Neutron scattering in O$_2$ adsorbent magnet

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Oxygen molecule is a simple magnetic element that carries $S = 1$ spin. While metal ions are constituents of various types of magnetic compounds, O$_2$ based magnets has been restricted to monolayer O$_2$ molecule adsorbed on the surface of several materials such as Aluminum or graphite [1, 2]. The adsorbed O$_2$ forms spin framework that reflects the surface structure of mother compound. For example $S = 1$ triangular lattice is realized in the O$_2$ adsorbed graphite. However the small amount of the adsorbed spins makes the magnetic property measurement difficult. Hence the metal based compound has been major substances for the study of magnetism.

Recently the adsorption of O$_2$ molecule in the nanochannel of some microporous compounds were reported [3]. In contrast with the surface adsorption, the oxygen molecules are intercalated deep inside the host compound and the adsorption is realized in the bulk crystal. Hence the O$_2$ based magnet with the bulk size is experimentally realized. In this pioneering work we observed the magnetic excitation of O$_2$ $S = 1$ spins in the O$_2$ adsorbed microporous compound [Cu(II)$_2$(bza)$_4$(pyz)]$_n$ (bza and pyz are benzoate and pyrazine, respectively) by neutron scattering technique.

Crystal structure analysis by x-ray diffraction showed that the adsorbed O$_2$ molecule forms isolated trimer [3]. Preliminary magnetic susceptibility measurements is consistent with the spin trimer model with $J \sim 2.0$ meV [4]. If this is the case a narrow band excitation would be observed at $\hbar \omega \sim 2.0$, 4.0, and 6.0 meV with the intensity modulation in inelastic neutron scattering (INS). [5]. Hence we performed initial experiment at PONTA spectrometer installed at 5G beamline.

However, we observed no intrinsic signal in the energy transfer range between 1 meV and 20 meV. This means that preliminary model is inconsistent with experiment. Then we performed the second experiment at HER spectrometer at C11 in guide hall. We repeat the measurements for both O$_2$ adsorbed and not adsorbed samples in the same experimental configuration.

Figure 1 shows a typical constant $q$ scan. Well defined sharp peak was observed at $\hbar \omega = 0.40$ meV. We confirmed the disappearance of the peak in not adsorbed sample. The peak position was independent of $q$. The intensity decrease with the increase of $q$ gradually and monotonically. The $\hbar \omega = 0.4$ meV mode is the only excitation that we observed in the energy range of $0.15 \text{ meV} < \hbar \omega < 20 \text{ meV}$. Furthermore we did not observe any sign for the intensity modulation.

The results mean that the observed peak is due to magnetic excitation from O$_2$ spins of $S = 1$. The $q$ independence means that the spin system is isolated. The absence of the intensity modulation means that the interaction between O$_2$ spins is too weak to be detected in INS. The only possible explanation for the excitation is that a single ion anisotropy of an O$_2$ spin of $S = 1$.

In summary we succeeded in the observation of the magnetic excitation in O$_2$ adsorbent magnet.

**References**

Fig. 1. Constant $q$ scan in the $O_2$ adsorbed $[\text{Cu(II)}_2\text{(bza)}_4\text{(pyz)}]_n$. 