Designing Metal-Organic Frameworks for sensing and optical devices

Kyle T. Smith,[a,b] Chloe A. Ramsperger,[a,b] Kye E. Hunter,[b] Tim J. Zuehlsdorff,[a] Kyriakos C. Stylianou[a,b]

Smithky9@oregonstate.edu

[a]Materials Discovery Laboratory (MaD Lab), [b]Department of Chemistry, Oregon State University, Corvallis, OR, 97331-4003 USA

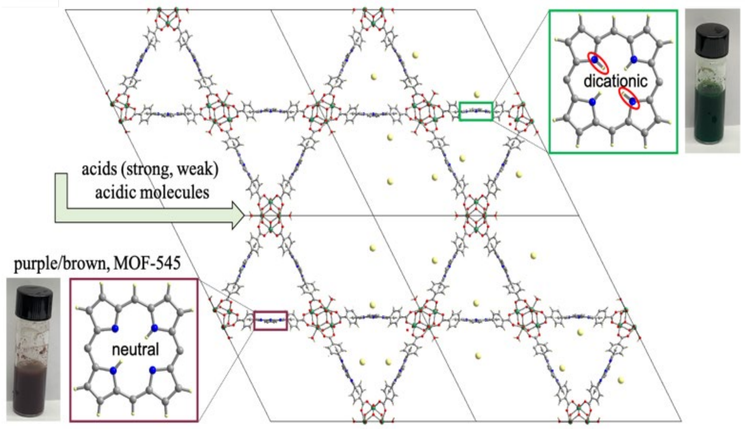
Abstract

Metal-Organic Frameworks (MOFs) are a class of materials with great promise for a variety of applications including gas capture, catalysis, sensing, and optical devices. Because of their wide applicability, they are uniquely suited to solve many of the challenges facing people in the twenty first century, namely the issues sustainability and environmental protection. Herein we investigated MOF-545 and BUT-10 for their optical properties and potential applications. MOF-545 demonstrated the potential to detect acidic pesticides due to bending of the porphyrin. Using BUT-10 as a basis, we created a series of new MOF materials with different emission colors for potential use in optical devices.

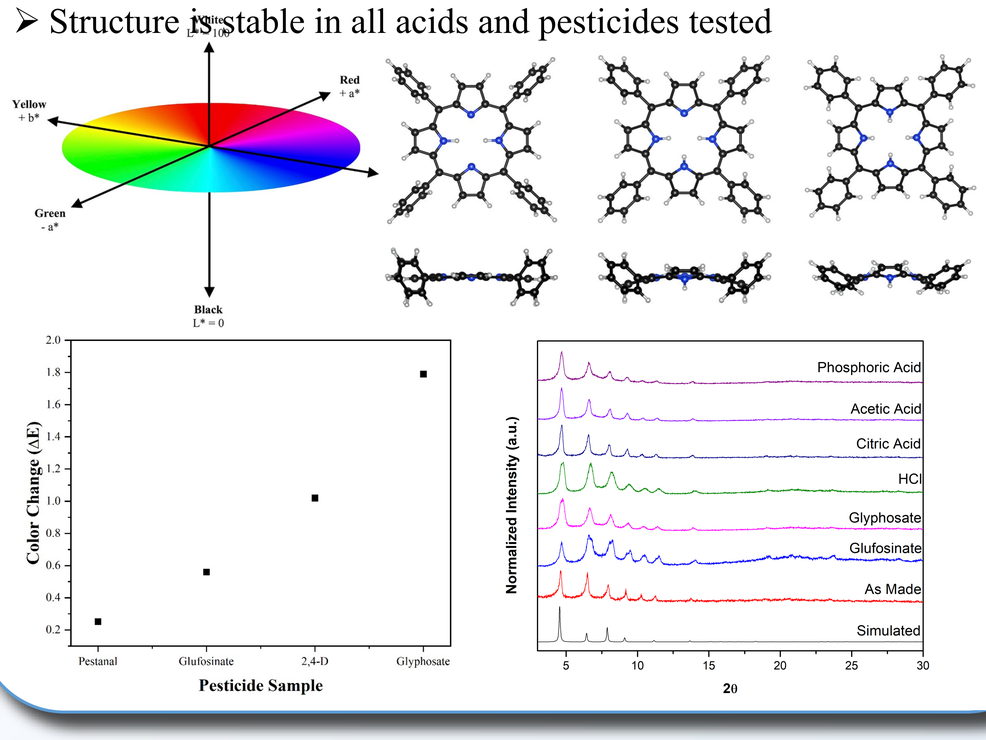
Introduction

- What is a Metal-Organic Framework (MOF)?
  - Porous, crystalline structures composed of metal centers coordinated to organic ligands
  - Easy to synthesize
- Chemistry within the MOF pores can be tailored by choice of ligand or coordination sphere of the metal
  - Luminescent ligands
  - Chiral ligands
  - Chromophores

