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Combining muon spin relaxation and DFT simulations of hydrogen trapping in Al_6Mn

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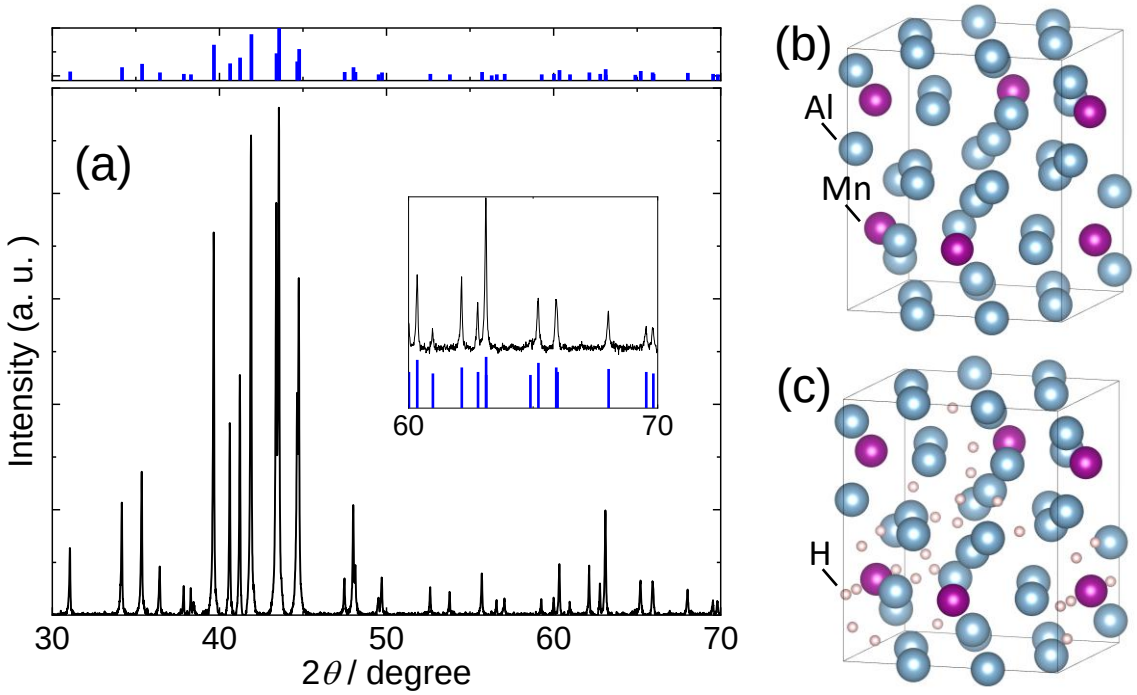


Fig. 1 Crystallographic characterization of Al_6Mn. (a) XRD pattern of the prepared Al_6Mn. The inset shows the magnified XRD spectrum ranging from 60 to 70 degrees, accompanied by the computed peak positions and intensities (represented by blue bars). (b) illustrates an Al_6Mn unit cell, while (c) depicts hydrogen situated within the Al_6Mn unit cell, which serves as a potential trapping site. Crystallographically equivalent sites for hydrogen locations are omitted for clarity.

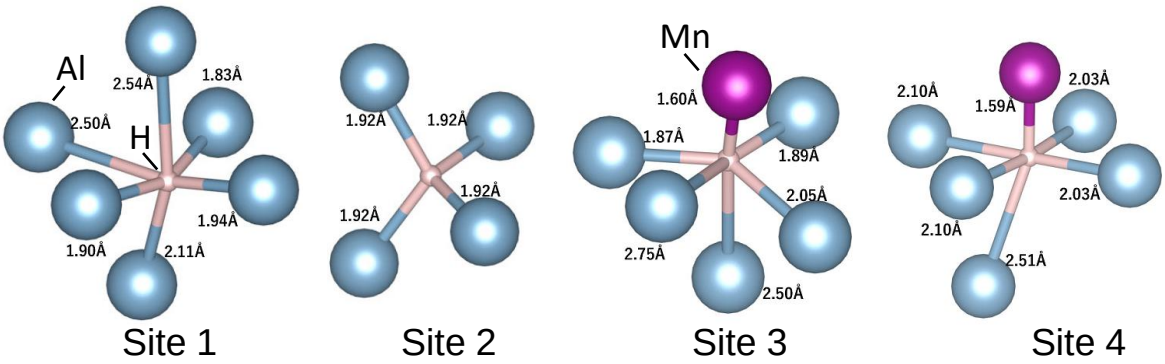


Fig. 2 Atomic configurations of the possible hydrogen trapping sites: site 1, distorted octahedral site of Al atoms; site 2, tetrahedral site of Al atoms; site 3, distorted octahedral site of five Al atoms and one Mn atom; site 4, different distorted octahedral site of five Al atoms and one Mn atom.

