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Entanglement between muon and I>1/2 nuclear spins as a probe of charge environment

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Quantum coherence between an implanted positively-charged muon and nuclei in a solid was first conclusively demonstrated using muon-spin spectroscopy experiments on simple ionic fluorides [1]. In this case the nuclear spin $I=\frac{1}{2}$ of the ¹⁹F nuclei couples to the muon spin through the dipolar interaction.

Here we identify the first example of muon spin quantum coherence in systems with nuclear spin larger than $\frac{1}{2}$. The effect is shown for vanadium intermetallic compounds which adopt the A15 crystal structure, and whose members include all technologically dominant superconductors.

The presence of $I \geq 1$ nearest neighbours (nn) nuclei implies the inclusion of quadrupolar interactions. The muon embedding in the crystal drastically alters the electric field gradient (EFG) at the nuclei nearest neighbours of the muon. Nevertheless, this perturbation can be effectively described with Density Functional Theory based simulations [2]. Once the muon site, the structural distortion and the charge perturbation induced by the muon are established through cost effective ab initio simulations, our modelling of the coherence is extremely accurate.

This case-study demonstrates that high-statistics measurements of systems in which the muon spin becomes entangled with nearby nuclear spins can yield information about small changes in local structure and charge order, even in the absence of magnetic ground states.

[1] J. H. Brewer, et al., Phys. Rev. B 33, 7813R (1986)

[2] P. Blaha, et al., Phys. Rev. Lett. 54, 1192 (1985)

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