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Local electronic structure of interstitial hydrogen in MgH_2 inferred from muon

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Metal hydrides have attracted attention as one of the candidate materials that can serve as safe and efficient hydrogen (H) storages. In particular, MgH_2 has great potential as a solid H-storage material because of its high storage capacity of 7.6 wt\%. However, its slow hydrogenation and dehydrogenation rates and the high decomposition temperature ($\sim$300°C) are major obstacles to the practical applications. Understanding the microscopic mechanisms of the H-related processes is key to engineering solutions to improve the H-intake/release kinetics and to lower the decomposition temperature. To this end, the information on the electronic state of interstitial H (which exists as an intermediate state in the reaction kinetics) is crucial in gaining insight into the rate-limiting processes.
The preceding studies on the microscopic state of H in MgH_2 have been mainly via computational approaches based on density functional theory (DFT), but there have been few experimental investigations to validate the prediction of DFT calculations. We have introduced muons as pseudo-H into MgH_2, and studied their electronic and dynamical properties in detail to elucidate the corresponding interstitial H states. As a result, we found two species of Mu states showing comparable yields; a paramagnetic state with relatively large hyperfine parameters (0.5-1.7 GHz) that undergoes rapid conversion to diamagnetic states, and a quasistatic diamagnetic state described by the Kubo-Toyabe relaxation function. In this talk, we discuss the correspondence between these Mu states and the predictions from the DFT calculations.

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