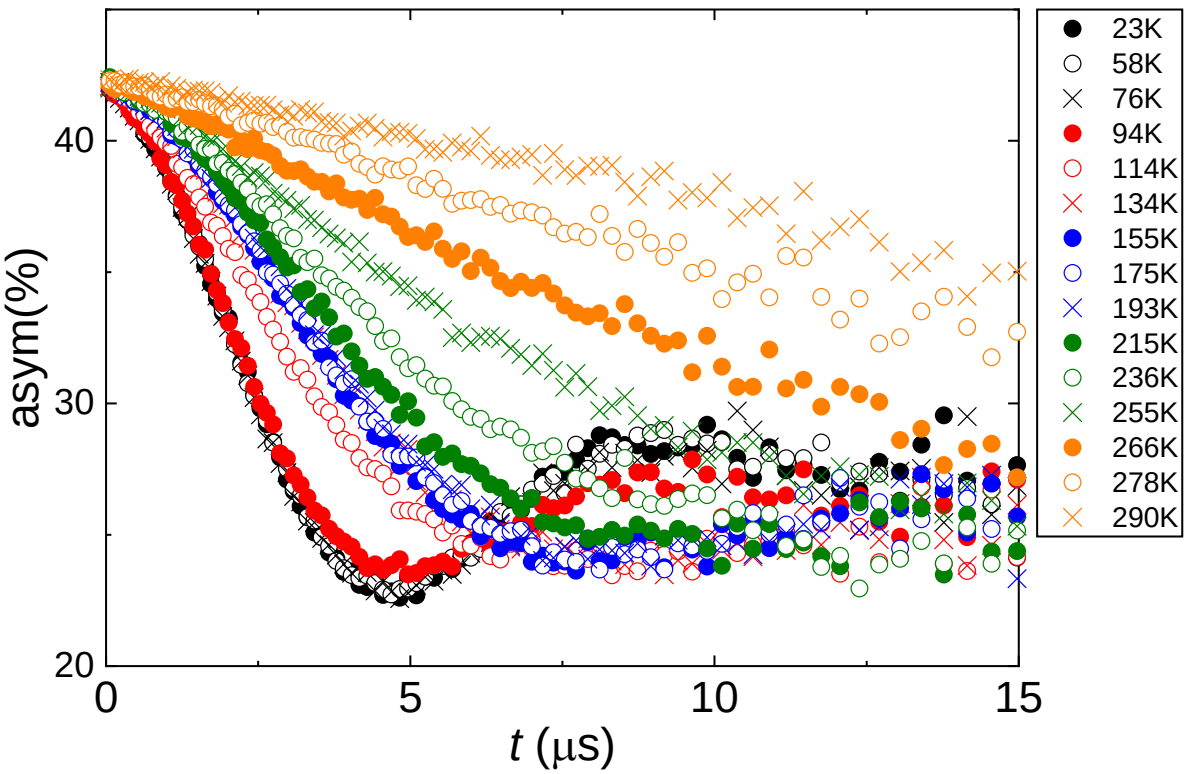


Fig. 3 Zero-field μSR spectra observed for Al_6Mn in the temperature range from 23 K to 290 K.

