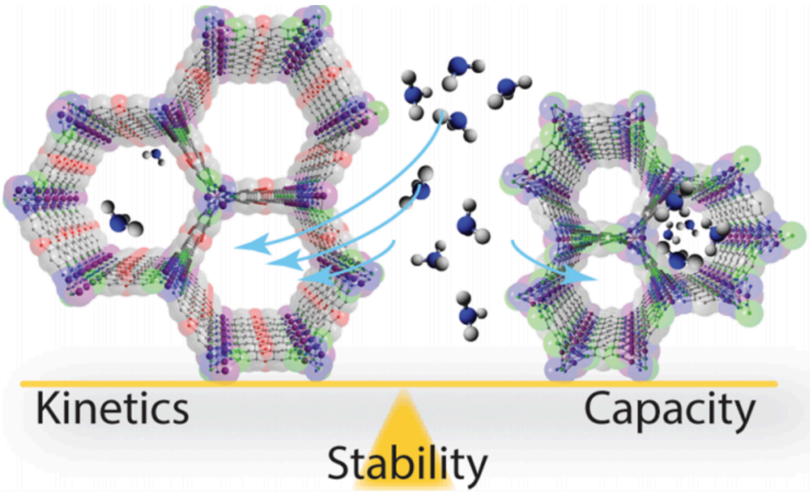
Controlled Gas Uptake in Metal−Organic Frameworks with Record Ammonia Sorption

Speaker:鍾承妤 Advisor:鄭沐政 老師 Date:2019/05/27

ABSTRACT

Ammonia is an irreplaceable feedstock for global agriculture and industry, but its toxicity and corrosiveness require advanced protection and mitigation. Furthermore, ammonia is produced at a rate of 140 million metric tons per year, making it among the largest volume chemicals on the planet. Here, authors report that a series of stable triazolate metal-organic frameworks containing open metal sites provide a unique platform for interrogating coordinating and gas sorption. Under conditions at 1 bar, Cu_2Cl_2BBTA adsorb up to 19.79 mmol NH_3 g^{-1}, exhibits the material with the highest NH_3 uptake among all MOFs. In addition, the stability trend of the isoreticular frameworks substituted with various metal ions (Co^{2+}, Ni^{2+}, Cu^{2+}) follows the metal-aquo substitution rate. Further, kinetic analyses correlate with the Knudsen flux model, demonstrating that this theoretical framework serves as a good baseline to predict the effects of modifying the pore size and the particle size on sorbent kinetic performance. Altogether, these results provide clear, intuitive descriptors that govern the static and dynamic uptake, kinetics, and stability of MOF sorbents for strongly interacting gas.



REFERENCE

1. Van Humbeck, J. F.; McDonald, T. M.; Jing, X.; Wiers, B. M.; Zhu, G.; Long, J. R. *J. Am. Chem. Soc.* 2014, 136 (6), 2432.
2. Doonan, C. J.; Tranchemontagne, D. J.; Glover, T. G.; Hunt, J. R.; Yaghi, O. M. *Nat. Chem.* 2010, 2 (3), 235.