SAND2017-7594D

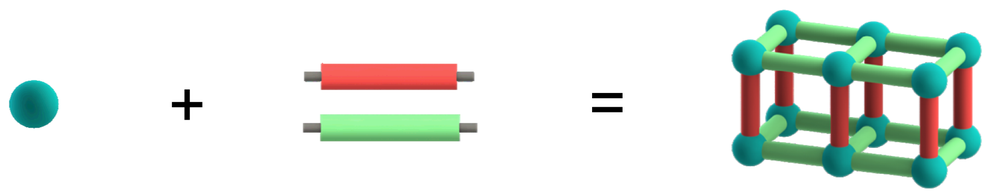
Metal-Organic Frameworks for Negative Thermal Expansion Materials

Ashley Bird[1] and Nicholas Burtch[2]

[1]The University of Texas at Austin
[2]Sandia National Laboratories

Background

Metal-organic frameworks (MOFs) are crystalline, nanoporous materials with exceptionally high surface areas and chemically tunable structures.



Metal Node | *Organic Ligand* | *Metal-Organic Framework*

Motivation

Negative thermal expansion (NTE) materials contract with increases in temperature. However, existing NTE materials are limited by tunability of the NTE and compatibility with PTE matrix.

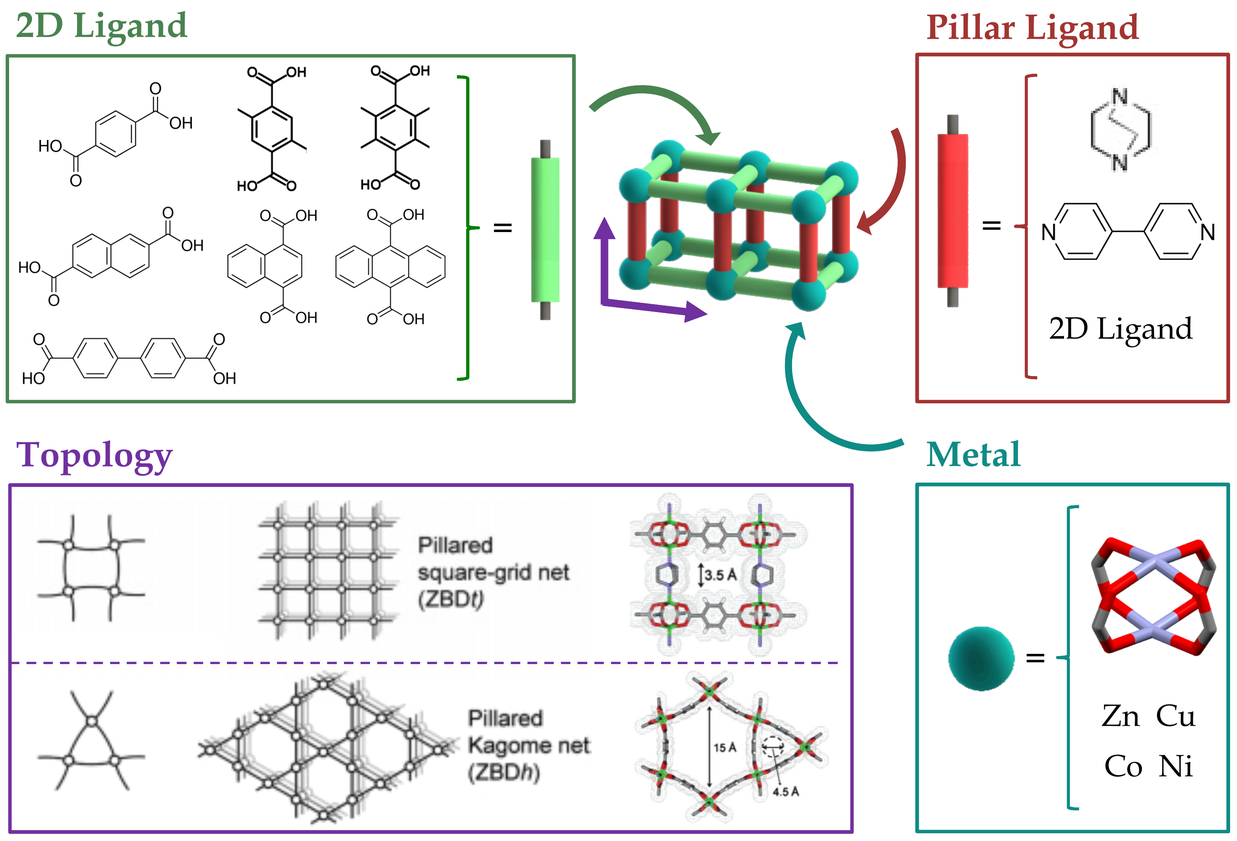
$$\alpha_l = \frac{1}{l}\left(\frac{\partial l}{\partial T}\right)_P$$

Coefficient of thermal expansion

Thermal expansion in materials can result in materials fracturing. Understanding the structure-property relationship of NTE MOFs can allow us to tune and apply these MOFs in materials to compensate for positive thermal expansion (PTE) and reduce strain leading to fracture.