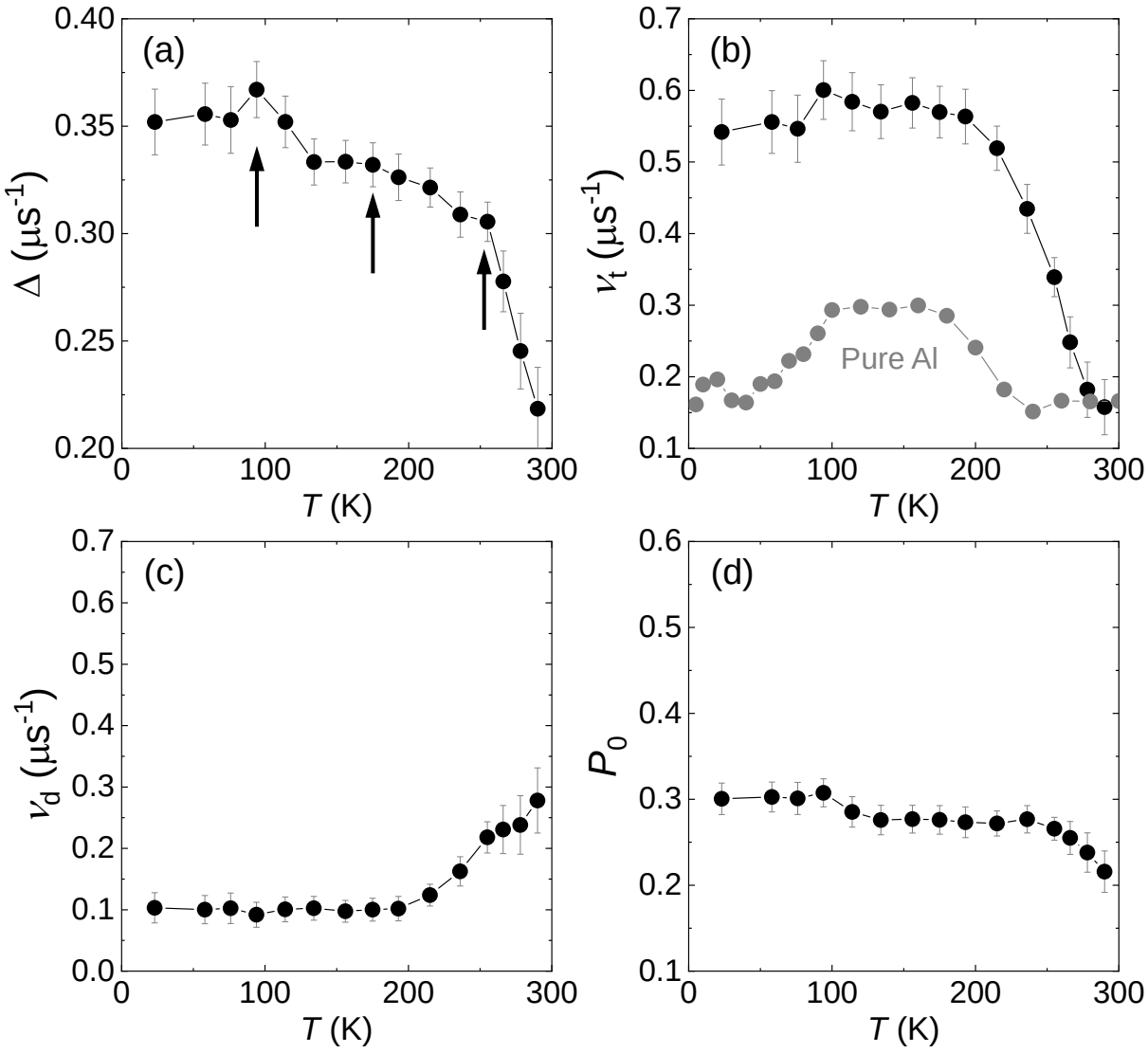


Fig. 4 Temperature-dependent variations in the extracted dipole field width (Δ), trapping rate (ν_t) (together with that of pure aluminum), detrapping rate (ν_d), and fraction of initially trapped muons (P_0) for Al_6Mn.

