

Electronic Supplementary Information

## Rational design of metal-organic frameworks with anticipated porosities and functionalities

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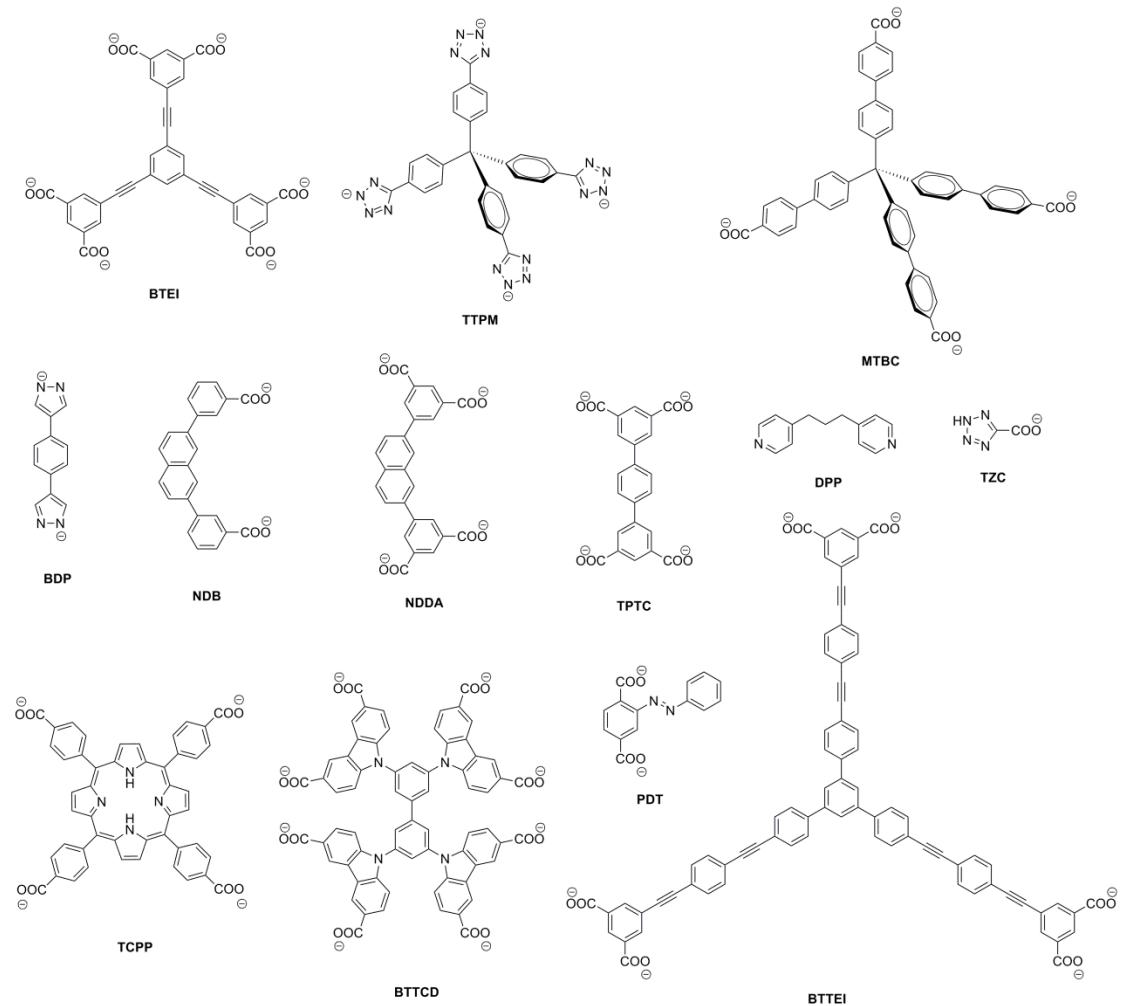
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## Section 1. The Chemical Structure of MOF Ligands



