Magnetic Interaction between Absorbed $O_2$ Molecules in Cu-Trans-1,4-Cyclohexanedicarboxylic Acid

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Cu-Trans-1,4-Cyclohexanedicarboxylic Acid (Cu-CHD) with one dimensional micropores, which can generate stable $O_2$-inclusion crystals at low temperature using adsorption conditions, has been extensively investigated.[1] In the case of the low $O_2$ adsorption, temperature ($T$) dependence of the magnetic susceptibility ($\chi$) shows the nonmagnetic ground state at low $T$. The magnetization is explained by the dimer model of $S=1/2$ with an antiferromagnetic exchange interaction although the oxygen molecule has $S=1$. In the case of the high $O_2$ adsorption, on the other hand, Curie-Weiss like behavior is observed in the low $T$ region.

Neutron scattering measurements were carried out using the cold neutron chopper spectrometer AMATERAS installed at J-PARC to clarify the magnetic interactions between absorbed $O_2$ molecules in Cu-CHD.

At low $T$, the dispersionless magnetic excitations were observed for both the low and high $O_2$ adsorption Cu-CHD samples, indicating that the absorbed $O_2$ molecules form clusters. These magnetic excitations for the low and high $O_2$ adsorption Cu-CHD samples can be explained by the $O_2$ dimer having nonmagnetic ground state and $O_2$ trimer having the magnetic ground state, respectively. On the other hand, the spin Hamiltonians do not explain the unique behavior of the observed magnetization.

In order to reproduce the magnetization qualitatively, we need to lower the level of the higher energies originally calculated from the spin Hamiltonians. The presumed energy scheme is consistent with the ab initio calculation including the intermolecular potential and spin states.[2] Since the absorbed $O_2$ molecules in micropores have the strong coupling between the magnetism and lattice, they are the interesting system with the multi degree of freedom.