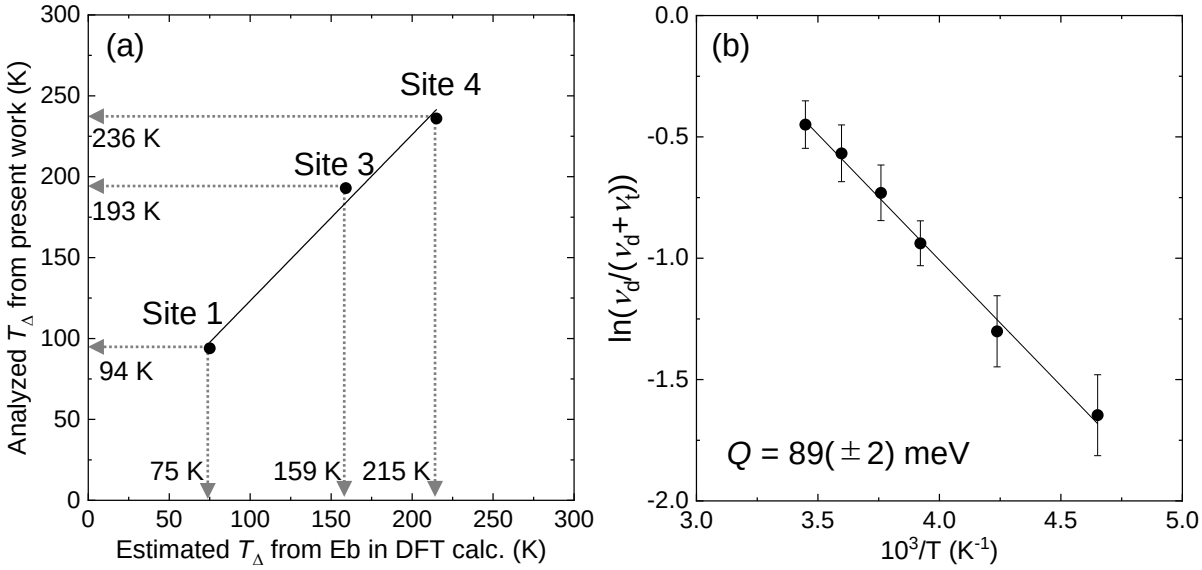
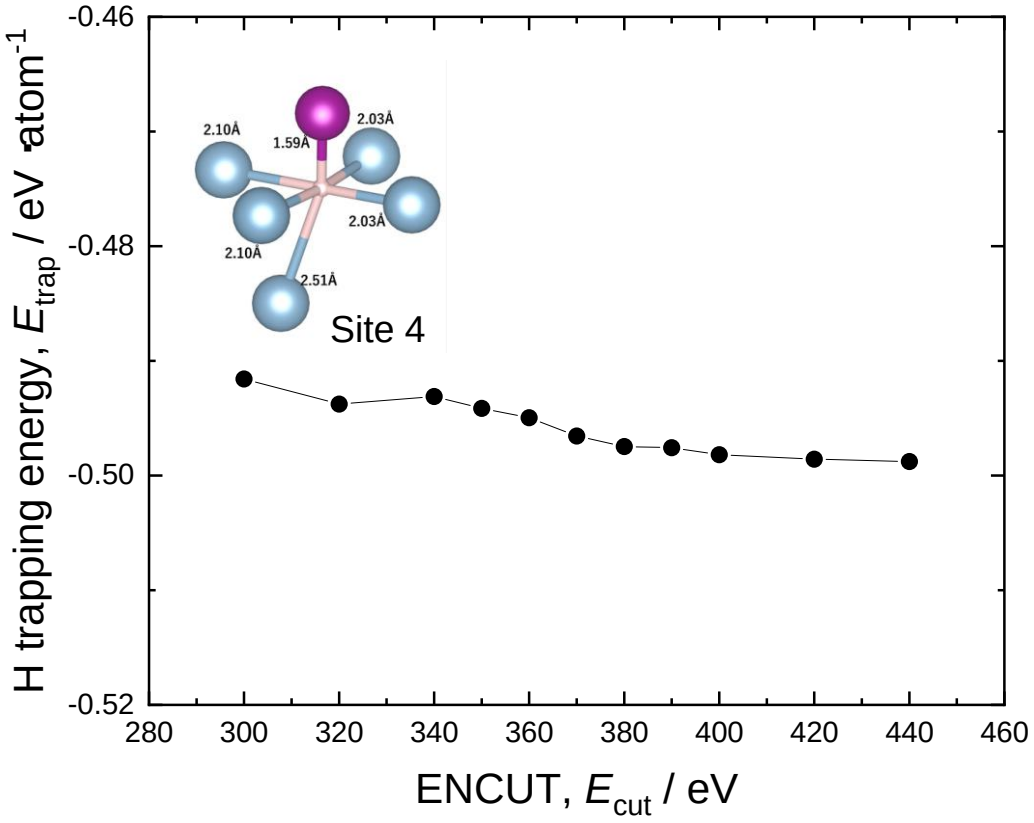


