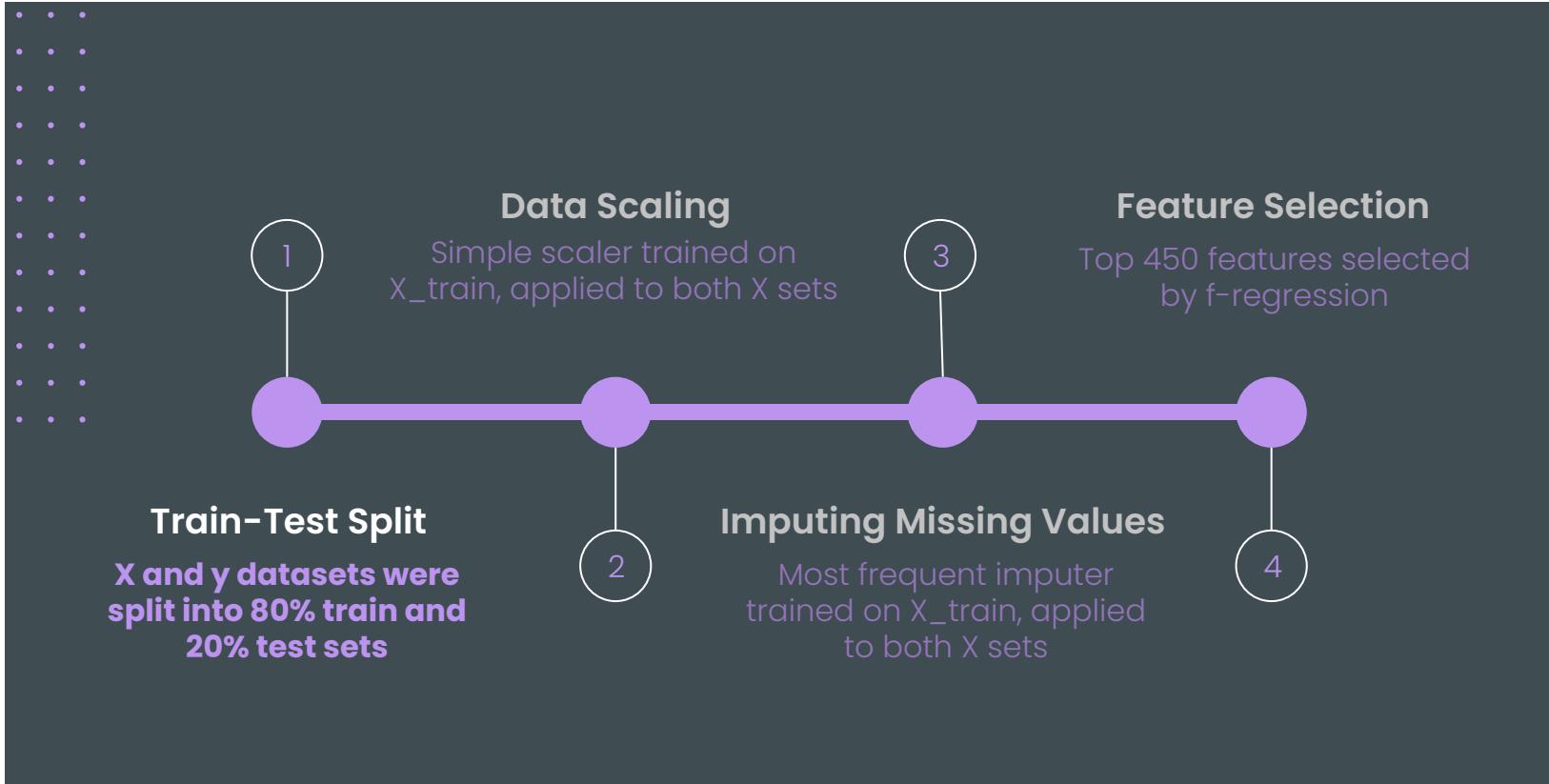


# Volumetric CO<sub>2</sub> Working Capacity

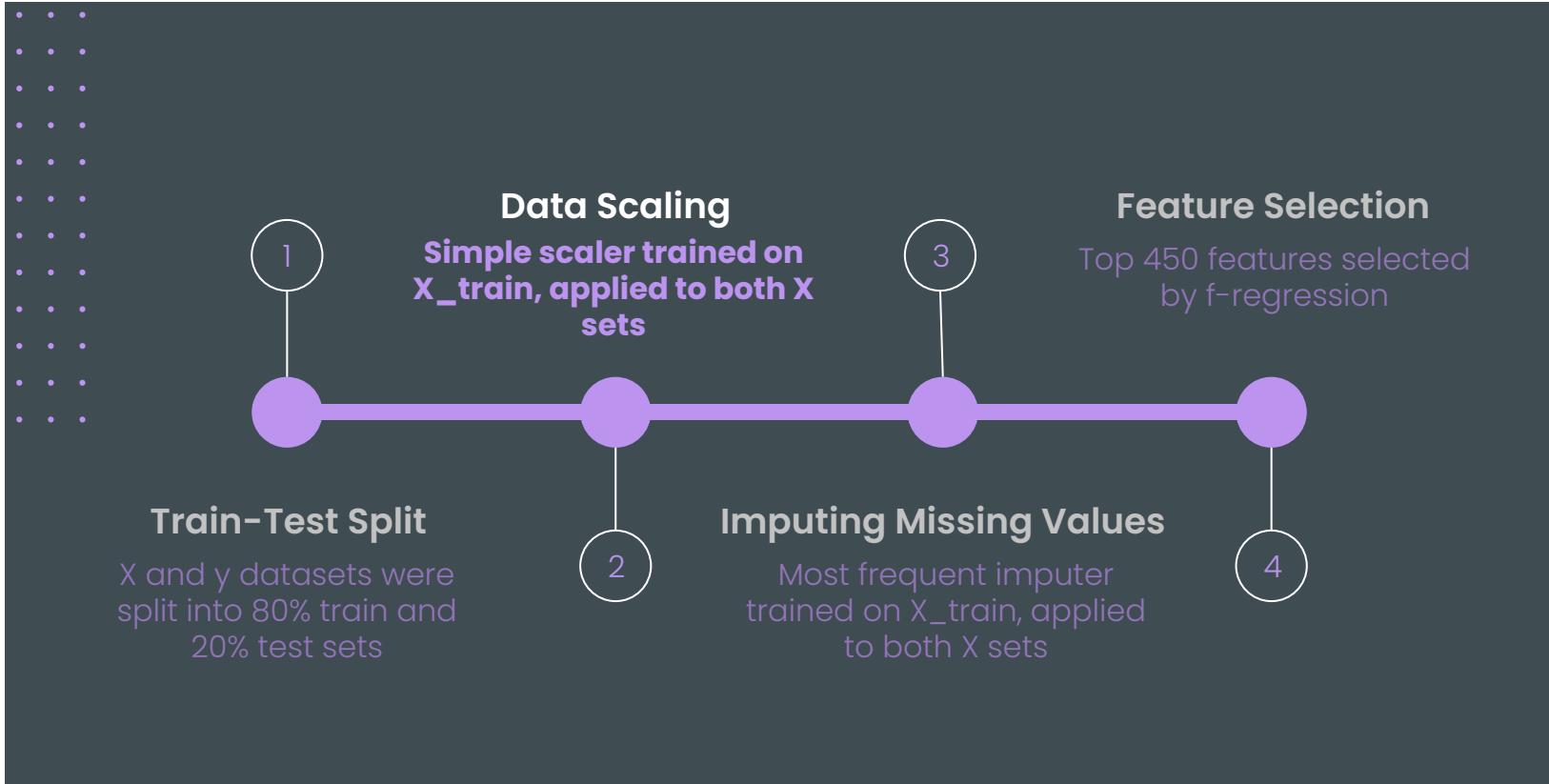
Target Metric Distribution



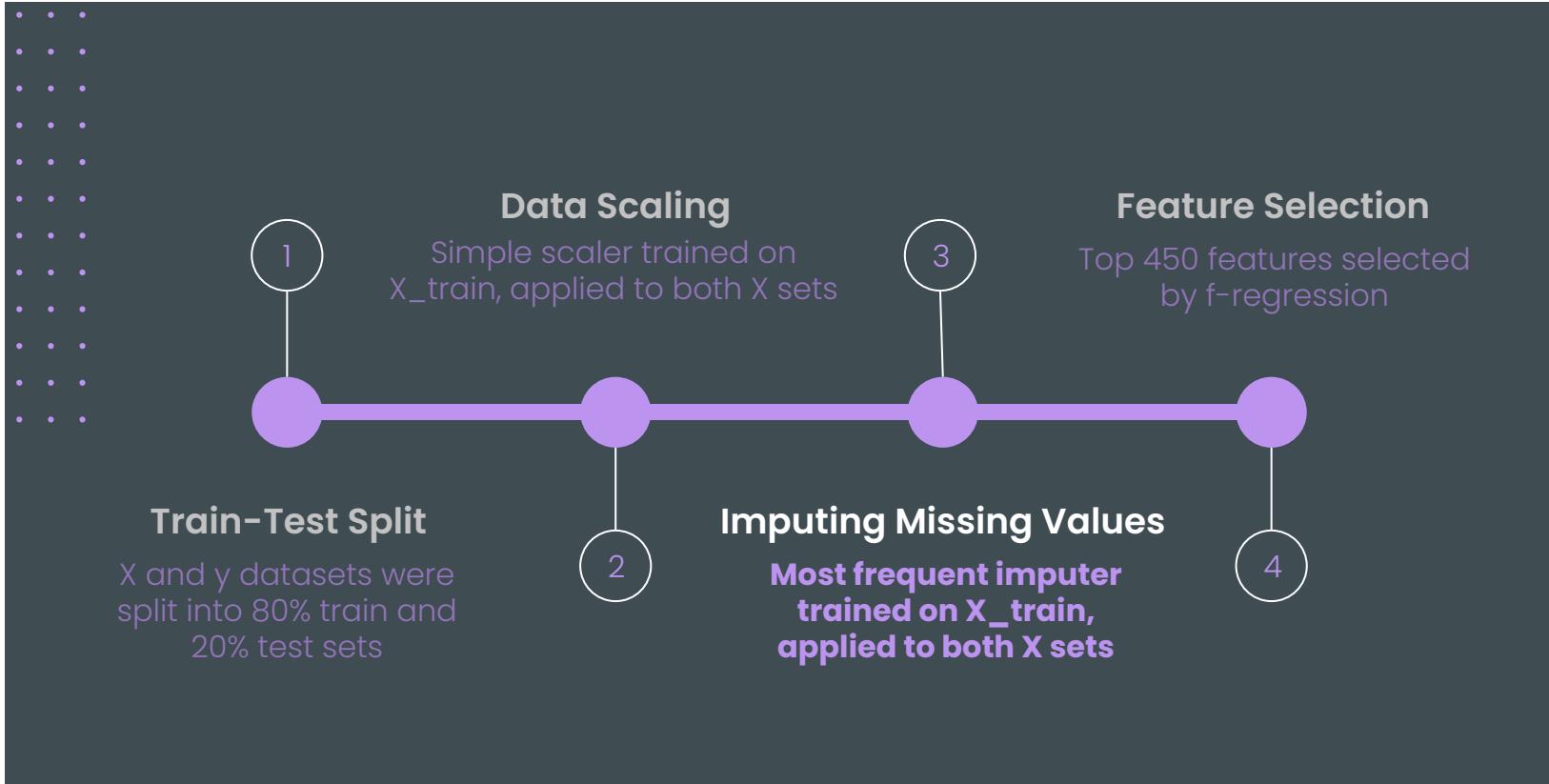
# Feature Engineering



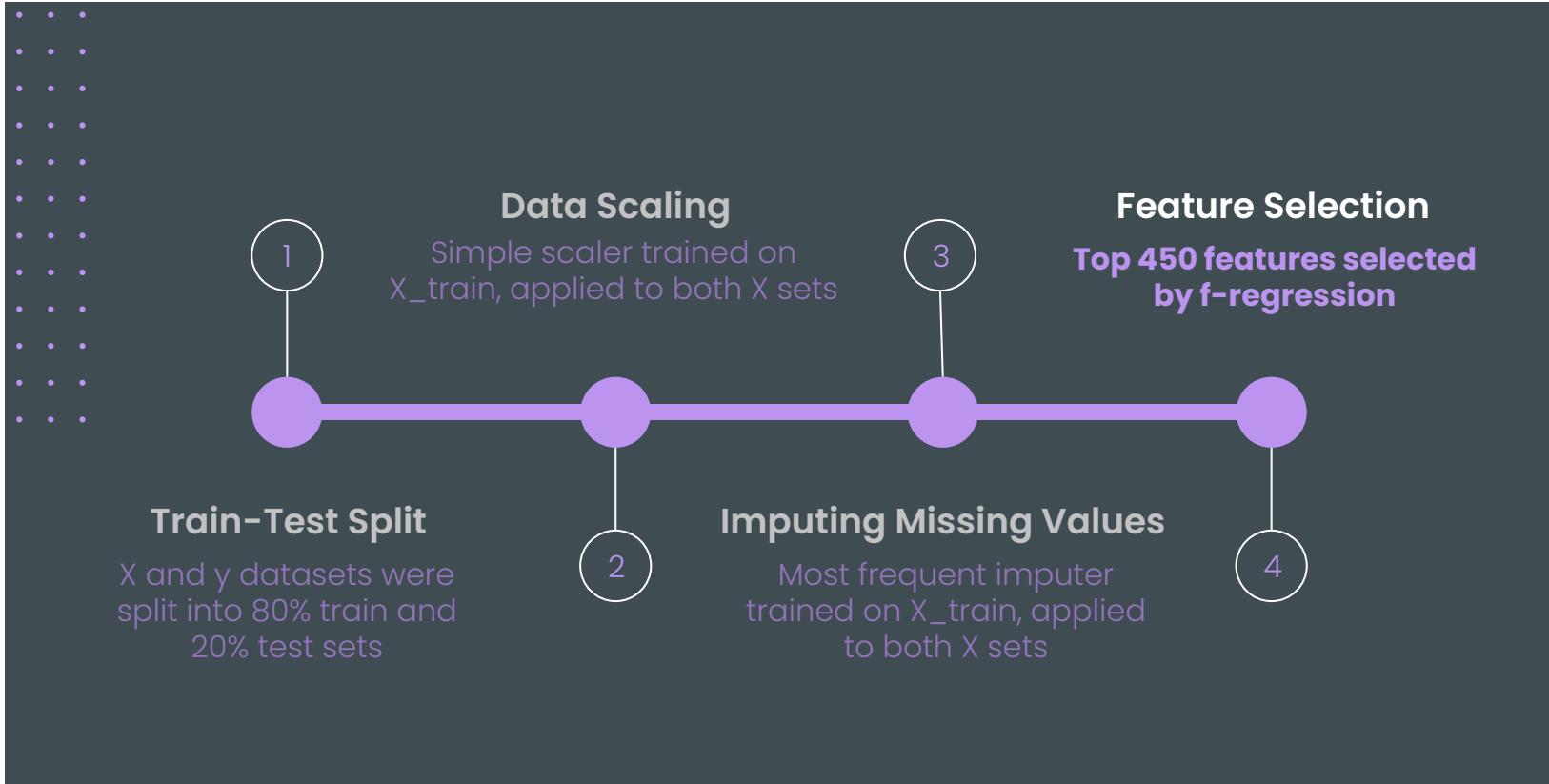
