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Title:

Volatile Gas Capture in Nanoporous Metal-Organic Frameworks (MOFs)

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The design and synthesis of nanoporous materials with built-in information for specific applications require critical understanding of host-guest interactions that occur at molecular level. The timely study presented herein focuses on the structure-property relationship between metal-organic frameworks (MOFs) and physisorbed volatile iodine (I_2) gas.

A main concern associated with nuclear energy as an alternative energy source is appropriate nuclear waste management. Radio-I_2 is a highly mobile gas resulted during nuclear fuel reprocessing or nuclear reactor accidents. It addresses particular challenges; the ^{129}I isotope has a very long half-life (1.57×10^7 years), and is involved in human metabolic processes. Therefore, its safe capture and storage is of utmost importance.

Here we report on the efficient capture of I_2 gas into known MOFs (ZIF-8 and HKUST-1), as well as novel materials developed in our group. High resolution synchrotron powder X-ray diffraction, pair distribution function analysis, and molecular modeling were used to identify structural details of I_2 binding locations in these systems. Two distinct I_2 sites were crystallographically refined in ZIF-8; they are centered over alternating 6-member ring windows in the material with sodalitic topology. Close monitoring of I_2-framework contacts reveals that adsorption is mainly due to favorable interactions with the 2-methylimidazole organic linker. The β-cages of ~1.2 nm in diameter act as molecular reservoirs, as the sorbed I_2 is confined within nanochannels, and cannot readily diffuse out. Incorporation of the I_2-loaded MOFs into glass composite materials as long-term waste forms was also investigated. This was monitored by thermal stability studies, electron microscopy, and chemical durability tests, which indicate that I_2 is successfully retained in the glass composite matrices.

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