Latent Variable Gaussian Processes and Bayesian Optimization Implementation to Determine Top-performing Metal-organic Frameworks

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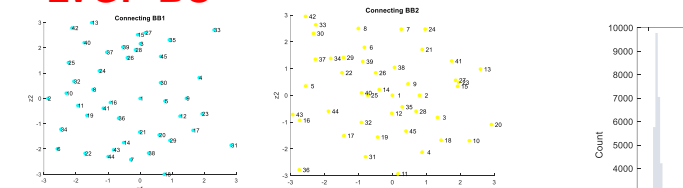**RANDALL SNURR**

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Research Objective

Metal-organic Frameworks (MOFs) are a class of nanoporous crystalline materials that are highly versatile and have a broad range of applications. Experimental synthesis cannot comprehensively explore the MOF-space, while common computation approaches such as high-throughput screening are computationally expensive. Our objective is to implement a novel computational method, Latent Variable Gaussian process (LVGP) and Bayesian optimization (BO), to study the MOF-space. This new approach is aimed to significantly reduce the computational cost by limiting the number of molecular simulations, while ensuring that top-performing MOFs are determined.
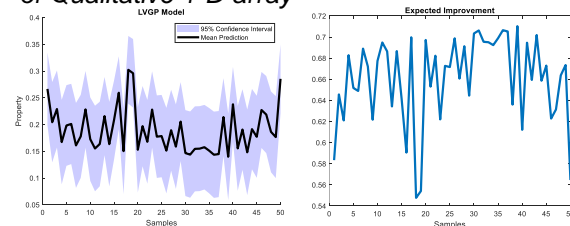
Metal-Organic Frameworks
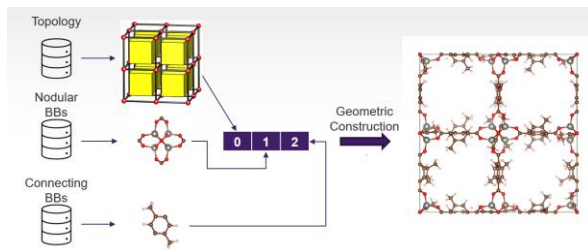
Qualitative 1-D array MOF representation by combining the building blocks labels that make up the MOF

Methodologies

Combined workflow of molecular simulations and LVGP-BO implemented in this work
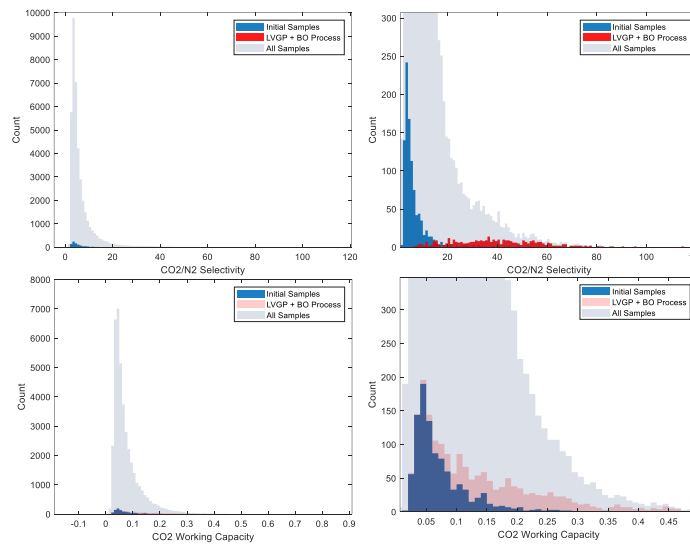
Discussion

- For a physical model with qualitive variables, a quantitative 2-D Latent Variable representation can explain the underlying effects on the property

- By only scanning less than 5% of the 40,500 sample dataset, LVGP-BO identified more than 80% of Top 25 best performing MOFs for CO_2 Working Capacity and N_2 / CO_2 Selectivity properties.
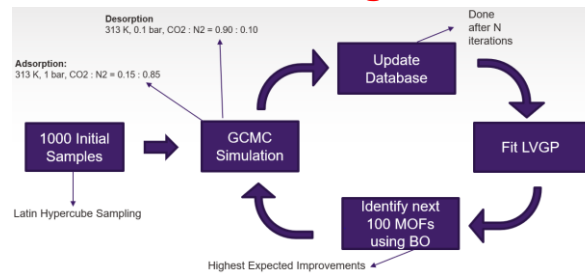
LVGP-BO

Quantitative 2-D Latent Space representation of Qualitative 1-D array

Constructed LVGP model to find top performing MOFs with BO through maximization of EI

Results

Conclusions

- Successfully implemented LVGP-BO to determine top-performing MOFs

- Automated the process to find potential MOFs with different topologies and different single objective functions

References

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