# DFT+$\mu$: a step change in muon spectroscopy

$\mu$

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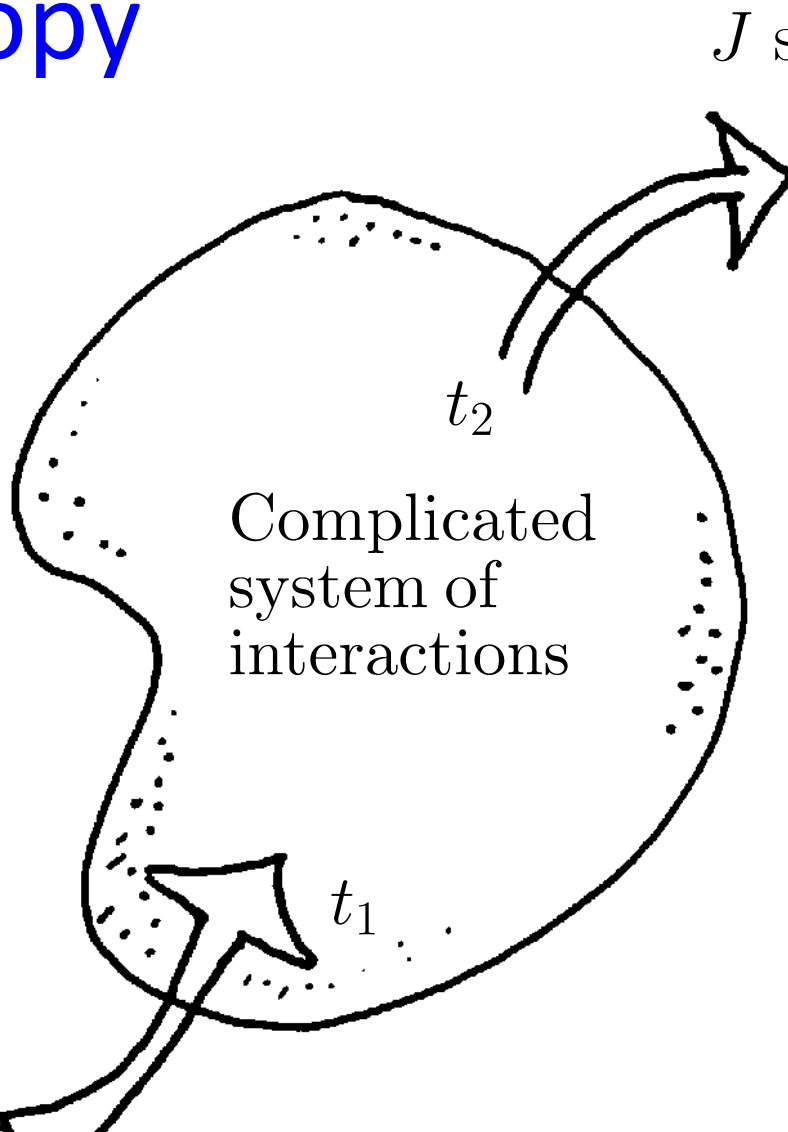

# Muon FAQs

- What is the muon site?
- Is the muon introducing a distortion?
- Is the muon changing what is being measured?

# The project in a nutshell

*"We now propose to advance the techniques, including quantum mechanical treatment of the muon, in order to address problems in condensed matter physics."*

# The people involved

- Oxford: Steve Blundell, Feliciano Giustino, Franz Lang
- STFC - ISIS: Francis Pratt
- Durham: Tom Lancaster, Stewart Clark, Matjaž Gomilšek, Ben Huddart