# Feature Engineering



# Feature Engineering

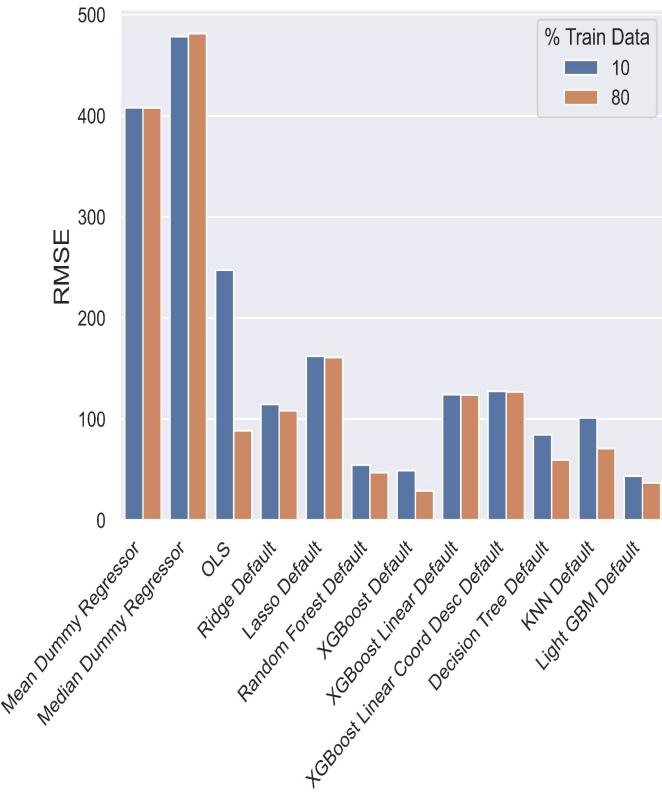


# Feature Engineering

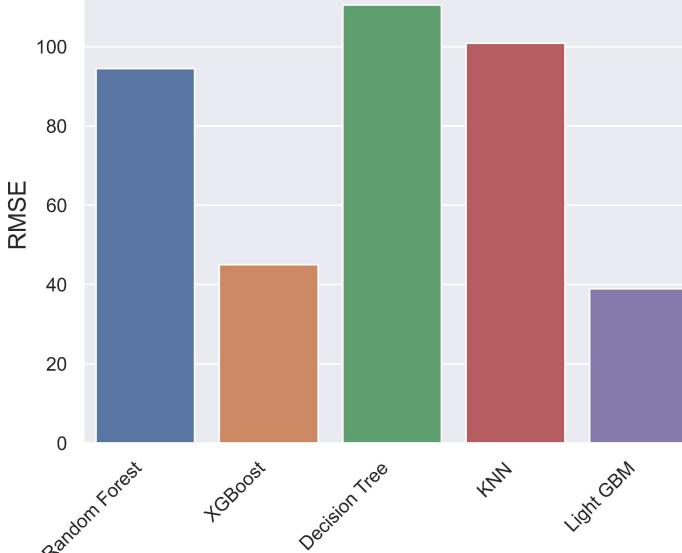


# Initial Models

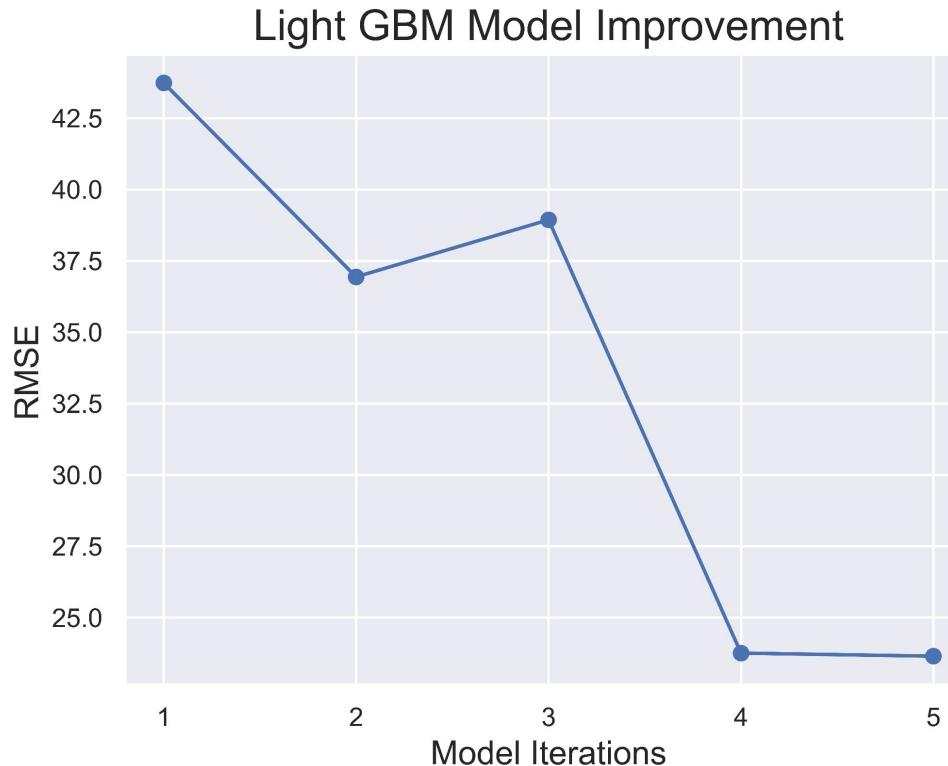
Default Model Scores



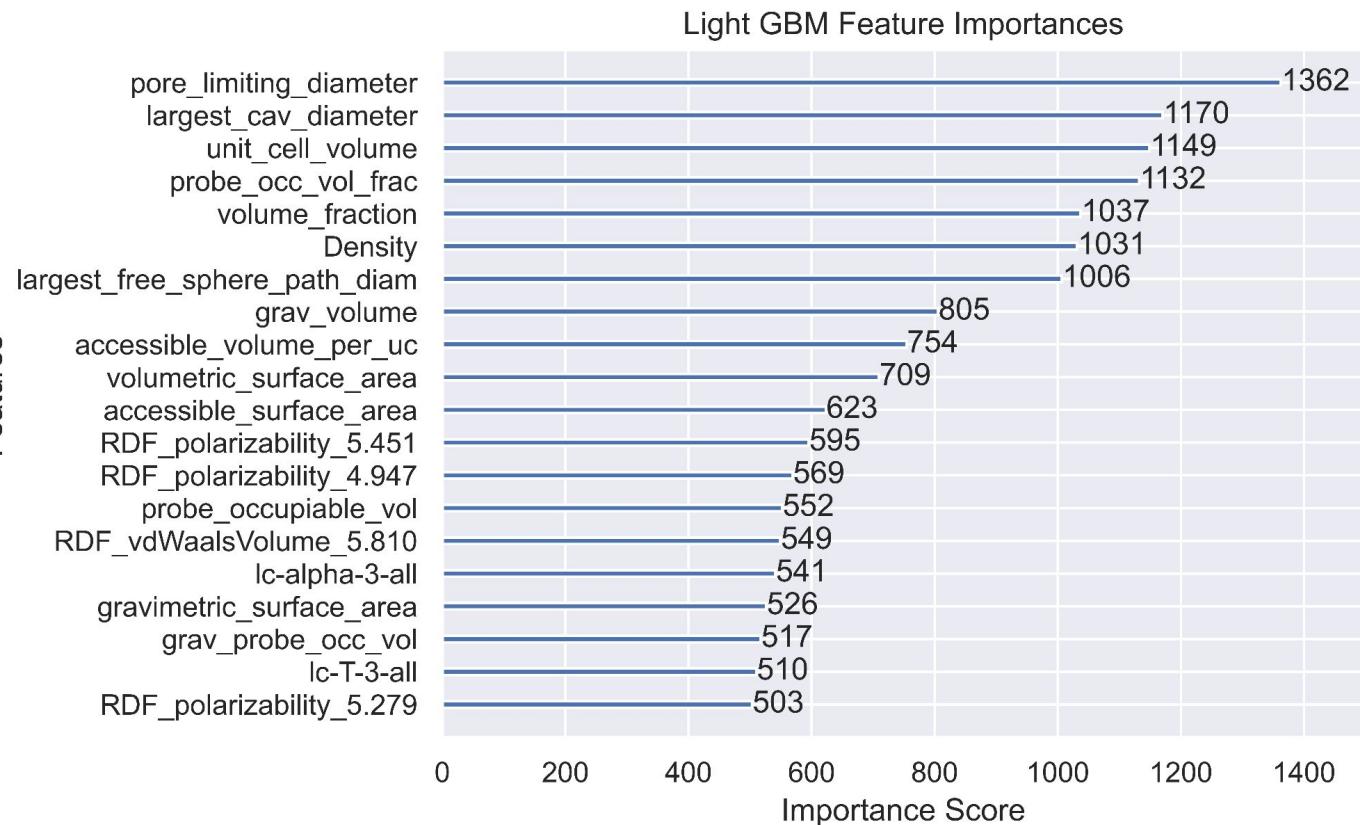