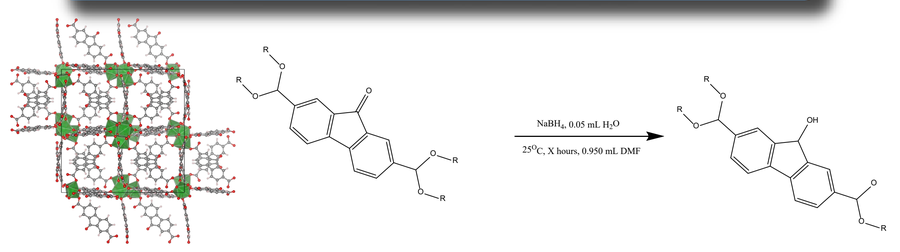
Pesticide Detection



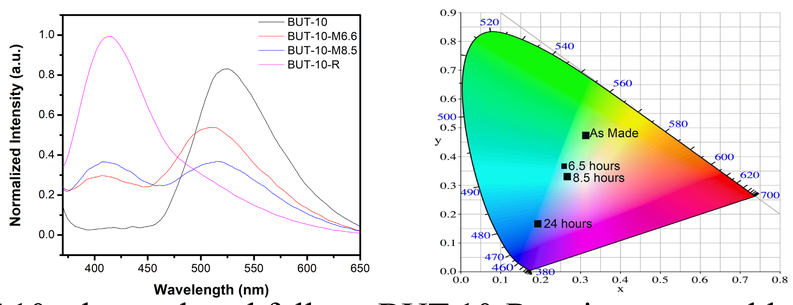
- MOF-545 is a porphyrin based MOF with octahedral Zirconium metal centers
- 15-20% of all pesticides in use are acidic
- We can reduce water testing times by creating portable, colorimetric sensors
- The porphyrin has two uncoordinated N sites that can be protonated, shifting the color from purple to green
  - Acidic pesticides can donate protons
  - Selectivity of pesticides based on subsequent complex formation
  - Protonation bends the porphyrin, resulting in color change
- Structure is stable in all acids and pesticides tested



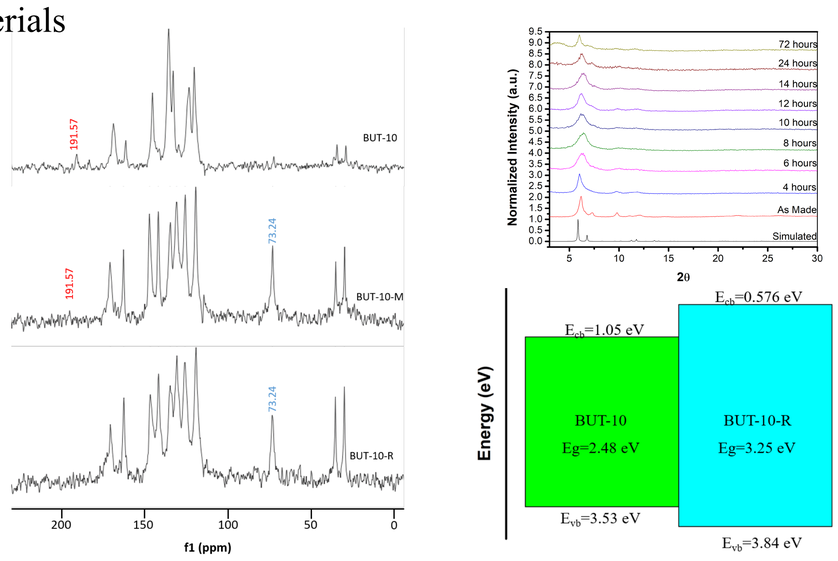
Multivariate MOFs



- BUT-10 is a fluorenone based MOF with 8-coordinate zirconium metal centers
- We can generate multiple versions of the structure by post synthetically reducing the fluorenone to fluorenol



- BUT-10 when reduced fully to BUT-10-R emits a strong blue color
- By altering reduction time, we get intermediate structures that have an emission between blue and green
  - Reduction confirmed via Fourier Transform Infrared Spectroscopy and solid state nuclear magnetic resonance Stability shown in powder X-ray diffraction
- Via optical measurements we can characterize the band gap of the materials



Conclusions

MOF-545 and BUT-10 demonstrate the variety of MOF applications. By investigating their optoelectronic properties we were able to not only able to demonstrate pesticide detection with MOF-545, but able to generate derivatives of BUT-10 with modified ligands capable of emitting different colors. These results demonstrate the capacity of MOFs to solve real world problems and help advance the toolbox for the creation of new MOF materials.