**Symmetry-Guided Design of Highly Porous MOFs**

**Scientific Achievement**
A novel Zr MOF, PCN-521, prepared from symmetry-guided synthesis, possesses the largest porosity and cavity size among all MOFs made from tetrahedral linkers.

**Significance and Impact**
This work has offered a general way of bottom-up design of stable, non-interpenetrated MOFs with desired topology and porosity.

**Research Details**
- MOFs with fluorite topology are highly desirable because of their large cavities and non-interpenetrated nature.
- Two components that are symmetrically complementary with each other should be selected: a 4-connected ligand and an 8-connected metal-containing cluster.
- Augmentation of 4-connected nodes in fluorite structure by MTBC ligand has generated a stable and highly porous MOF with its cavity size of $20.5 \times 20.5 \times 37.4 \, \text{Å}$.
- Isostructural MOFs can be made from Hf clusters.


(a) The crystal structure of fluorite (left) and PCN-521 (right).
(b) The building blocks of PCN-521 (left: MTBC ligand; right: Zr cluster)
(c) The fluorite topology of PCN-521

Work was performed at Texas A&M University.