Initial Hyperparameter Tuning Results

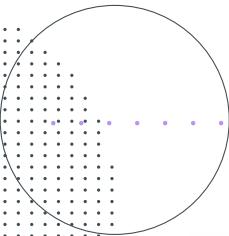


## Light GBM Progression

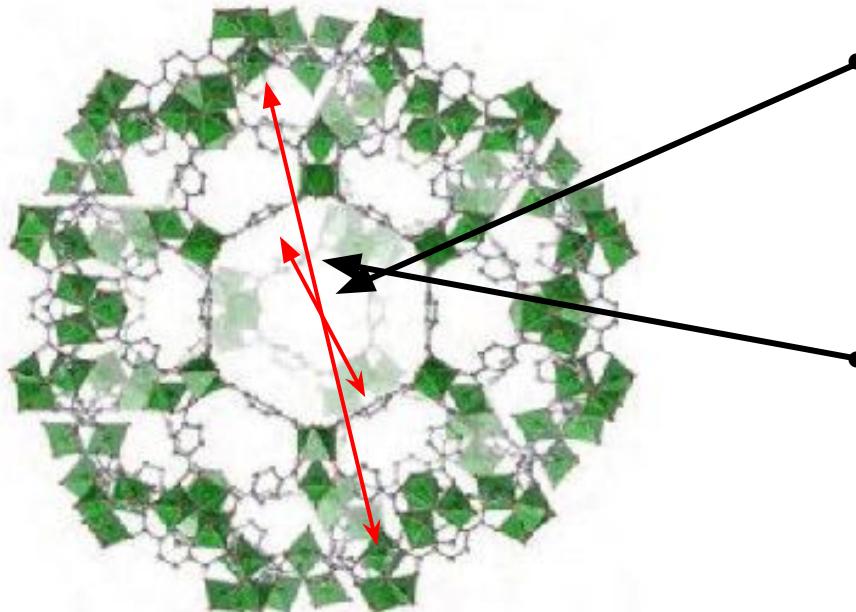


# Model Importances





## Pore Limiting and Largest Cavity Diameters



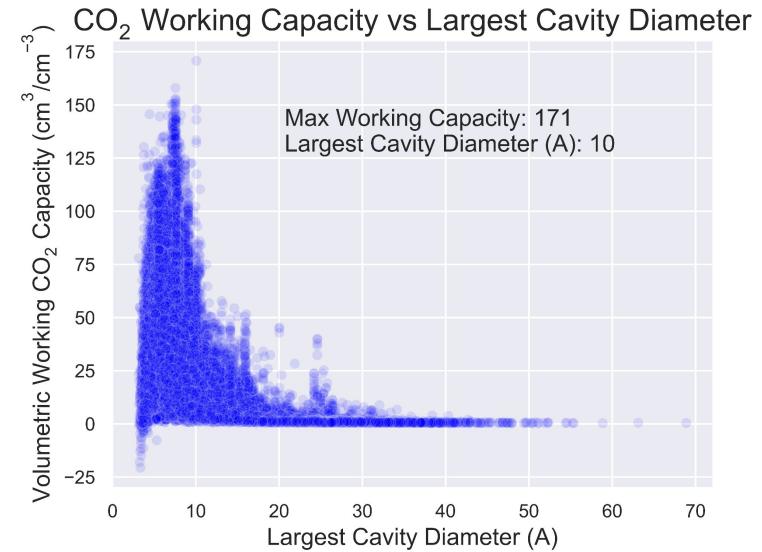
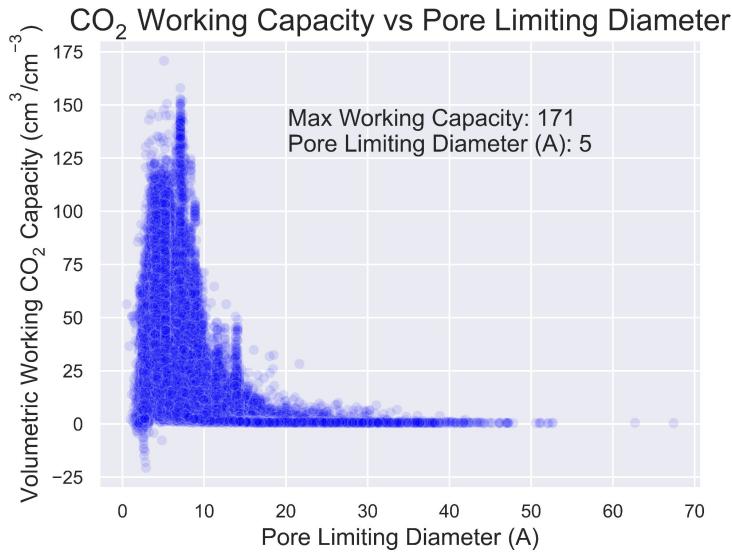
