Data-Driven Design of Electroactive Metal-Organic Frameworks

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Abstract

Metal-organic frameworks (MOFs) are versatile materials with tunable crystal structures, morphologies, and chemistries, offering diverse physical and chemical properties. Though typically electrically insulating, specific combinations of organic and inorganic components can impart electrical conductivity and redox activity in MOFs [1], [2]. Electronic structure theory methods like Density Functional Theory (DFT) offer valuable insights into the fundamental chemistry and physics of these materials, and are being used to study them extensively. However, the virtually limitless chemical space of MOFs presents a significant challenge in identifying optimal candidates for specific applications. The computational expense that comes with DFT is another major obstacle in the identification and discovery of novel electroactive MOFs. To tackle these challenges, in this work we exploit machine learning approaches such as novel active learning methods [3] to accelerate the discovery of these MOFs in a data-driven manner.

References

[1] L. S. Xie, G. Skorupskii, M. Dincă, *Chem. Rev.* (2020), **120**, 8536.
[2] J. Calbo, M. J. Golomb, A. Walsh, *J. Mater. Chem. A* (2019), **7**, 16571.
[3] A. Jose, E. Devijver, N. Jakse, and R. Poloni, Journal of the American Chemical Society (2024), **146**, 6134–6144.