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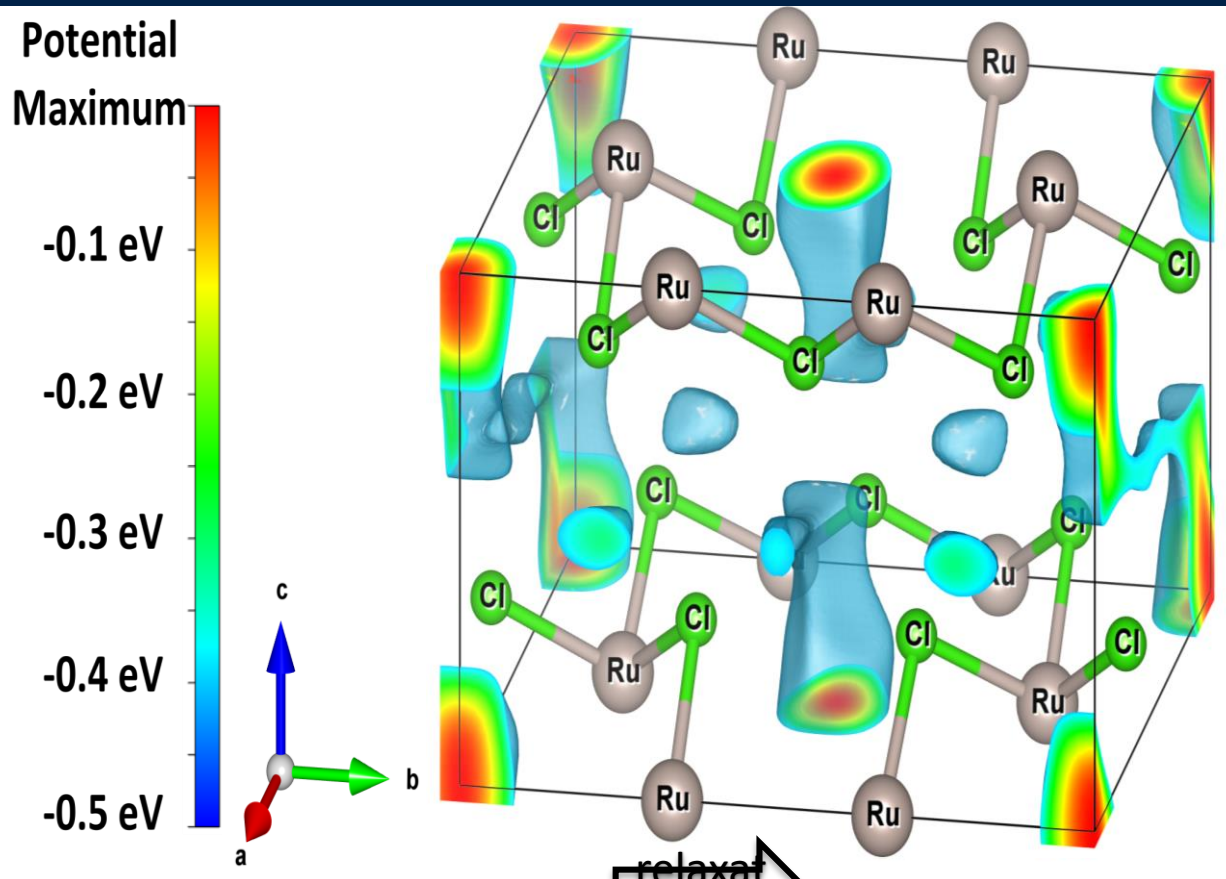
# DFT+μ calculation




relaxation

| Atom | WP | SS | x | y | z |
|---|---|---|---|---|---|
| Ru | 4g | 2 | 0 | 0.33441 | 0 |
| Cl | 4i | m | 0.73023 | 0 | 0.23895 |
| Cl | 8j | 1 | 0.75138 | 0.17350 | 0.76619 |
| Mu1 | 2a | 2/m | 0 | 0 | 0 |
| Mu2 | 4i | m | 0.14 | 0 | 0.36 |
| Mu3 | 4g | 2 | 0 | 0.2 | 0.5 |
| Mu4 | 2d | 2/m | 0.5 | 0 | 0.5 |

| Atom | ΔE (meV) | NN-ion | NN dist. |
|---|---|---|---|
| Mu1 | 0 | Cl (8j) | 1.39 Å |
| Mu1' | 1 | Cl (4i) | 1.39 Å |
| Mu3 | 110 | Cl (8j) | 1.36 Å |
| Mu4 | 115 | Cl (4i) | 1.34 Å |
| Mu2' | 130 | Ru | 1.56 Å |

powder: F Lang *et al.*, PRB **94** (2016), 020407(R)  single crystal: F Lang *et al.*, in preparation

