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Summary of Doctoral Dissertation

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Title of Doctoral Dissertation

The muon-spin resonance (μSR) and density functional theory (DFT) study of $YBa_2Cu_3O_6$
($YBa_2Cu_3O_6$ のミュオンスピン緩和法（μSR）および密度汎関数法（DFT）による研究)

The insight of magnetic properties of the mother compound of superconductor, $YBa_2Cu_3O_6$, is the main key to understand the nature of superconductivity mechanism, $YBa_2Cu_3O_{6+x}$. The muon-spin resonance (μSR) firstly reported the presence long-range antiferromagnetic ordering in $YBa_2Cu_3O_6$ which disappear with doping and superconductivity appears. In addition to this the μSR has greatly contributed to reveal magnetic properties of the high-Tc superconductor. On the other hand, two main limitation in interpreting the μSR experimental data are the unknown muon position and how large muon perturb the host system. This study developed a computational technique to estimate muon site in $YBa_2Cu_3O_6$ by using density functional theory (DFT) with additional Hubbard parameter, U, (DFT+U) to treat $YBa_2Cu_3O_6$ as strongly correlated system. The DFT+U calculation showed that the muon's perturbation significant only to the neighboring ions. In order to get complete description of muon as local magnetic probe, the zero-point energy (ZPE) vibration must be considered. The ZPE caused the muon does not occupy single point but distributed around local minimum potential which related to the muon's wave function.

The μSR experiments on single crystals of $YBa_2Cu_3O_6$ were carried out in Paul Scherrer Institute and detected three distinct muon-spin precession components which correspond to the three different muon site. The DFT+U calculation also showed that three different muon site in $YBa_2Cu_3O_6$. The internal field calculation on the basis point dipole model with assuming spin reside in Cu^{2+} ion is not match with the internal field which deduced from experiment. The spin is found to be distributed in the real space due to the strong hybridization of Cu *3d* orbital with surrounding O *2p* orbital (covalency effect). This spin behavior related to the spin density in crystal which directly probe by implanted muon. The internal field evaluation on the basis of spin density has strong dependence on the U value. The carefully tuning of the U value was done and allow us to determine the suitable U value for $YBa_2Cu_3O_6$.

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Finally, the study has indicated that the important to consider local crystal deformation of the system caused by muon and ZPE of muon in discussion the μSR data. It also pointed out that the covalency effect play crucial role in discussion of magnetism in $YBa_2Cu_3O_6$. The U is determined to be 6.7 eV for $YBa_2Cu_3O_6$.