Metal–organic frameworks and applications

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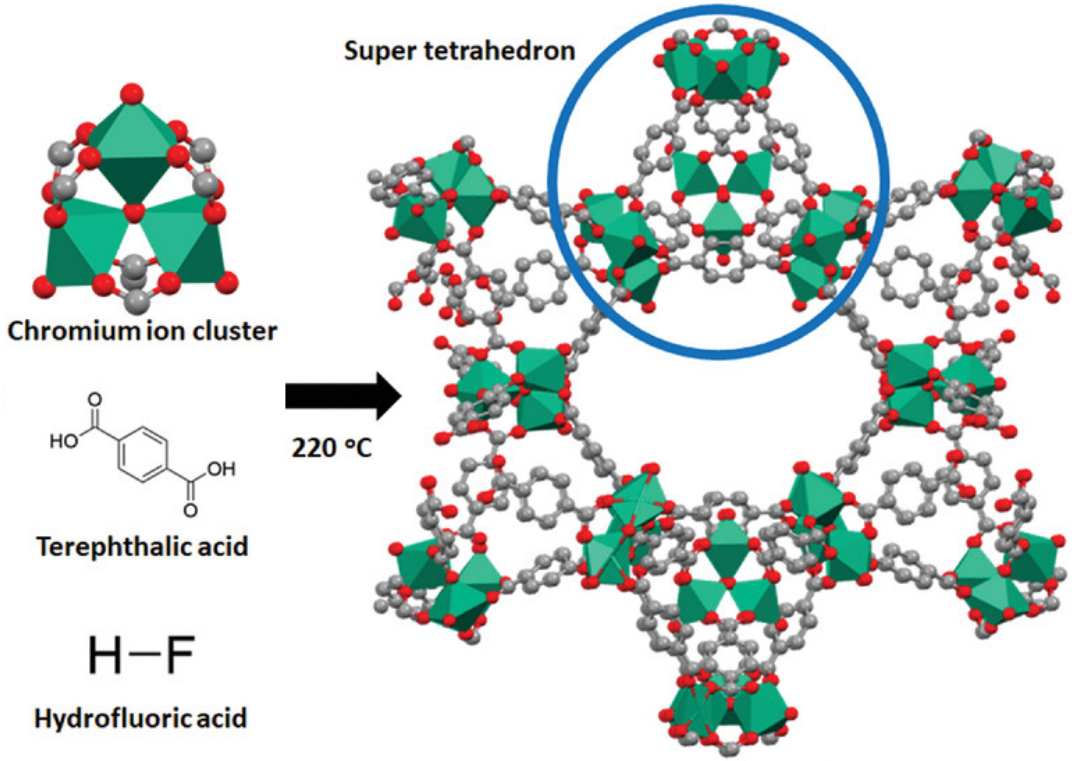
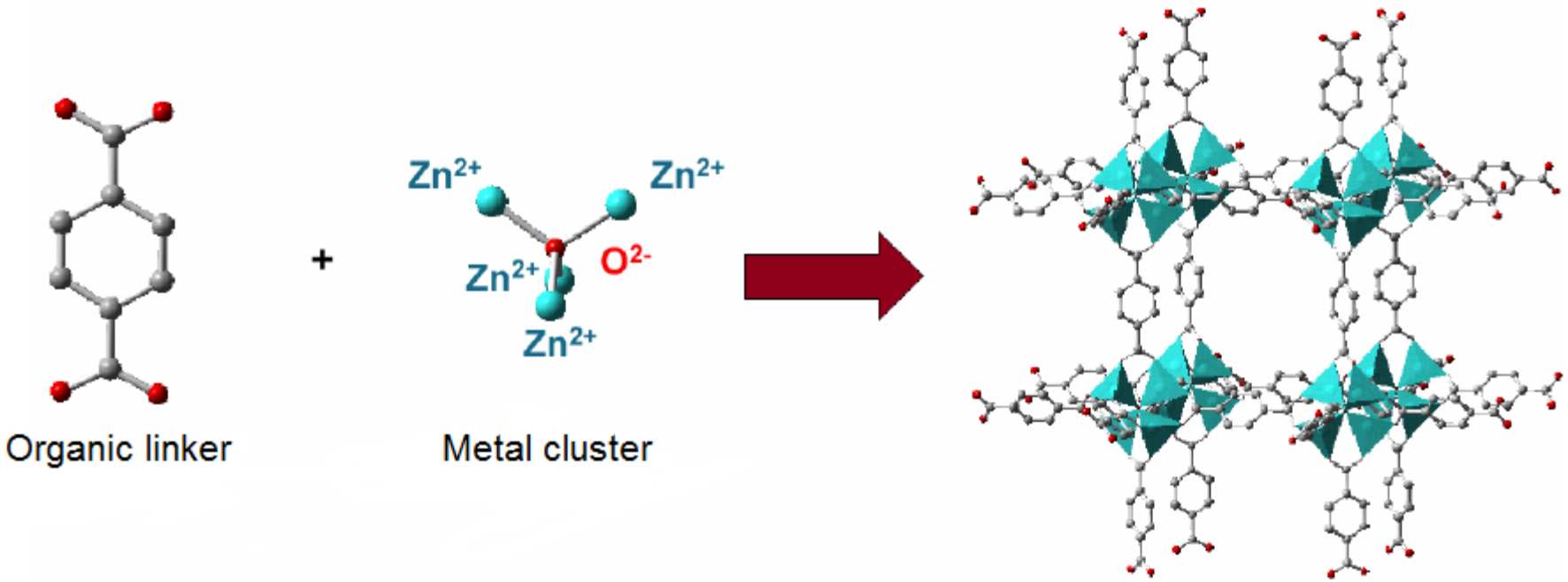
Metal–organic frameworks