**Scheme S1** The chemical structure of all the ligands mentioned in this review

## **Section 2. Abbreviations and Acronyms**

IMP: Imperial College London (Nomenclature of a series of MOFs)

MOF: Metal-Organic Framework

MOP: Metal-Organic Polyhedra

NU: Northwestern University (Nomenclature of a series of MOFs)

PCN: Porous Coordination Network

PCP: Porous Coordination Polymer

PSM: Post-Synthetic Modification

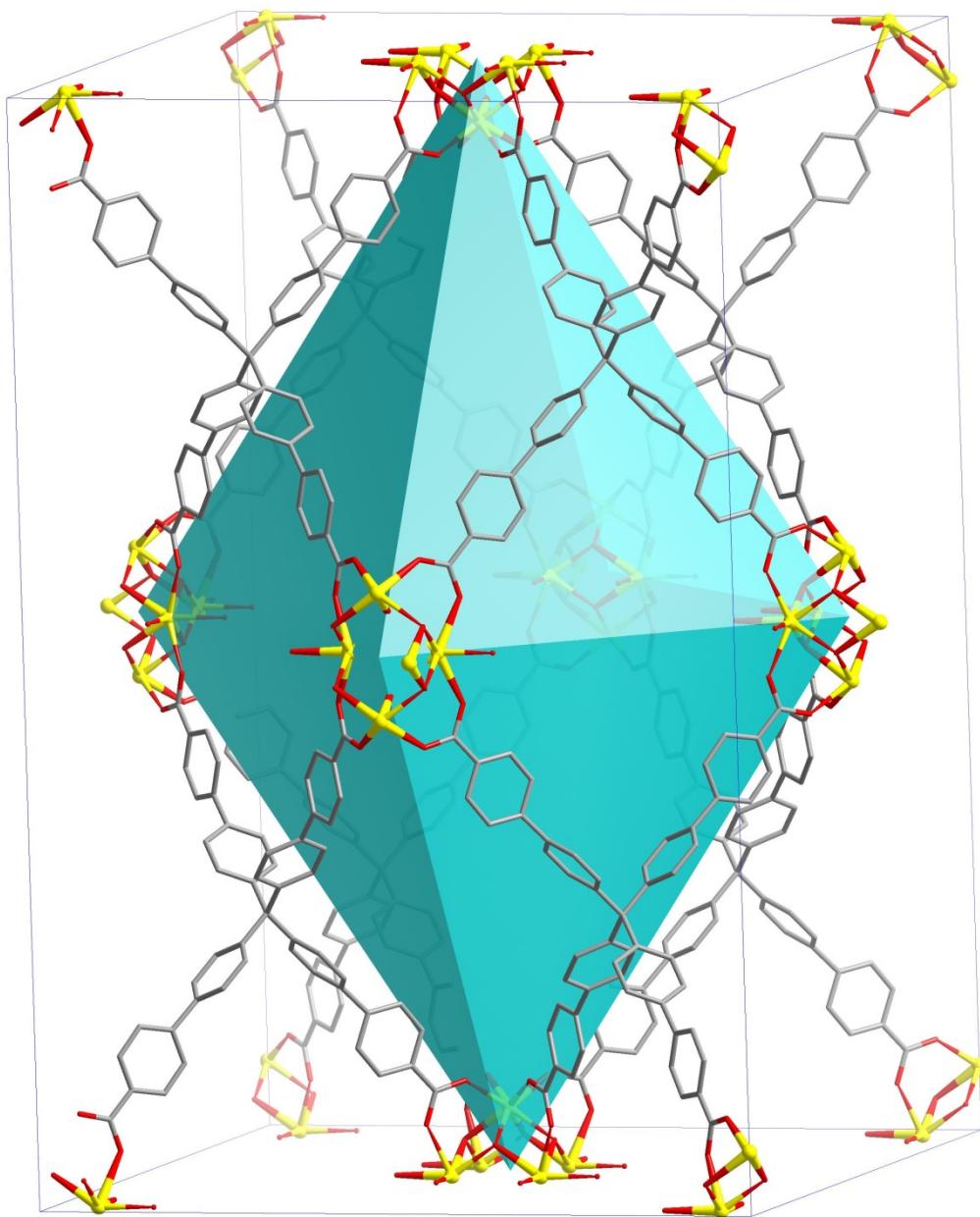
SBU: Secondary Building Unit

SMT: Single Molecular Trap

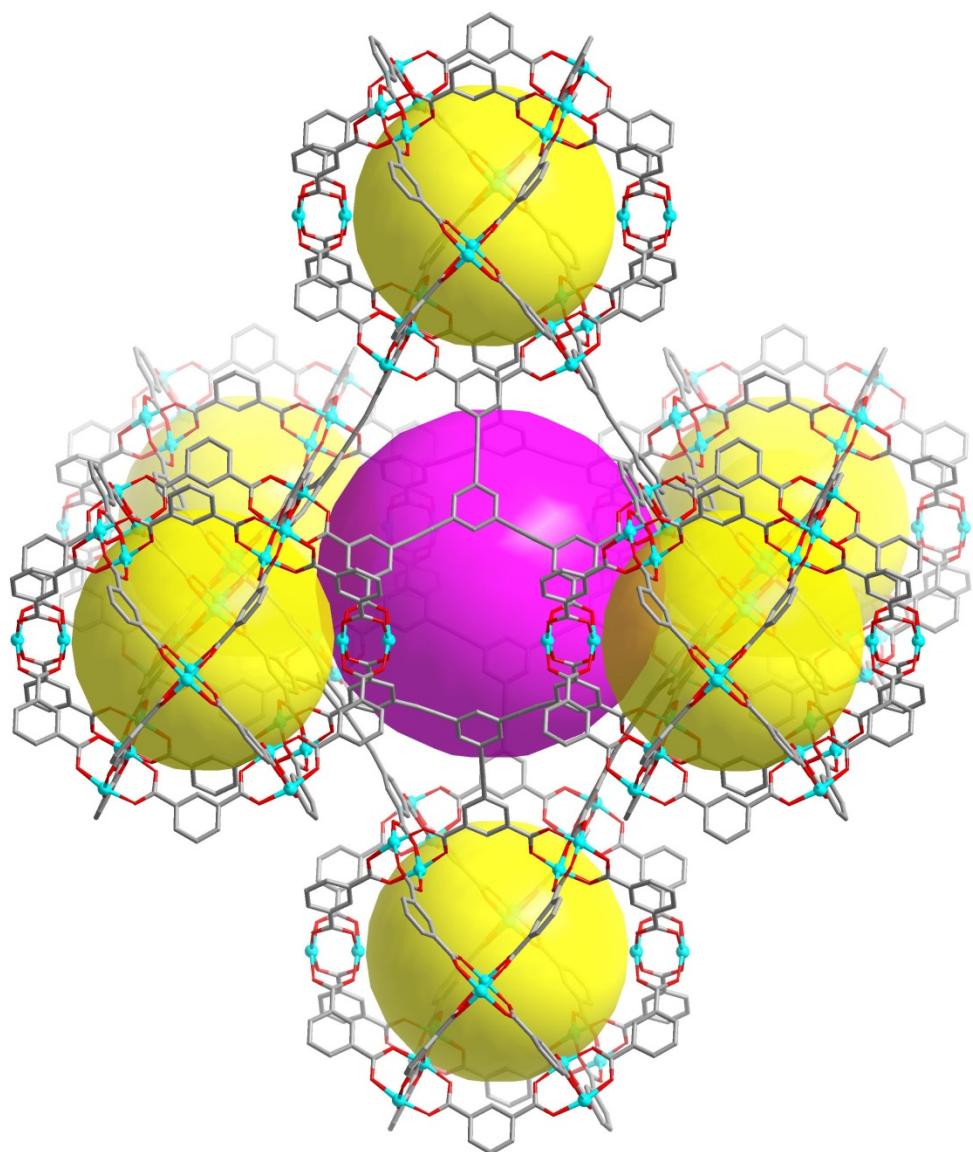
UiO: University of Oslo (Nomenclature of a series of MOFs)

