University of Louisville
Department of Chemistry

Christine Phipps

Literature Seminar

When: September 17, 2020
Time: 2:30 PM
Location: Microsoft TEAMS

Metal Organic Frameworks for Cooperative CO_2 Capture

Abstract

CO_2 is the most abundant greenhouse gas in the atmosphere. Atmospheric CO_2 contributes to the greenhouse gas effect leading to global warming as well as ocean acidification. CO_2 is an important synthetic material in chemistry that can be used to make urea, methane, and a variety of other carbon containing compounds. However, to be used for synthetic purposes, CO_2 first needs to be captured from the atmosphere. Zeolites and polymers have been evaluated for their efficiency of CO_2 capture, but metal organic frameworks are the most promising area. Metal organic frameworks (MOFs) are porous coordination polymers ideal for CO_2 capture due to their permanent porosity, high surface area, functionalized pore surface, and tunable binding affinity. While a typical MOF captures CO_2 by pore opening or closing processes, MOFs using a novel cooperative mechanism exploit the Lewis acidity of CO_2 for CO_2 capture[1]. Using a systematic evaluation of the MOF M_2(dobpdc) where M = Mn, Mg, Fe, Co, Ni, Zn and dobpdc = dioxidobiphenyl the CO_2 capture properties can be modified. Changing the metal in the MOF modifies the metal- amine bond strength where the weaker the metal amine bond, the easier it is for CO_2 insertion[2]. Altering the amine sterics were also found to have an effect on the thermodynamics of CO_2 insertion where bulkier amines on the N-M bond increased the thermodynamics for insertion, while bulkier amines on the unbound amine in the pore were found to decrease the thermodynamics of CO_2 capture[3]. The chemistry of the cooperative CO_2 capture by Mg_2(dobpdc) is reliant on two Lewis basic sites and modifying one of the Lewis basic sites to an alcohol was found to decrease the thermodynamics of adsorption. If only one Lewis basic site is present, there is minimal CO_2 capture[4]. When the number of Lewis basic sites is increased from two to four an increase in CO_2 capture is observed as well as an increase in the thermodynamic driving force[5].

References:

1. Li, J. Et al. *Chem. Rev*. **2012** *112*, 869–932
2. McDonald, T et al. *Nature* 2015 *519*, 303–308
3. Siegelman, R. et al. *J. Am. Chem. Soc*. **2017**, *139*, 10526-10538
4. Mao, V.Y., et al. Angew. Chem. Int. Ed. **2020** *59*, 2-12
5. Kim et al., *Science* **2020** *369*, 392–396