

# Analysis of Hydrogen Molecules Chemisorbed on Cu Ions Confined in Solid Nanospace

T. Ohkubo(A), K. Takahara(A), A. Itadani(A), O. Yamamuro(B), and Y. Kuroda(A)  
(A) *Fac. Sci., Okayama Univ.*, (B) *ISSP-NSL, Univ. Tokyo*

We have reported specific adsorption properties of gas molecules on copper-ion-exchanged MFI-type zeolite (CuMFI). Specifically, monovalent Cu ions exchanged in MFI zeolite can strongly interact with an adsorbed molecule even at room temperature. In our previous report, we showed the possibility from the IR measurements which indicated the existence of the specific adsorption sites on CuMFI treated at 873 K [1]. However, it is quite difficult to investigate the adsorption phenomena with ordinary methods and, herein, we performed the inelastic neutron scattering (INS) measurements for CuMFI adsorbed by hydrogen and tried to elucidate the adsorption sites to interact strongly with hydrogen.

INS experiments were carried out on hydrogen-chemisorbed CuMFI by using AGNES spectrometer. At first, we measured the spectra of original CuMFI which was evacuated at 873 K in a quartz tube and then transferred into an aluminum holder in a helium-exchanged globe box. Hydrogen molecules were directly installed into the holder at 0.1 MPa and 77 K through the center stick. To obtain the INS spectrum of chemisorbed species, we cooled down to 8 K and evacuated physically adsorbed molecules and the molecules in the bulk phase.

Fig. 1 shows the difference INS spectrum of adsorbed hydrogen molecules at 8 K. We could observe two kinds of INS bands at 1.08 and 1.72 cm<sup>-1</sup>, respectively. Eckert et al. assigned the INS band of hydrogen-coordinated tungsten complex observed at 0.95 cm<sup>-1</sup> as the rotational tunneling of side-on-type coordinated hydrogen [2]. Therefore, these two bands strongly indicate the existence of two kinds of strong or chemical adsorption sites on the CuMFI

surface. However, our results did not agree with the band positions observed at 0.80 and 1.37 cm<sup>-1</sup> reported by Georgiev et al. by using CuMFI [3]. These differences may be due to the differences of surface composition such as Si/Al ratio or the variation of local structure around a monovalent Cu ion. The present results revealed that the two kinds of adsorption sites can act as specific sites for hydrogen whose interaction strength is similar to that observed for side-on-type coordinated hydrogen of a complex.

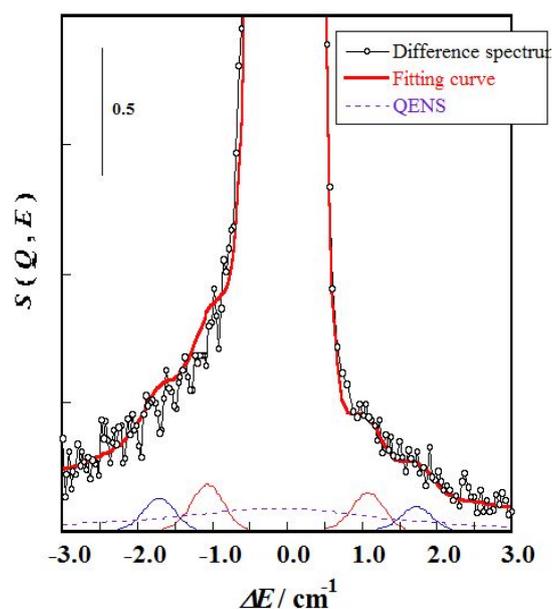


Fig. 1. Difference INS spectrum of adsorbed hydrogen on CuMFI.