UMC: Unsaturated Metal Center

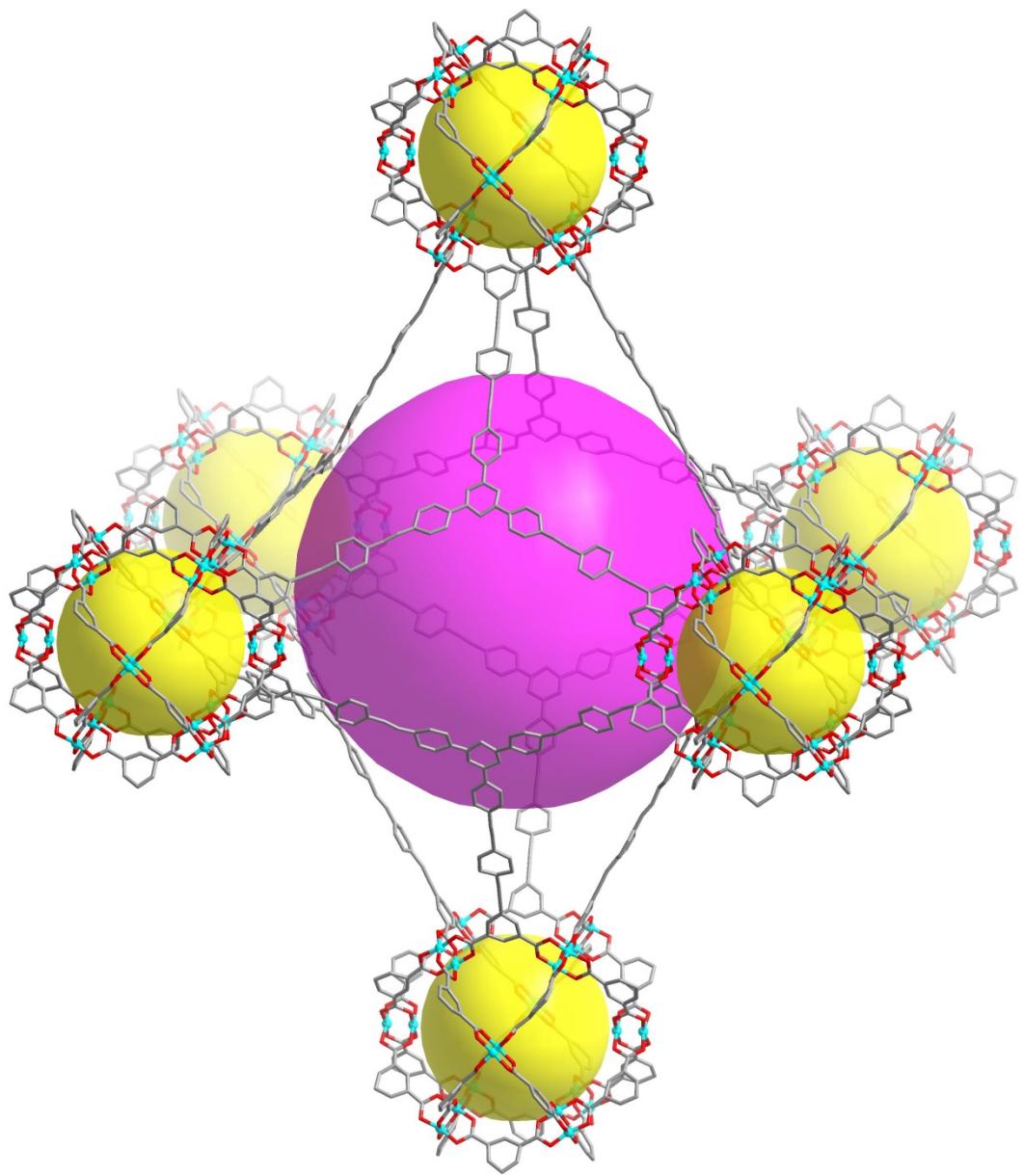
**Section 3. High-Resolution Pictures of Some Selected MOF Structures**



