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What can we learn from muon-stopping site analysis?

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Two of the most fundamental limitations of the muon-spin spectroscopy (μ^+SR) technique are the lack of knowledge of the muon stopping site, and the uncertainty surrounding the degree to which the muon distorts its local environment. Over the past decade there has been significant progress in calculating muon stopping sites using *ab initio* methods, particularly density functional theory (DFT). These methods can provide significant insight into how the muon probes the system, thereby enhancing the information that can be extracted from a μ^+SR experiment.

Establishing the degree to which the muon perturbs it environment can be crucial for confirming that the phenomena observed by the muon are intrinsic to the system under study. Here we investigate the muon stopping states in a range of correlated electron systems. 1) In superconductors that exhibit time-reversal symmetry breaking, where spontaneous magnetic fields have been observed using μ^+SR, we show how knowledge of the muon stopping site shows how the muon is a faithful probe that provides sensitivity to the intrinsic magnetism in the system [1]. 2) By calculating the muon site and its associated hyperfine interactions in the quantum spin-liquid candidate 1T-TaS_2 we can model how the muon couples to diffusing spinon excitations [2]. Here we are also able to compute details of the muon's own diffusion between sites. 3) Calculating the distribution of magnetic fields at the muon site allows us to link the μ^+SR spectra directly to the underlying magnetic structure. We discuss the use of this approach in skyrmion-hosting systems, whose phase diagrams comprise several complicated incommensurate magnetic structures as a function of magnetic field and temperature.

[1] B. M. Huddart *et al.* Phys. Rev. Lett. **127**, 237002 (2021).

[2] S. Mañas-Valero *et al.*, npj Quantum Mater. **6**, 69 (2021).

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