Utilization of Metal-Organic Frameworks to Degrade Per- and Polyfluoroalkyl Substances in Aqueous Solutions

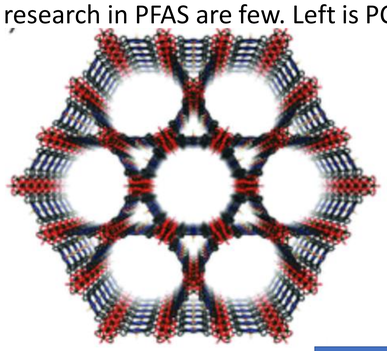
Dominique Dang, Hannah Tjitradjaja, Yangyang Liu
Department of Chemistry, California State University, Los Angeles, CA 90032

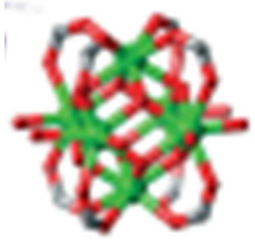
Abstract

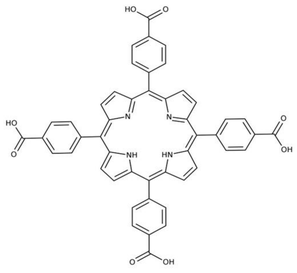
Per- and polyfluoroalkyl substances (PFAS) are known to last for years in the environment before degradation and have been linked to causing negative health effects. Current solutions for degrading PFAS include granular activated carbons and ion exchange resins however these methods are not perfect solutions due to reasons such as low absorption capacity, taking days to reach equilibrium and inefficiency towards certain PFAS. Metal-organic frameworks (MOFs) have the potential to be solutions towards degrading PFAS due to certain characteristics possessed such as large surface areas and high pore volumes.

Background

Background: A family of chemicals called per- and polyfluoroalkyl substances (PFAS) are also known as forever chemicals due to the long amount required for these chemicals to degrade. PFAS are compounds that have carbon chains of varying length with Fluorines attached to each carbon. Perfluorinated will have completely fluorinated chains whilst Polyfluorinated will have at least one carbon chain not completely fluorinated. PFAS have been linked to various negative health effects such as higher risks of cancer and high blood pressure. MOFs are metal nodes such as Zirconium and Titanium which are connected by an organic ligand. MOFs are known for their large surface areas, and pore volumes leading to great candidates for absorption related applications. MOFs have been seen in applications such as heavy metals though research in PFAS are few. Left is PCN-222, middle is the Zr cluster and the right is TCPP.







Acknowledgements

The work conducted for this poster was made possible by the Chemistry and Biochemistry REU program and Dr. Sode.

Li, Rui, et al. "Systematic study on the removal of per-and polyfluoroalkyl substances from contaminated groundwater using metal–organic frameworks." *Environmental Science & Technology* 55.22 (2021): 15162-15171.

Li, Rui, et al. "Efficient removal of per-and polyfluoroalkyl substances from water with zirconium-based metal–organic frameworks." *Chemistry of Materials* 33.9 (2021): 3276-3285.

Feng, Dawei, et al. "Zirconium-metalloporphyrin PCN-222: mesoporous metal–organic frameworks with ultrahigh stability as biomimetic catalysts." *Angewandte Chemie International Edition* 51.41 (2012): 10307-10310.

Methodology

- Synthesis of the MOF (steps dependent on MOF being synthesized such as Ti-TCPP, NU-1000 and PCN-222.)
- Use an application called Mercury to obtain what an ideal PXRD of the MOF being made should look like
- Verify the structure of the MOF with the Powder X-Ray Diffraction or PXRD.
  - Should the graph be too noisy, the MOF is then washed thrice and ran under the PXRD again.
  - If peaks end up missing or the graph completely flatlines, a new batch of MOFs are created.
- With the MOF successfully verified by the PXRD, the sample is placed in the vacuum and dried.
- Afterwards the sample is put under the Gas Sorption Analyzer. Pore sizes as well as surface areas are examined. Should the values for these two traits be found lacking, the MOF is again cleaned and vacuum dried and ran under gas sorption again.
- With the MOF ready for use, it is applied to a vial containing a PFAS called perfluorooctanoic acid (PFOA).
- Orbitrap-LCMS is used to verify successful absorption of PFOA by the MOF.
- A small metal plate with a UV/LED light on each side has the vial containing the PFOA and MOF in it is placed into a dark hood and tested under Orbitrap-LCMS.

Results and Discussion

As mentioned before in the Methodology section, a machine called the PXRD is utilized to verify that the structure synthesized is indeed the one it was intended to be. An application named Mercury gives one an ideal graph of what their MOF is ideally supposed to look like. Below this contains an ideal image of what PCN-222 is supposed to look like versus a sample of PCN-222 ran under the PCN-222. The left image being the Mercury graph or ideal graph versus the PCN-222 ran under the PXRD.