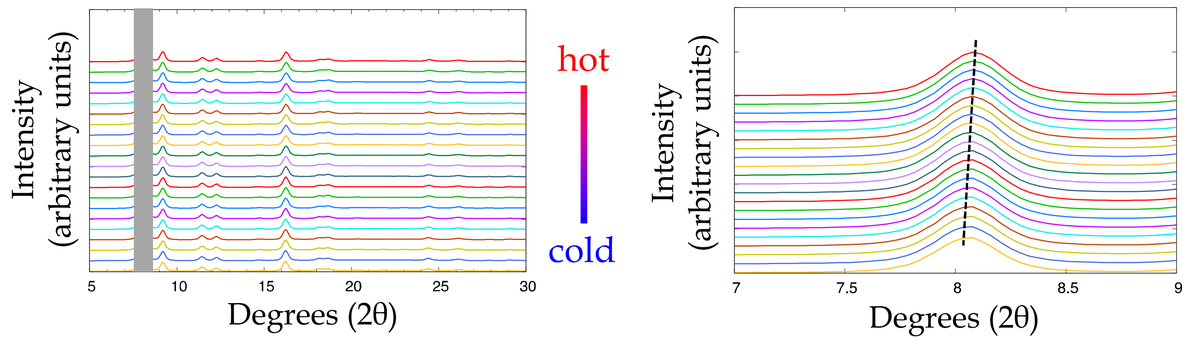
Structures

The structure-property relationship is explored by varying 2D ligands, pillar ligands, metals, and topology.

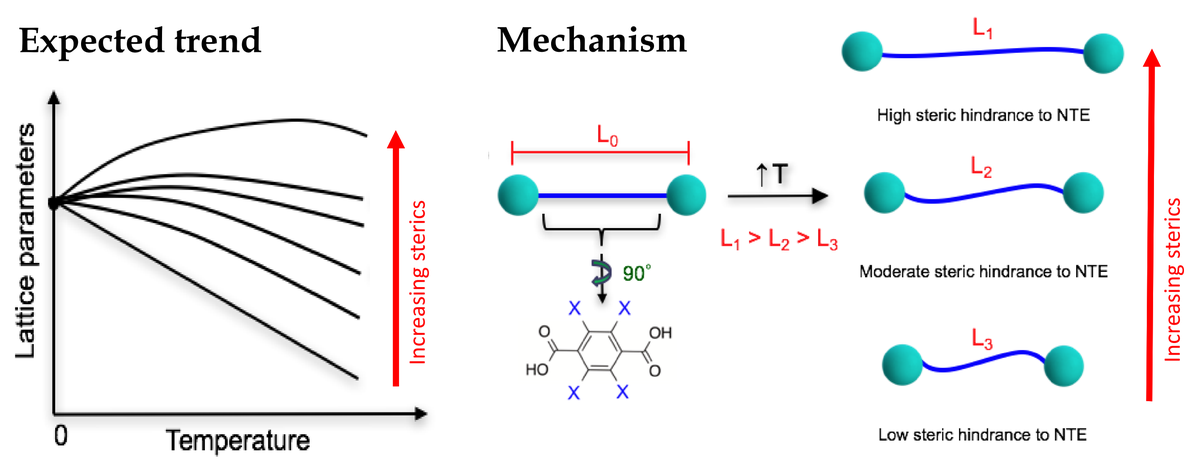


Analytical Methods

The NTE coefficient is determined using X-Ray Diffraction (XRD). Lattice parameters are calculated from the diffraction patterns, which can be used to find the coefficient of thermal expansion.

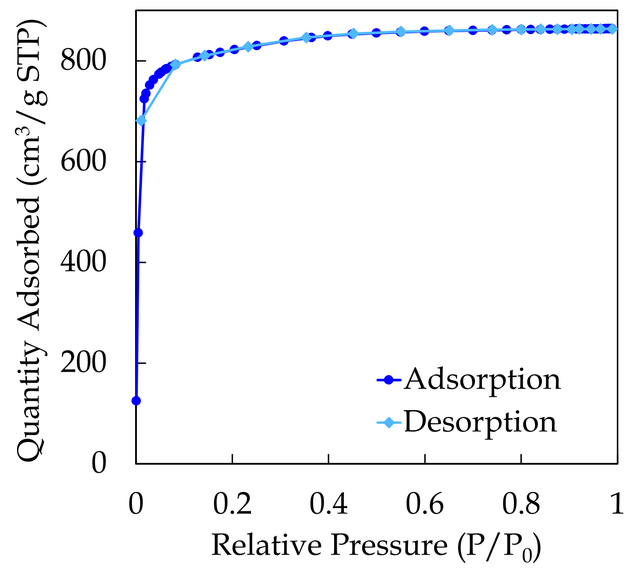


Based on the proposed mechanism for NTE, the thermal expansion can be tuned by changing the ligand functionality. Ligands with high steric hindrance are expected to have PTE while those with low steric hindrance would have NTE.



Results and Future Direction

Various MOFs have been synthesized. Before measuring XRD, the MOFs are activated by removing any guest molecules from the pores, and BET (Brunauer–Emmett–Teller) surface areas are determined by nitrogen adsorption/desorption.



Isotherm for IRMOF-1.
BET Surface Area: ~3460 cm³/g

The next step is to collect XRD patterns for each variation over a temperature range and determine the thermal expansion coefficient.

Acknowledgements

This work was funded through the Sandia National Laboratories Truman Fellowship Program, which is funded by the Sandia Laboratory Directed Research and Development (LDRD) Program.

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.