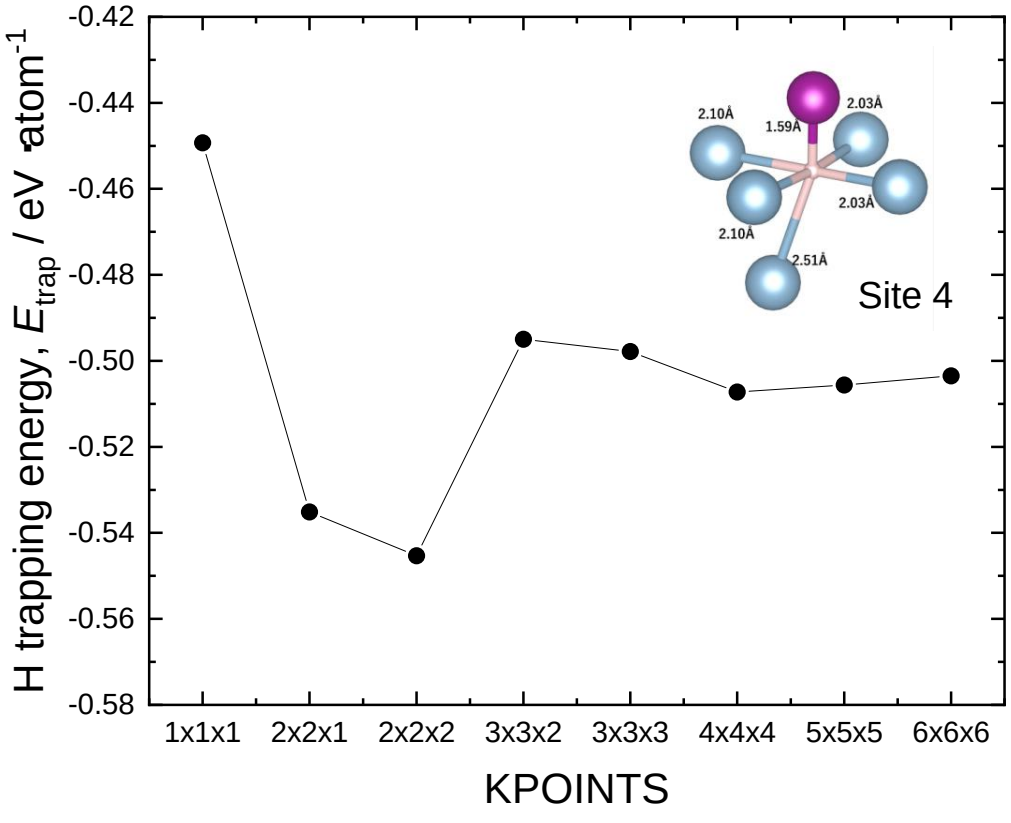
Fig. 5 (a) Correlation between the T_Δ estimated from the $-E_{trap}$ obtained in DFT calculations of hydrogen (refer to Table 1) and T_Δ analyzed from the present muon experiments (refer to Fig. 4(a)). The site numbers in Fig. 5(a) correspond to those in Fig. 2 and Table 1. (b) Arrhenius plot constructed using the trapping and detrapping data of muons extracted for Al_6Mn between 215 K and 290 K.

Table 1 Hydrogen trapping energy ($-E_{trap}$), hydrogen trapping site density, calculated Δ peak temperature (T_{Δ}), and expected dipole field width at each hydrogen trapping site (Δ)

Site	$-E_{trap}$ (eV/atom)	Site density (site/nm^3)	T_{Δ} (K)	Δ (1/μsec)
1	0.168	37.3	75	0.36
2	0.312	9.3	137	0.35
3	0.364	37.3	159	0.43
4	0.495	18.6	215	0.42



E_{trap} vs. ENCUT at Site 4 in Fig. 2



E_{trap} vs. KPOINTS at Site 4 in Fig. 2