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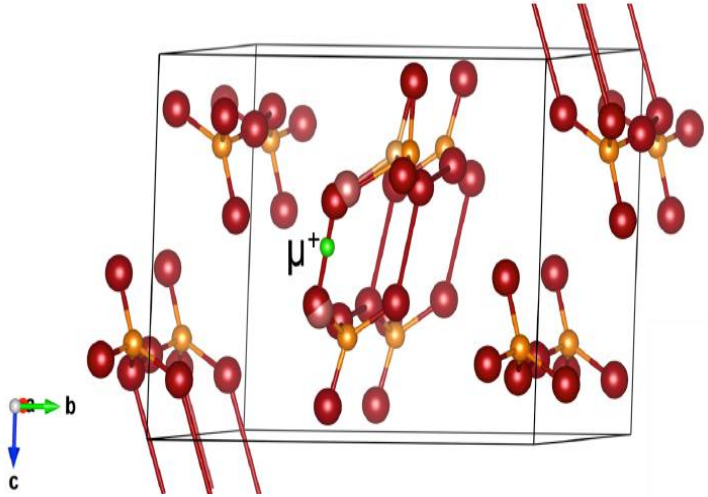
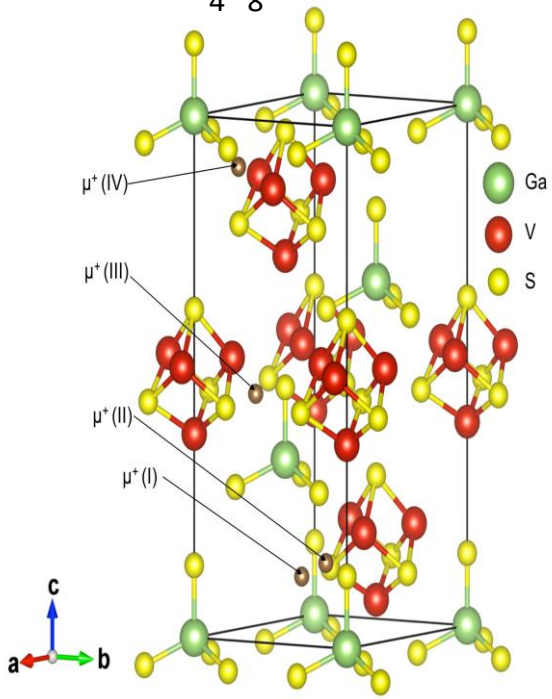
## Molecular spin ladder $(Hpip)_2CuBr_4$



