Reticular Chemistry to Predict Metal-Organic Frameworks Topology
Javier Fonseca, Tenghua Gong and Sunho Choi

Opportunity

- Metal–organic frameworks (MOFs) enable compositional and structural diversity and allow the incorporation of chemical information within structures to explore further levels of functionality beyond traditional solid-state materials.
- Metal–organic frameworks applications: energy storage, gas storage, gas separation, water purification, catalysis, biomedical applications, etc.
- Challenge: To design and predict new crystalline MOFs.

Approach

- Reticular synthesis [1].
- The geometric principle of construction of reticular chemistry is applied to address the challenge of designing and predicting new crystalline MOFs.
  - Based on the identification of a small number of preferred topologies (networks).
  - Based on the identification of rigid molecular building blocks (secondary building units).
  - Determining MOFs with permanent porosity.

Impact

- Three new metal–organic frameworks with different potential applications were designed by applying the geometric principle of construction of reticular chemistry.
  - Zn$_4$O(BPDI)$_3$
    - Proof of concept
    - CO$_2$ capture
    - H$_2$ storage
  - [Zr$_6$(μ$_3$−O)$_4$(μ$_3$−OH)$_4$(BPDI)$_6$]
    - Drug delivery
    - CO$_2$ capture
    - Water purification
  - [Ce$_6$(μ$_3$−O)$_4$(μ$_3$−OH)$_4$(BPDI)$_6$]
    - Water purification
    - CO$_2$ and SO$_x$ capture
    - Catalysis