Modeling Metal-Organic Frameworks for Water Harvesting and Catalysis

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Metal-organic frameworks (MOFs) are versatile platforms for various applications including catalysis for complex reactions and water harvesting. I will first present our ongoing efforts to understand and design the water-filling mechanism for water-harvesting MOFs.[1]
I will then describe our combined computational and data-driven study of MOF-supported catalysts for propyne dimerization. Utilization of machine learning algorithms in conjunction with experimental data can not only predict superior catalytic materials, but also under which experimental conditions they are most optimal.[2]

[1] N. Hanikel, X. Pei, S. Chheda, H. Lyu, W. Jeong, J. Sauer, L. Gagliardi, and O. M. Yaghi, *Evolution of water structures in metal-organic frameworks for improved atmospheric water harvesting*, Science, 2021, 374, 454–459.
[2] [1] K. E. McCullough, D. S. King, S. Chheda, M. S. Ferrandon, T. A. Goetjen, Z. H. Syed, T. R. Graham, N. M. Washton, O. K. Farha, L. Gagliardi, and M. Delferro *High-throughput experimentation, theoretical modeling, and human intuition: lessons learned in metal-organic framework-supported catalyst design*, ACS Central Science ASAP (2023) DOI: 10.1021/acscentsci.2c01422