**Pore Limiting Diameter:**

largest opening to cavities of the MOF

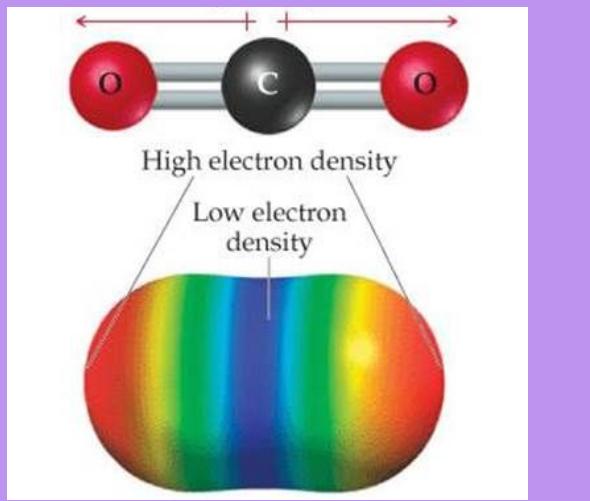
**Largest Cavity Diameter:**

largest opening inside of the MOF

# Pore Limiting and Largest Cavity Diameters



# Adsorption Fundamentals

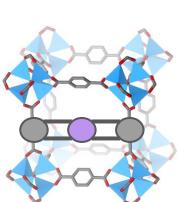


- Polar/polar
  - Positive attracting negative
- Polar/non-polar
  - CO<sub>2</sub> bumps into the MOF and sticks temporarily

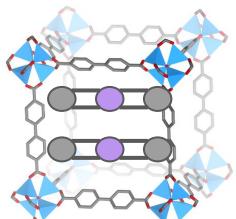
# Unit Cell Volume



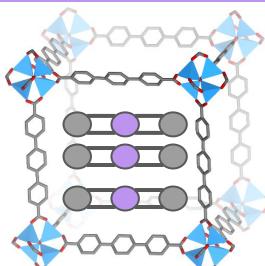
Zn-based MOFs:



