Scientific Achievement

A database was developed consisting of metal-organic frameworks containing anion groups as structural pillars; the structural properties of each MOF were characterized with DFT and tested for Xe/Kr gas separation to determine potential indicators of separation ability.

Significance and Impact

Xe and Kr are both individually useful, however current separation techniques are costly and energetically expensive; discovering materials that may be efficient in separation would make the process much more efficient and low-impact.

Research Details

The database was constructed using DFT to optimize anion-pillar structures made from various transition metals, fluorine groups, and ligands

- Xe/Kr screening was carried out by tracking the Henry coefficient ratios, working capacities, and regenerabilities of each MOF during separation
- SIFSIX-6-Cd-i had the best balance between working capacity and separation selectivity