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Muonium states in semiconducting transition metal dichalcogenides

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The usual response of muonium to an external magnetic field is dominated by the hyperfine interaction, which causes the observed spectrum to show the transition frequencies between different muonium spin states. However, we have recently discovered an unconventional magnetic muonium state in 2H-$MoTe_2$ where the muonium acts a magnetic impurity, which polarizes the local electronic magnetic moments [1]. For sufficiently small externally applied fields, the "magnetic" muonium effectively behaves as a diamagnetic muon in a local magnetic field. Here, we show experimentally that in 2H-$MoTe_2$ the magnetic muonium coexists with another conventional, non-magnetic muonium state (Fig. 1b). The latter is axially symmetric with a hyperfine coupling of $A_{\parallel}$=1426(1) MHz and $A_{\perp}$=1368(3) MHz, corresponding to an effective Bohr radius of $\approx$ 0.82 Angstrom. The hyperfine coupling remains fairly constant, as a function of temperature, until the state disappears around the same temperature where the magnetic muonium disappears as well. We employ density functional theory calculations to reveal that this is linked to the presence of two muonium sites in the compound: one within the van der Waals gap that becomes magnetic, and a second one inside the layer, that is conventional. A similar behavior is also observed in 2H-WSe_2 (Fig. 1a), indicating that this is a more general feature of semiconducting transition metal dichalcogenides.

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

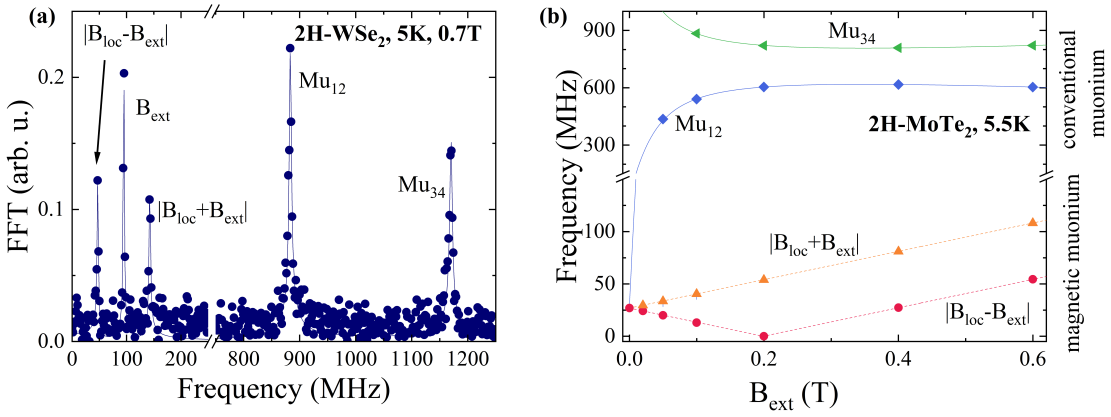

Figure 1: (a) Local field distribution in 2H-WSe_2 at 5K in a 0.7T transverse field. (b) Applied field dependence of the oscillation frequencies in 2H-$MoTe_2$ at 5.5K.

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