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Local electronic structure of dilute hydrogen in gallium oxide

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Gallium oxide β-Ga_2O_3 is currently drawing much attention as a material for high-voltage power devices because of its large band gap (E_g ~4.9 eV). We investigated the electronic structures of muon as a pseudo-hydrogen in β-Ga_2O_3 in which the dilute hydrogen is under the central focus as a crucial factor for the bulk conducting properties. We demonstrate by μSR study combined with the first principles calculations that muons in β-Ga_2O_3 have two electronic structures: a state corresponding to hydrogen that acts as an electron donor (Mu_1), bounded to three-coordinated oxygen, and a hydride-like state in rapid motion (Mu_2). Furthermore, we imply from the Hall effect measurements that the fractional yield of Mu_2 exhibits a close link with the mobility and density of the carriers (electrons).
In the presentation, we will compare our results with those of previous study and discuss the electronic structures of Mu_1 and Mu_2 in terms of our recently proposed ambipolar model of muon in oxides.

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