- **Metal–organic frameworks** (**MOFs**) are a class of porous polymers consisting of metal clusters (also known as Secondary Building Units - SBUs) coordinated to organic ligands to form one-, two- or three-dimensional structures. The organic ligands included are sometimes referred to as "struts" or "linkers", one example being 1,4-benzenedicarboxylic acid (BDC).



MOF structure and synthesis



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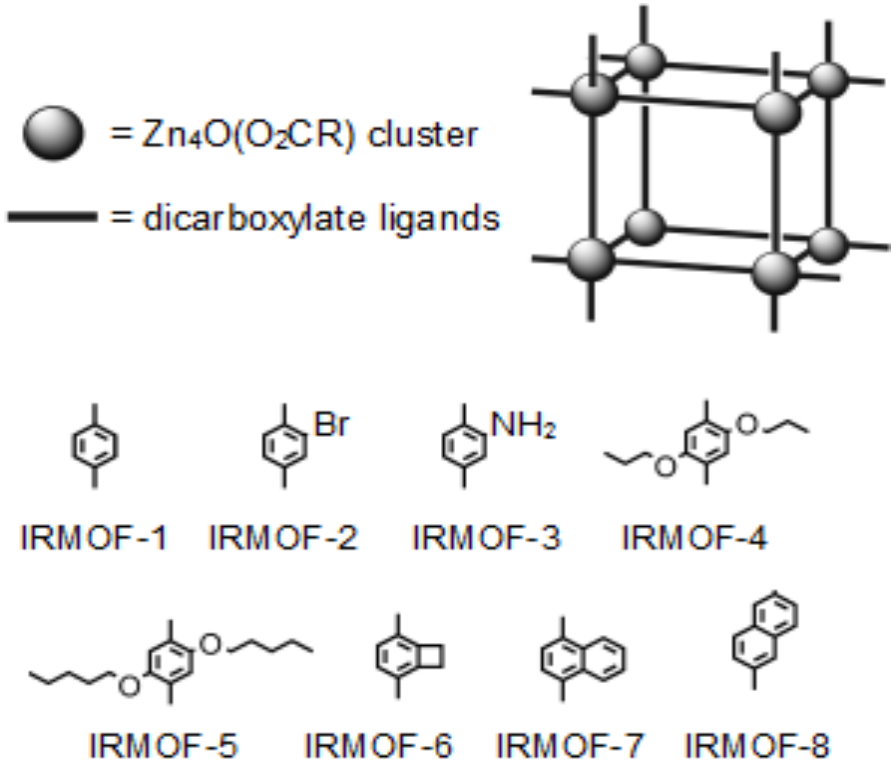