MOF-5 / IRMOF-1

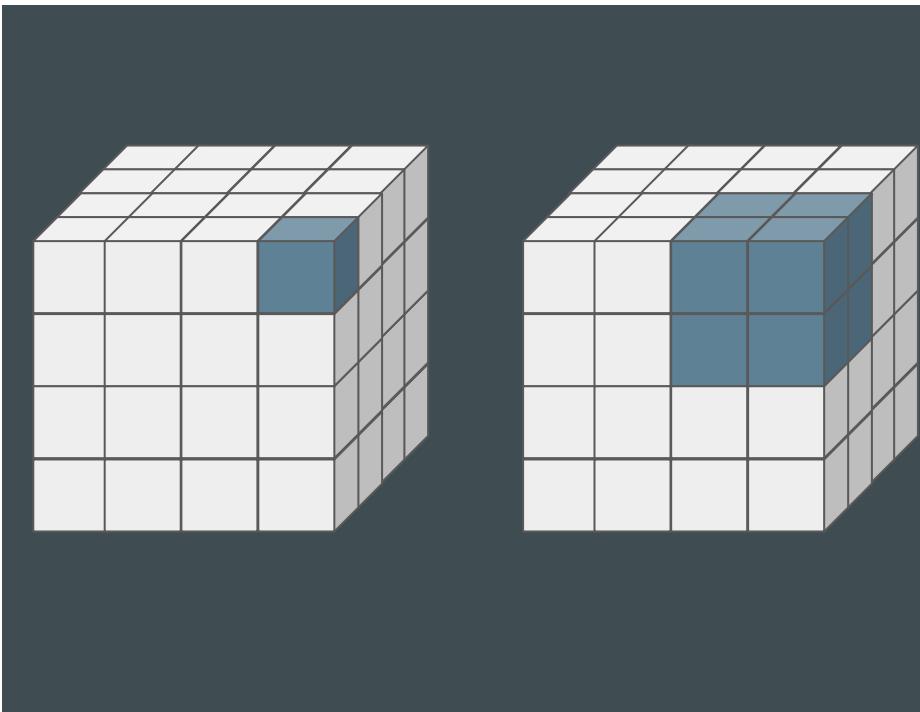


IRMOF-10



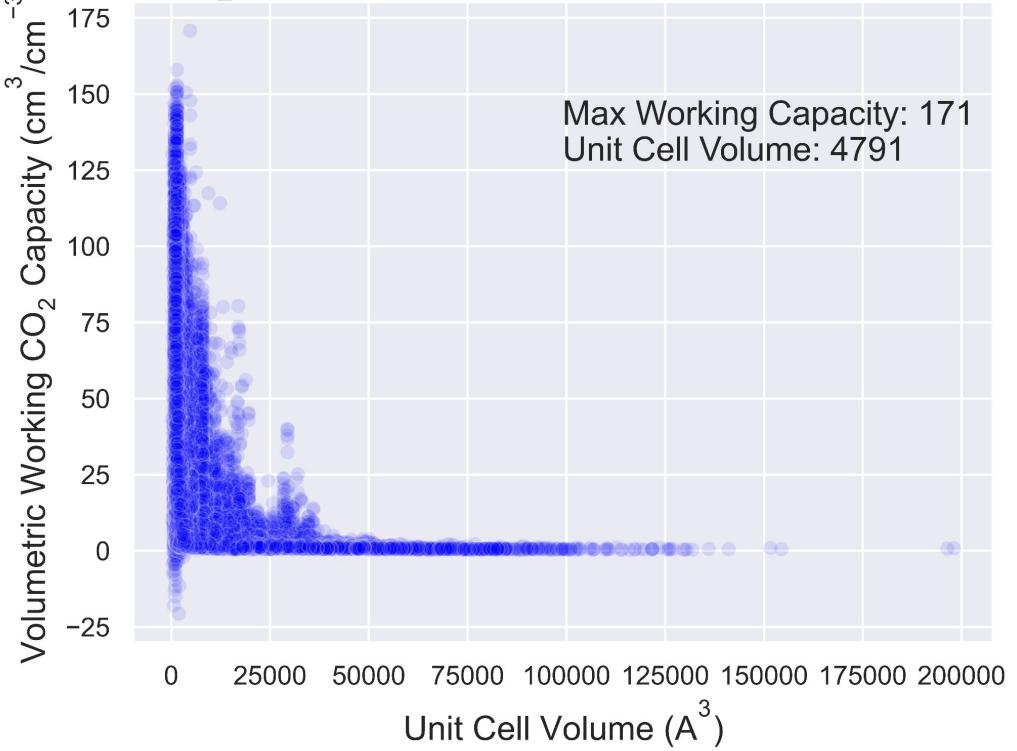
IRMOF-16

Source: <https://www.mn.uio.no/kjemi/>



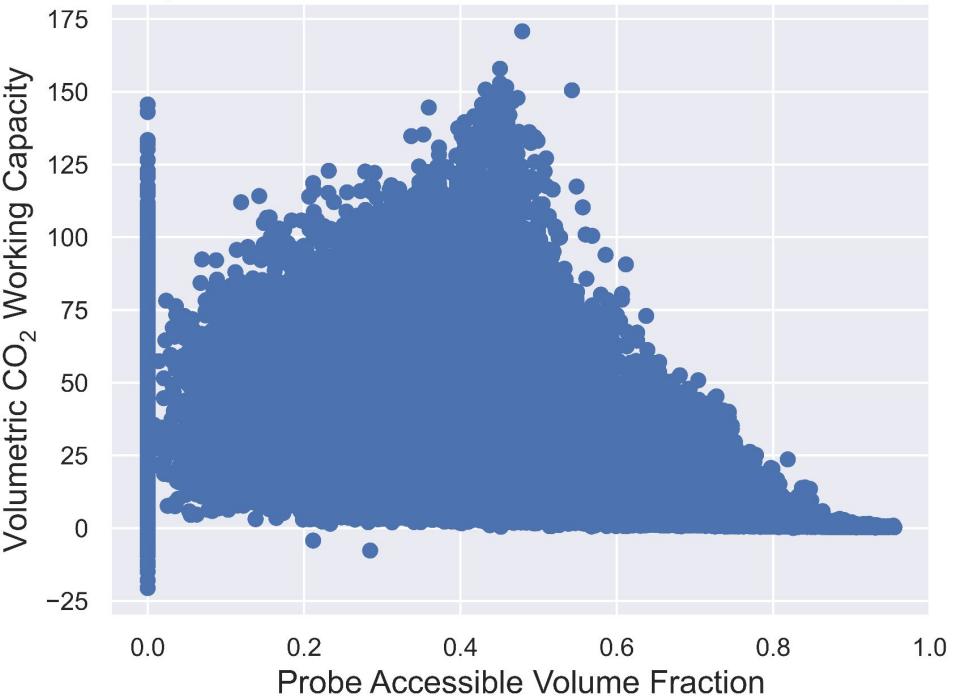
# Unit Cell Volume

CO<sub>2</sub> Working Capacity vs Unit Cell Volume

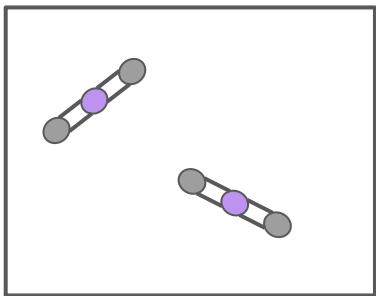


# Probe Accessible Volume Fraction

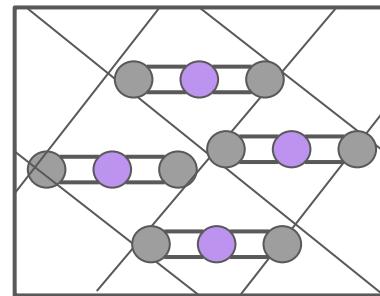
Relationship Between Volume Fraction and Working Capacity