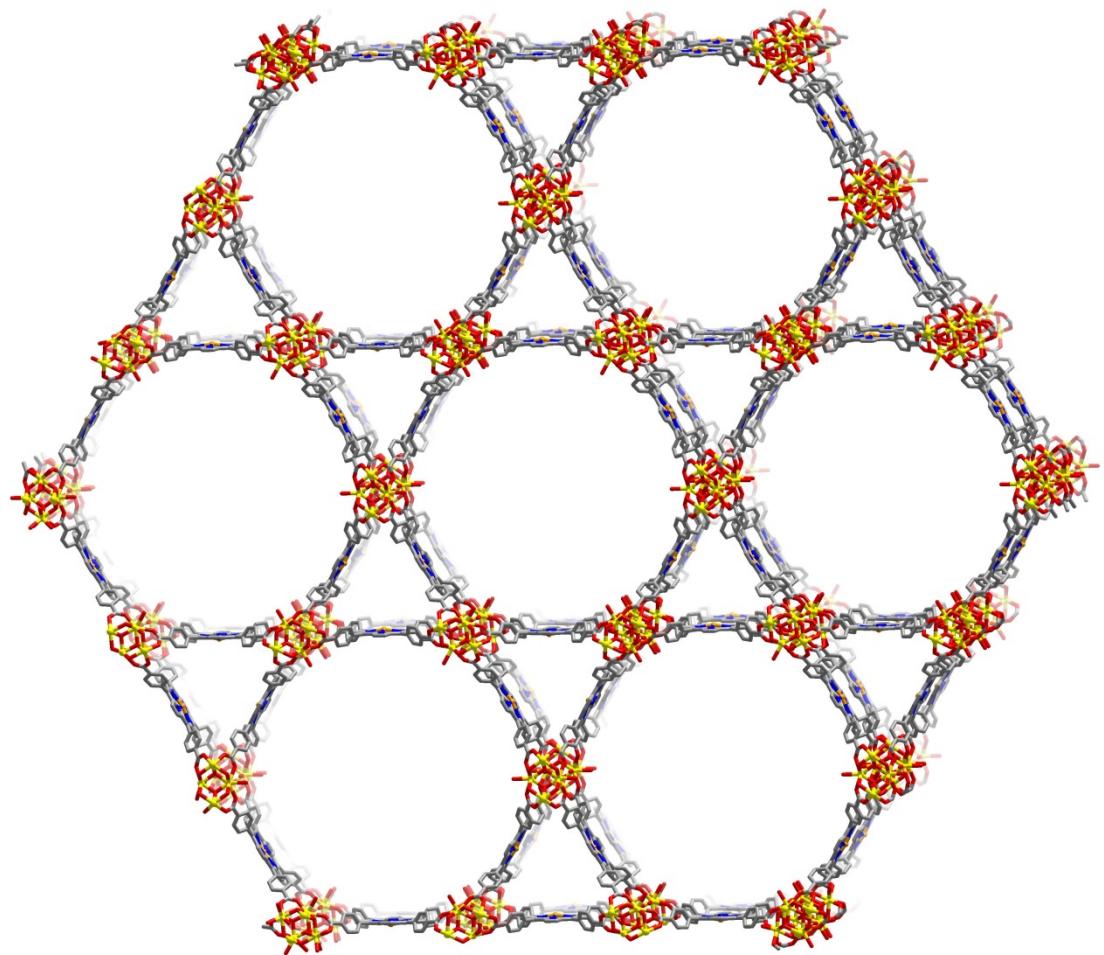
**Figure S1** The crystal structure of PCN-521