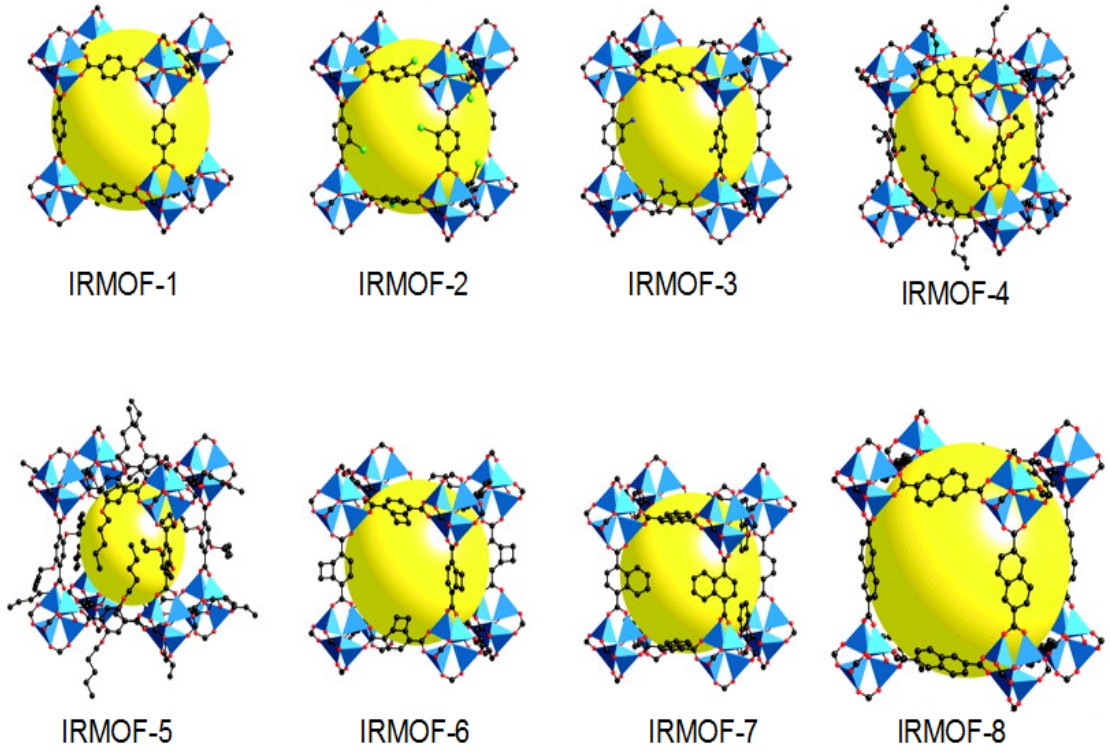

MOF structure and synthesis

- Solvothermal synthesis at low temperature (< 250 ^{o}C)
- Microwave irradiation

  - Conditions: pH, solvent, concentration, and temperature
  - Common polar solvents: water, dimethyl/ethyl formamides, dimethyl sulfoxide or acetonitrile
  - Characteristics of the ligand: bond angles, molecular length, etc. and of the metal ion play a very important role in the structure of MOF

MOF structure and synthesis - Post-synthetic modification

- Ligan functionalize
- Metal exchange
- Open coordination sites

MOF characteristics- porosity

Name	Chemical formula	Pore size (Å)	Window size (Å)	Specific surface area ($cm^2\ g^{-1}$)	Pore volume ($cm^3\ g^{-1}$)
MOF-5	$[Zn_4O(O_2C–C_6H_4–CO_2)_3]$	12	8	2900	0.61–0.54
IRMOF-3	$Zn_4O[O_2C–C_6H_3(NH_2)–CO_2]_3$	10.15	<8	2160	0.63
HKUST-1/ MOF-199	$[Cu_3\{(C_6H_3–(CO_2)_3\}_2]$ or $[Cu_3(BTC)_2]$	9.0	-	692	0.33
MIL-53	$Al(OH)[O_2C–C_6H_4–CO_2]\cdot[HO_2C–C_6H_4–CO_2H]_{0.70}$	8.5	8.5	1140	0.57
MIL-100	$Cr_3F(H_2O)_3O[C_6H_3–(CO_2)_3]_2$	25–30	4.8–8.6	3100	1.16
MIL-101	$Cr_3X(H_2O)_2O[(O_2C–C_6H_4–CO_2)]_3$, X = F/OH	29–34	12–14.7	5900	2.38

MOFs applications

- Gas Adsorption
  - Hydrogen storage
  - CO2 capture
  - Gas separation
  - Water vapor capture and dehumidification
  - Desalination/ion separation
  - Drug delivery
- Semiconductors
- Catalysis

MOF applications – Catalysis

- The metal clusters of the MOF framework;
- Functionalized linker (e.g., acid or base function);
- Active species immobilized in the MOF framework (e.g., supported complexes, metals, metal oxide cluster or enzymes).