

Supplementary Information: Bayesian optimization of nanoporous materials

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September 27, 2021

S1 Influence of the number of COFs used to initialize BO

We study how the number of COFs, randomly selected from the library, used to initialize BO affects the search efficiency of BO in Fig. S1.

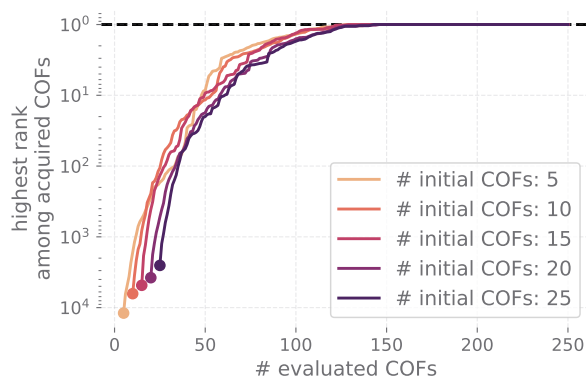


Figure S1: How does the number of COFs used to initialize the GP surrogate model for BO influence the search efficiency of BO? Here, we show the search efficiency curves of BO when initialized with different numbers of COFs (solid points).