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Beta detected NMR of ^8Li in 2H molybdenum ditelluride

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Layered transition-metal dichalcogenides (TMDs) are proposed as building blocks for van der Waals (vdW) heterostructures. Semiconducting TMDs are further prone to host magnetic impurities, e.g. at defects or interstitials. Here we investigate the behavior of interstitial $^8\text{Li}^+$ implanted into 2H-MoTe₂ at depths of ~ 110 nm with β -detected NMR. We find that unlike muons [1], the $^8\text{Li}^+$ does not show any signature of induced magnetism. We confirm this result by density functional theory, which identifies the Li stopping site at the 2a Wyckoff position in the vdW gap and shows the absence of Li-induced electronic spin polarization. Both, the spin lattice relaxation (Fig. 1c) and the resonance lines (Fig. 1a) show evidence for Li diffusion or a site change above 200K. The line shape of $^8\text{Li}^+$ is found to consist of quadrupolar satellites on top of a broad central peak (Fig. 1a). Therefore, we employ a frequency comb measurement, where four frequencies, $\omega_0 - 3\omega_{\text{comb}}$, $\omega_0 - \omega_{\text{comb}}$, $\omega_0 + \omega_{\text{comb}}$, and $\omega_0 + 3\omega_{\text{comb}}$ corresponding to the first-order quadrupolar satellite transitions are excited simultaneously as a function of ω_{comb} . This offers an enhanced sensitivity to the quadrupolarly split portion of the line. Using this method, we find a small decrease of the quadrupolar frequency with increasing temperature (Fig. 1b), showing the typical behavior associated with thermally excited phonons.

[1] J. A. Krieger, et al., arXiv:2206.03051 (2022)

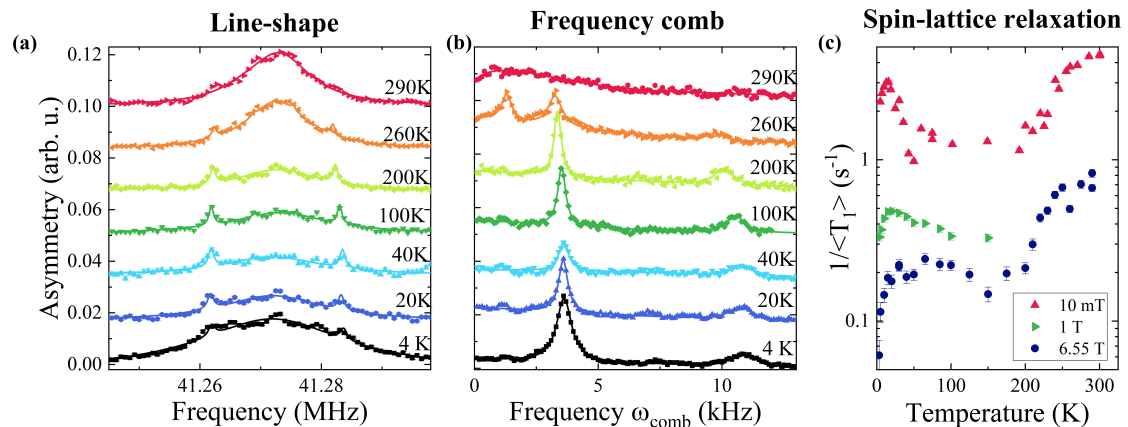


Figure 1: (a) $^8\text{Li}^+$ line shape and (b) frequency comb in 2H-MoTe₂ at different temperatures, which are offset for clarity. (c) Temperature dependence of the spin lattice relaxation rate at different applied fields.

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