Pore Surface Engineering with Controlled Loadings of Functional Groups via Click Chemistry in Highly Stable Metal–Organic Frameworks

Scientific Achievement
Highly stable isoreticular Zr-MOFs offer an ideal platform for pore surface engineering by anchoring various functional groups with controlled loadings onto the pore walls, endowing the MOFs with tailor-made interfaces and powerful applications.

Significance and Impact
The work develops an approach for pore surface engineering of stable MOFs to realize desired composition, density and function.

Research Details
- Azide groups with desired contents are introduced into highly stable isoreticular Zr-based MOFs.
- Quantitative click reactions with alkynes occur to afford various functional groups with controlled loadings on the pore wall surfaces.
- The functionalized MOFs remain stable and the engineered pore surfaces are readily accessible, thus providing more opportunities for powerful applications of MOFs.

Work was performed at Texas A&M University.

Schematic illustration of the general strategy for pore surface engineering of Zr-MOFs with precise control over composition, density, and functionality by two steps: (1) introduction of azide groups into the MOF with a desired loading (0 - 100%) by simply changing molar ratio of CH₃⁻ and N₃⁻ appended ligands; (2) grafting of various functional groups onto the pore walls of the MOF via the click reaction between azide and alkyne groups in quantitative yield. The green spheres: Zr₆ clusters.


Work was performed at Texas A&M University.