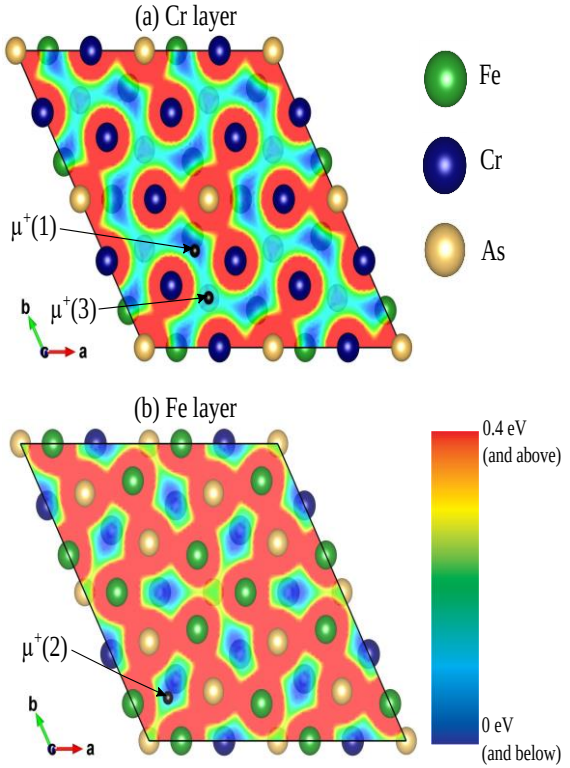

T. Lancaster *et al.*, submitted to J. New Phys. (2018)

## Skyrmion-hosting $GaV_4S_8$




K. J. A. Franke *et al.*, submitted to Phys. Rev. B (2018)

## "Nonmetallic metal" FeCrAs




B. M. Huddart *et al.*, in preparation

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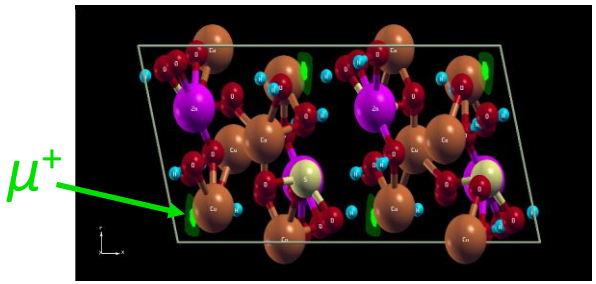
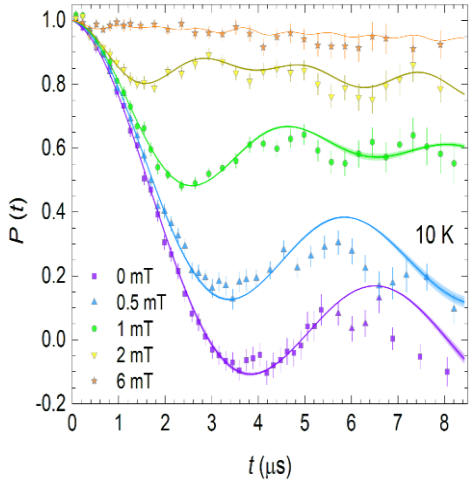
## Zn-brochantite

kagome quantum spin liquid

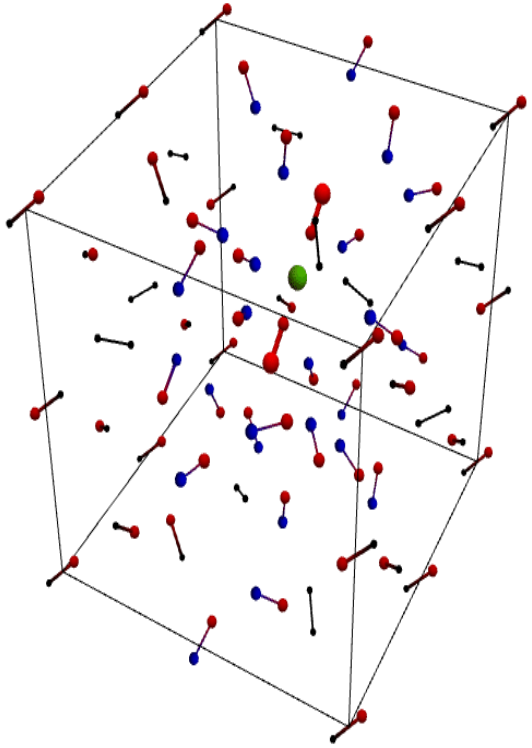



**$\mu^+$–OH complex**

**Quantum entanglement of muon spin**

## Solid nitrogen

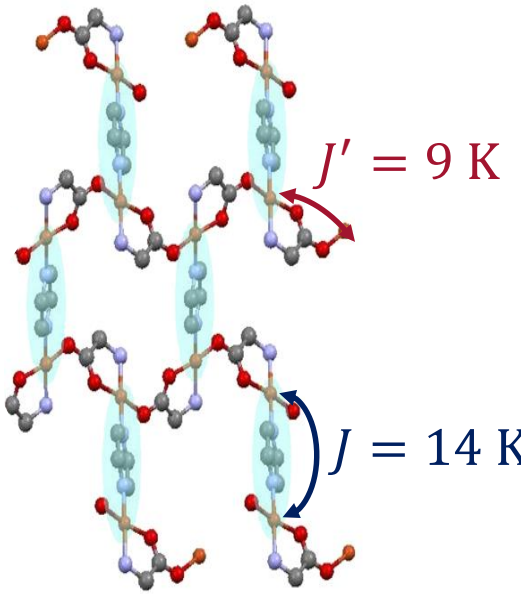


**$N_2$–$\mu^+$–$N_2$ complex, dipoles**

**Quantum muon diffusion, ZPE, tunnelling, Bloch waves**

## [Cu(pyz)(gly)](ClO$_4$)

magnetic BEC




**Exchange interactions**

**Muon sites, local fields**

# Impact

2019 workshop: “Muons and materials modeling”

- We have budgeted to accommodate around 30 delegates at an STFC-organized workshop

# Summary

- This is a central problem to users of the technique
- It is also a very visible problem to non-users
- Democratizing the techniques for use by all must be a goal…

…but to do that we need a firm basis of understanding.