RISE:2018
RESEARCH, INNOVATION AND SCHOLARSHIP EXPO
Graduate
Category: Engineering and Technology
Degree Seeking: PhD
Abstract ID# 2149

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Reticular Chemistry to Predict Metal-Organic Frameworks Topology

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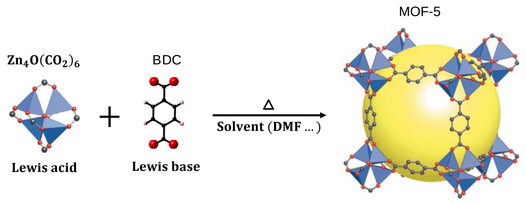
Opportunity

- **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.

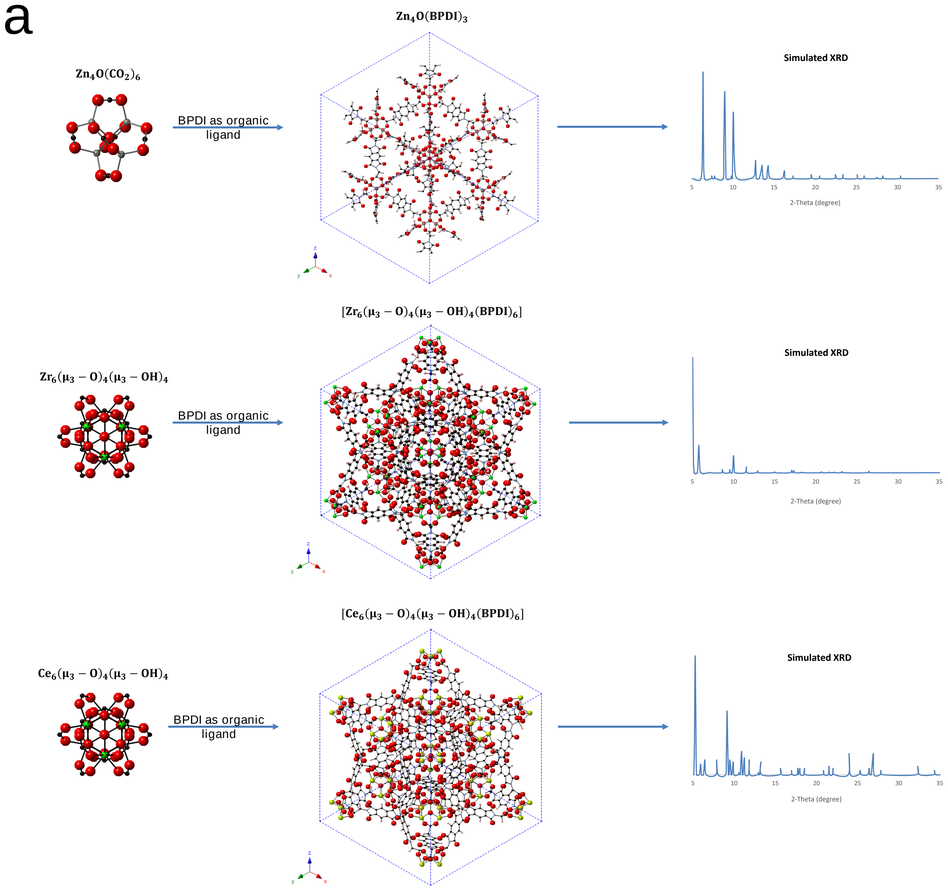
Approach

- 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.

Data



Impact

- Three new metal−organic frameworks with different potential applications were designed by applying the geometric principle of construction of reticular chemistry.
  - $Zn_4O(BPDI)_3$
    - Proof of concept
    - $\mathbf{CO_2}$ capture
    - $\mathbf{H_2}$ storage
  - $[Zr_6(\mu_3-O)_4(\mu_3-OH)_4(BPDI)_6]$
    - Drug delivery
    - $\mathbf{CO_2}$ capture
    - Water purification
  - $[Ce_6(\mu_3-O)_4(\mu_3-OH)_4(BPDI)_6]$
    - Water purification
    - $\mathbf{CO_2}$ and $\mathbf{SO_x}$ capture
    - Catalysis

[1] H. Furukawa, K. E. Cordova, M. O'Keeffe, O. M. Yaghi. Science 341 (2013)