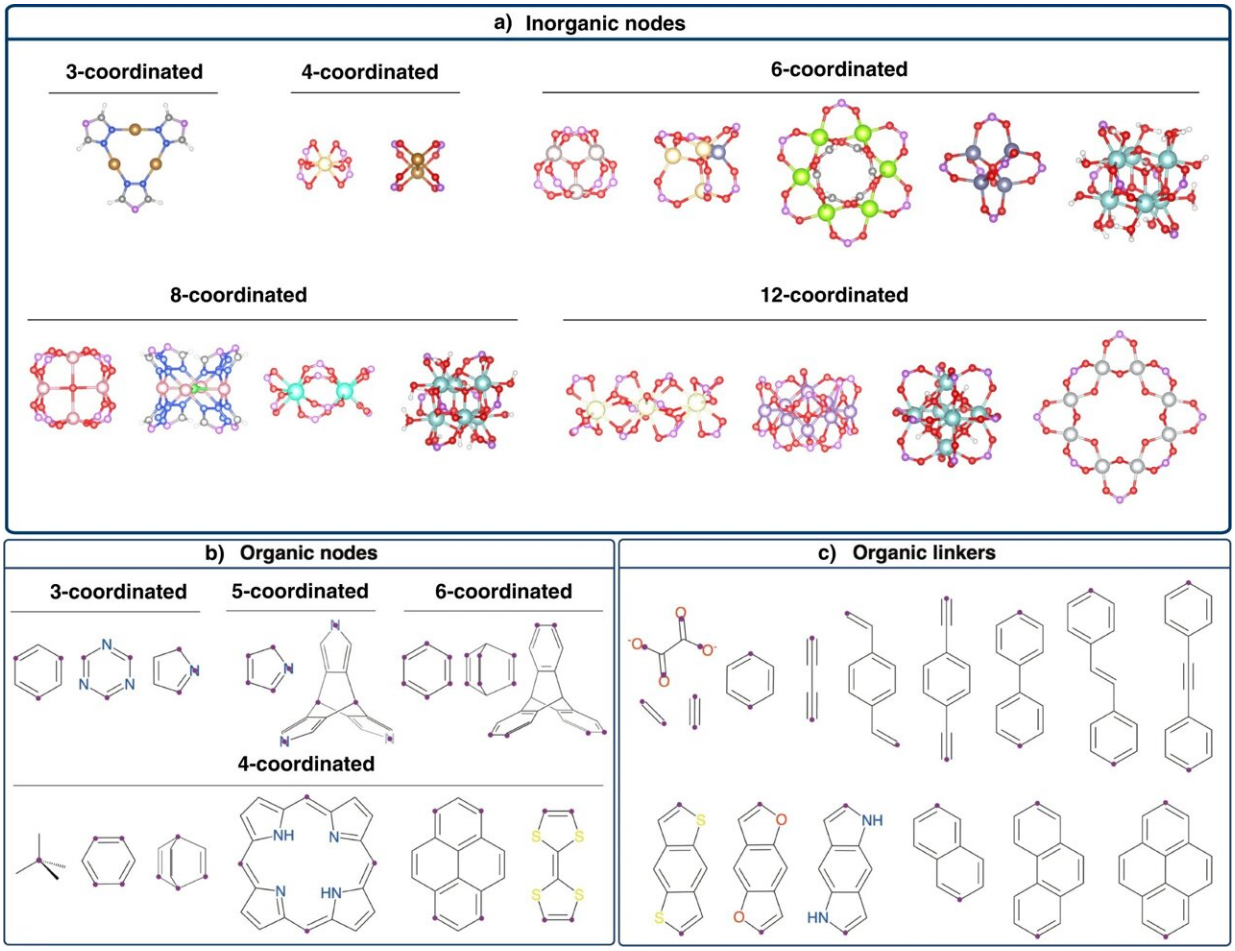
Too hot to handle: Study tests the thermal conductivity of metal organic frameworks

March 13 2023, by Kat Procyk



Building blocks that are used to build 10,194 hypothetical MOFs containing 1015 topologies. **a** inorganic nodes; **b** organic nodes; **c** organic linkers. The connecting points to other building blocks are represented with violet circles. Credit: *npj Computational Materials* (2023). DOI: 10.1038/s41524-022-00961-x

Metal organic frameworks, or MOFs, are kind of like LEGOs.

The pieces are simple to connect, yet they're capable of building highly sophisticated structures. These structures can be used to filter toxic gases out of the air or to store fuel for natural or hydrogen gas-powered engines.

LEGOs melt when they interact with heat. But, what happens to MOFs?

A new study from the University of Pittsburgh Swanson School of Engineering found that MOFs heat up significantly when they soak up gases and if they get too hot, they stop working.

"This study helps us determine which MOFs can soak up gases and dissipate that heat efficiently, ultimately moving MOFs closer to practical commercial implementation," Chris Wilmer, associate professor of chemical and petroleum engineering at Pitt and co-author, explained.

The team used computational screening of thermal conductivity in over ten thousand MOFs, which required over a million hours of supercomputing power. They learned MOFs with high densities, small pores, and four-connected metal nodes are more capable of conducting heat. On the other hand, those with extremely large pores are not.

"There are millions of different types of MOFs one can design, so it can be hard to determine the best one for the job," said Meiirbek Islamov, a Ph.D. student at Pitt and first author on the study. "This study allows us to be more accurate as we create them in a lab."

Wilmer and his coauthors, who include researchers from Pitt, UC Berkeley, Carnegie Mellon University, and the Colorado School of Mines, focus on designing MOFs with excellent thermal properties.

Wilmer has been widely cited for his previous work on using computer simulations to predict the properties of MOFs.

The findings are published in the journal *npj Computational Materials*.

More information: Meiirbek Islamov et al, High-throughput screening of hypothetical metal-organic frameworks for thermal conductivity, *npj Computational Materials* (2023). DOI: 10.1038/s41524-022-00961-x

Provided by University of Pittsburgh

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