Direct Observation of Hydrogen Molecules adsorbed in a Coordination Polymer

Yoshiki Kubota[a], Masaki Takata[b], Ryotaro Matsuda[c], Ryo Kitaura[d], Susumu Kitagawa[c], Tatsuo C. Kobayashi[e], Kenichi Kato[b], Makoto Sakata[f], [a]*Dept. of Physics, Osaka Prefecture Univ., Osaka.* [b]*JASRI/SPring-8 & CREST(JST).* [c]*Kyoto Univ.* [d]*Toyota Central R&D Labo.,Inc..* [e]*Okayama Univ.* [f]*Nagoya Univ., Japan.* E-mail: kubotay@center.osaka-wu.ac.jp

Hydrogen is a very important material for the development of a clean energy system. The use of physisorption in microporous coordination polymers is one of the most promising candidates for the hydrogen gas storage. The fundamental structural information of adsorbed H_2 molecules is indispensable for the rational synthetic strategy of these materials. Although the weakest X-ray scattering amplitude of hydrogen has made it difficult to determine the structure of H_2 molecules, we have succeeded in direct observation of H_2 molecules adsorbed in the nanochannels of the coordination polymer by the *in-situ* synchrotron powder diffraction experiment of gas adsorption and the MEM/Rietveld charge density analysis [1].

The H_2 molecules were found to be adsorbed without any chemical bonding to the host framework, in the condition that they can be easily adsorbed and released. The position of H_2 molecule was displaced from the center of the nanochannel. It was located near the metal-oxygen unit near one corner of the rectangular nanochannel. The size of the H_2 molecule is suited to the size of the pocket of the cavity. The structural information of H_2 molecule at the beginning stage of gas adsorption was obtained. That gives us the guideline for the design of high performance hydrogen gas storage materials.

[1] Y. Kubota, et al., *Angew. Chem. Int. Ed.*, 2005, **44**, 290-293.

Keywords: gas storage materials, microporous coordination polymer, synchrotron powder diffraction