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Structures and Gas Storage Performance of Metal-organic Framework Materials at High Pressures YANG SONG, YUE HU, YINING HUANG, University of Western Ontario — Metal Organic Frameworks (MOFs), are crystalline nanoporous materials comprised of small metal clusters connected three-dimensionally by polyfunctional organic ligands. MOFs have been widely studied due to their high porosity, surface area and thermal stability, which make them promising candidates for gas capture and storage. In the MOF family, Zeolitic Imidazolate Frameworks (ZIFs) have attracted much attention because of their promising applications for CO_2 storage. In contrast to the extensive studies under ambient conditions, most ZIFs have only been studied under pressure in a very limited range. It is known that pressure can provide an effective driving force to achieve structural modification which includes changes in pore size, opening and geometry, channel shape and internal surface area. Subsequently, these pressure-induced changes will affect the sorption selectivity, capacity and access to the binding sites of the porous materials. Here, we report the first in situ high-pressure investigation of several ZIFs by FTIR spectroscopy. We observed rich pressure-induced transformations upon compression in different pressure ranges. Furthermore, the reversibilities of these transformations upon decompression were also examined. Finally, the performance of CO_2 storage of selected ZIFs at high pressures will be addressed. Our observation and analyses contribute to the understanding of chemical and mechanical properties of ZIFs under high-pressure conditions and provide new insight into their storage applications.

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