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The Nanoporous Materials Genome in Action

Abstract

The attractive feature of Metal Organic Frameworks (MOFs) is that by changing the ligand and/or metal, these nanoporous crystals can be chemically tuned to perform optimally for a given application. This unique chemical tunability allows us to tailor-make materials that are optimal for a given application. The promise of finding just the right material seems remote however: because of practical limitations we can only ever synthesize, characterize, and test a tiny fraction of all possible materials. To take full advantage of this development, therefore, we need to develop alternative techniques, collectively referred to as Materials Genomics, to rapidly screen large numbers of materials and obtain fundamental insights into the chemical nature of the ideal material for a given application.These computational materials genomics initiatives have been so successful that we have created a new problem: what to do with so much data? In this presentation we will discuss different computational strategies to deal with a large amount of data. We illustrate on the use of these strategies by addressing the following questions: How the find the best material for a given application? How to find materials with similar pore shape? How to design a material that optimally binds CO2? And, what can we learn from failed experiments?