# Probe Accessible Volume Fraction



1.0 (gaseous  $\text{CO}_2$ )



0.1 - 0.9  
(some MOF, some  $\text{CO}_2$ )



0.0 (no  $\text{CO}_2$ )

# Summary

- Light GBM regression model had 22.83 RMSE
- Top 4 most important features:
  - Pore limiting diameter
  - Largest cavity diameter
  - Unit cell volume
  - Probe accessible volume fraction
- General goal: Create a dense framework with channels roughly 8 angstroms wide

## Future Work

### Dig Deeper

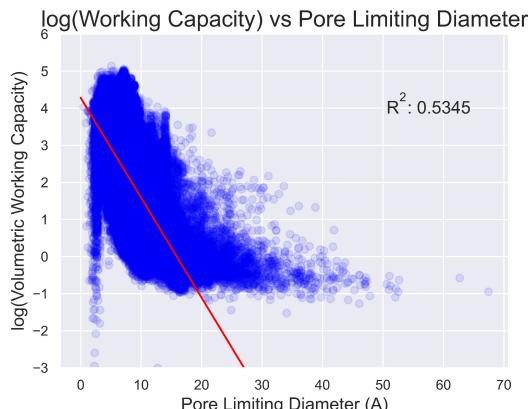
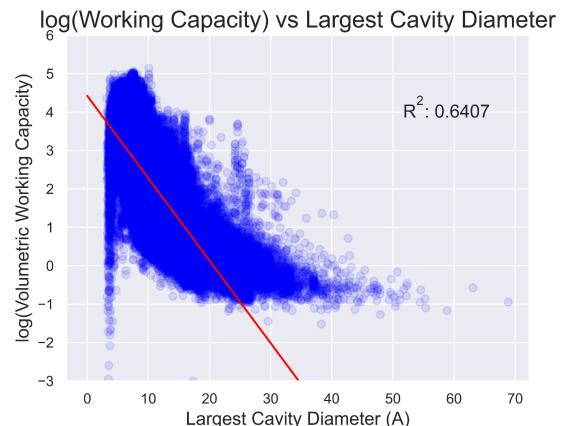
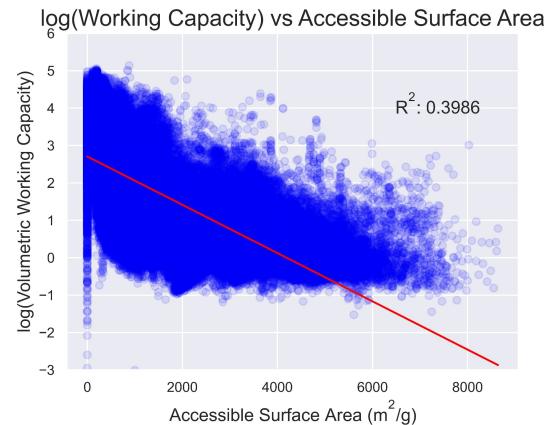
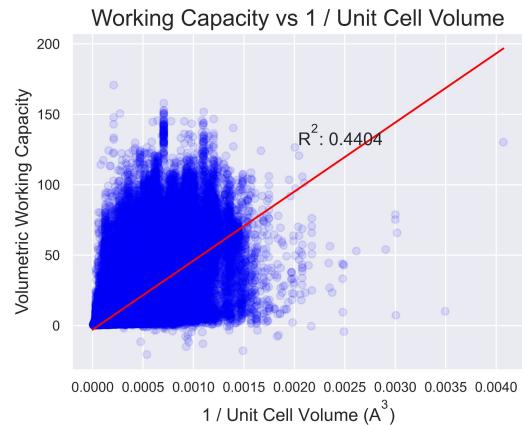
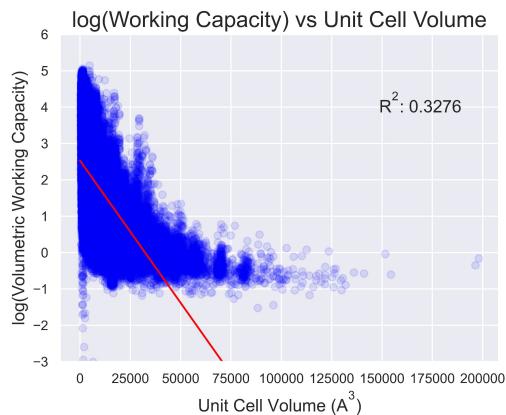
- Add features from other databases
- Find experimental data to compare vs theoretical

### Collaboration

- Work with research groups
- Recommend and synthesize specific MOFs

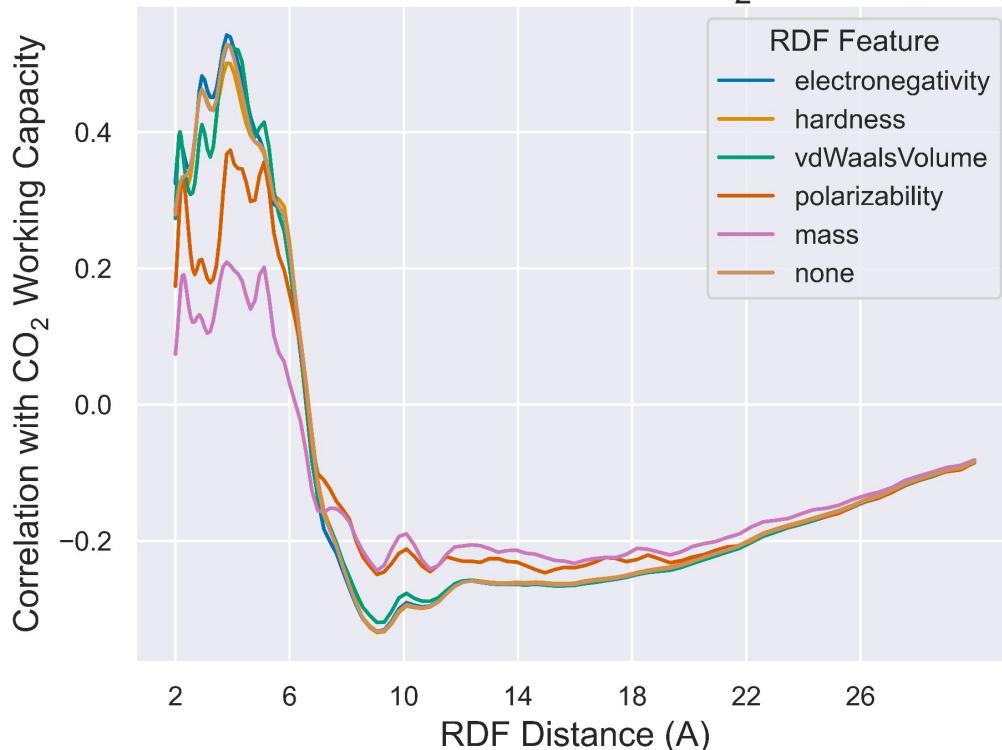
# Questions?

