Contribution ID: **72** Type: **Poster Presentation**

Electronic Structure of Mu as Pseudo-H in RuO2: Comparison with Other Rutile-Type Oxides

While ruthenium oxide RuO_2 with a rutile structure has long been regarded as a Pauli paramagnetic metal, it has recently attracted much attention as a candidate for the "altermagnet". The existence of an antiferromagnetic (AFM) order, essential for the altermagnet, has been claimed by recent neutron diffraction study [1]. However, the reported Ru magnetic moment size $|m_{\mathrm{Ru}}| = 0.05\mu_{\mathrm{B}}$ is close to the detection limit, necessitating verification by other experimental techniques. We investigated the magnetic ground state of a high-quality RuO_2 single crystal (residual resistivity ratio > 1500) using μSR.
We found no clear evidence of AFM order from 5 K to 400 K [2]. DFT calculations using dilute hydrogen (H) simulating muon ruled out the possibility that muons occupy sites where the internal magnetic field cancels out for the reported AFM structure. These results indicate that the reported AFM order is unlikely to exist in the bulk of RuO_2. Furthermore, the upper limit of the $|m_{\mathrm{Ru}}|$ was found to be ~1% of the reported value.
Thus, understanding the local electronic structure of muons is crucial for evaluating the internal magnetic field in μSR. In this presentation, we will address the defect structures of interstitial muon in other rutile oxides and discuss their systematic understanding.

References
[1] T. Berlijn et al., Phys. Rev. Lett. 118, 077201 (2017)
[2] M. Hiraishi et al., Phys. Rev. Lett. 132, 166702 (2024)

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Session Classification: Poster session 2

Track Classification: Magnetism