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Hydrogen impurity in MgO as seen by the muonium analogue

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We present a joint muSR and ab-initio study of the hydrogen impurity in magnesium oxide (MgO). Muon spin rotation measurements at magnetic high-fields reveal the presence of a diamagnetic configuration and of a muonium state, confirming an hyperfine interaction of 3.9(1) GHz at T=6K 1. The temperature dependence of these states is followed up to room temperature, revealing a conversion of the muonium to the diamagnetic state. Ab-initio density-functional theory (DFT) calculations further characterize the local atomistic (or microscopic) structure of these two configurations, the atomic muonium state corresponding to an interstitial location in the magnesium oxide lattice and the diamagnetic configuration corresponding to an oxygen-bound location.

1 R. F. Kiefl et al., Phys. Rev. B 34 (1986) 1474

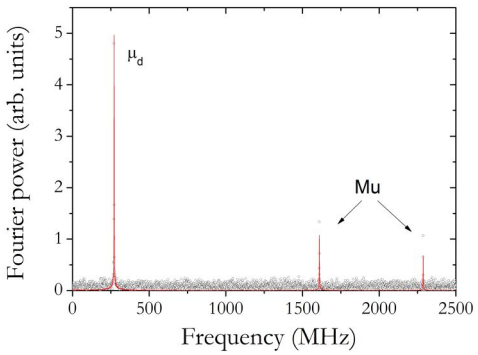

Figure 1: FFT of MuSR spectrum of MgO at T=6K and B=2T.

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