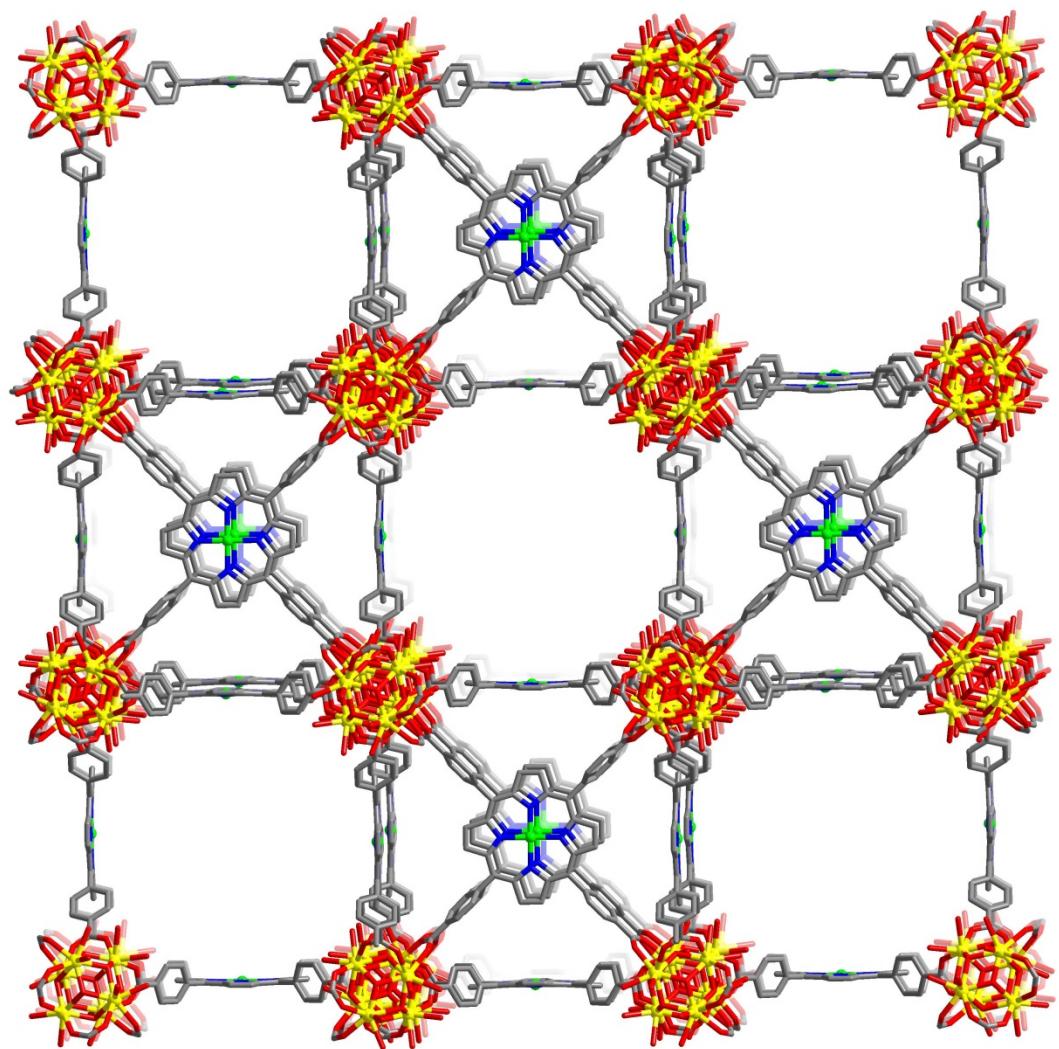
**Figure S2** The crystal structure of PCN-61



**Figure S3** The crystal structure of NU-110



**Figure S4** The crystal structure of PCN-222



**Figure S5** The crystal structure of PCN-224

## **Section 4. Funding Resources of All Contributors**

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