# Appendix



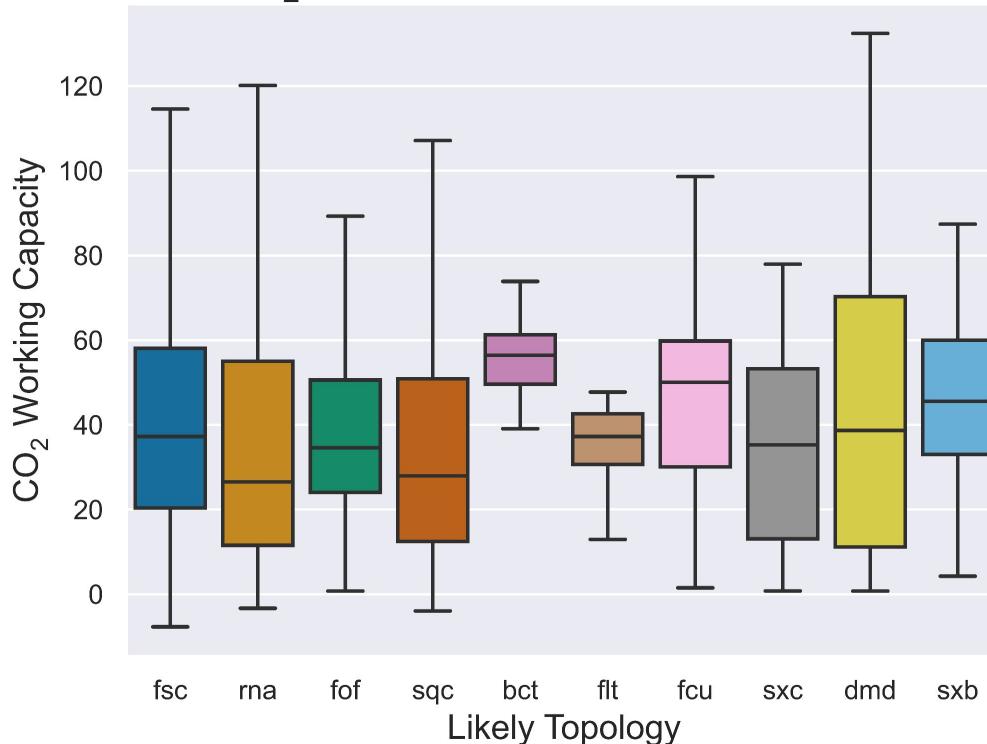
# Appendix

## RDF Distance Correlations with CO<sub>2</sub> Working Capacity



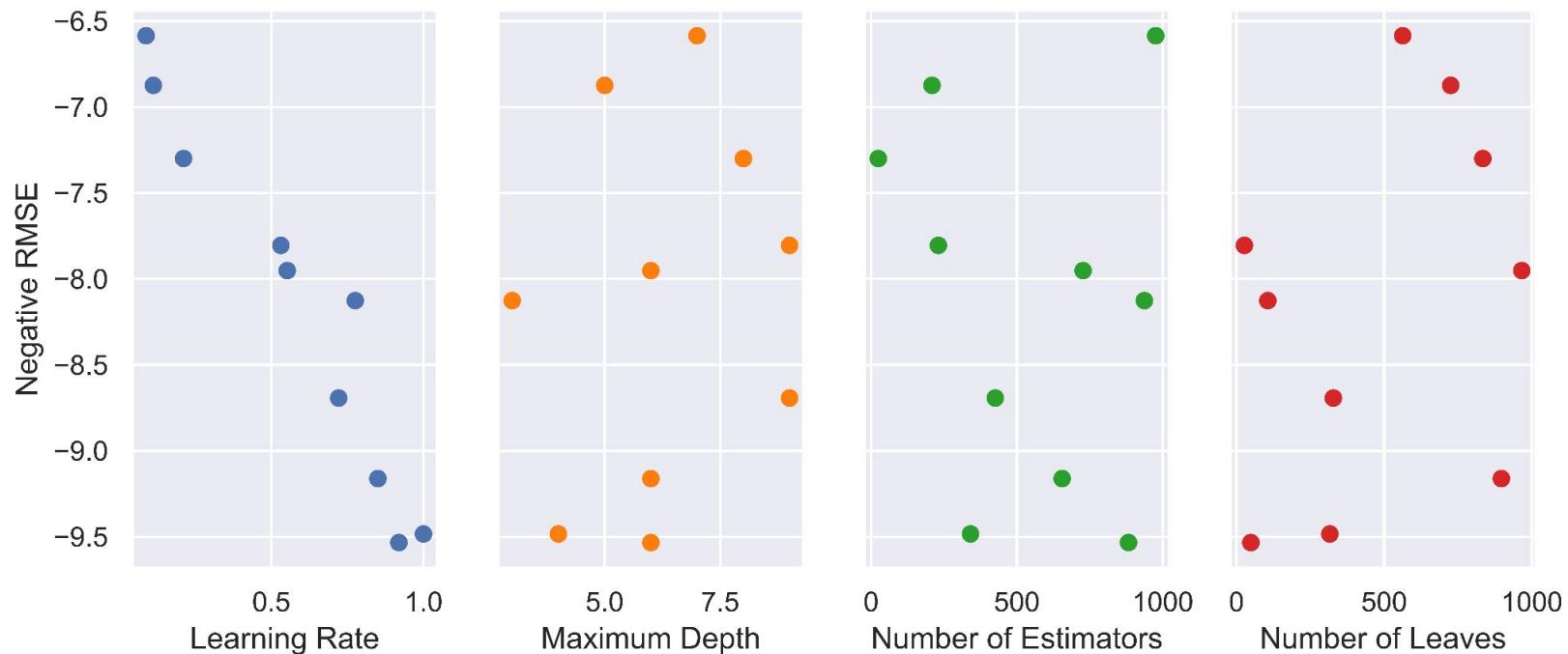
# Appendix

CO<sub>2</sub> Working Capacity by Topology



# Appendix

Light GBM Initial Tuning Results



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