Muon sites in spin ladders and skyrmion-hosting materials

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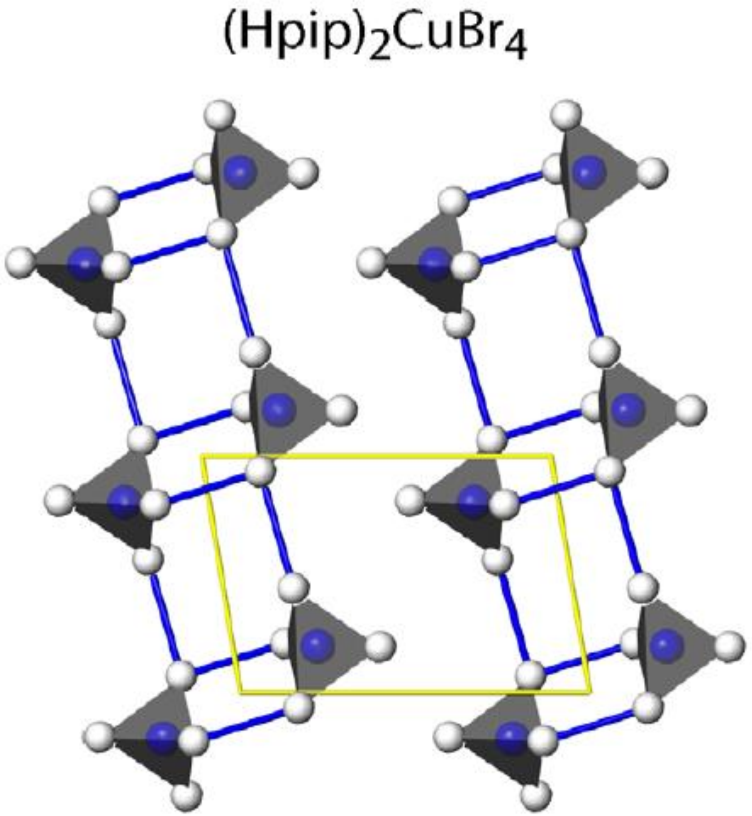
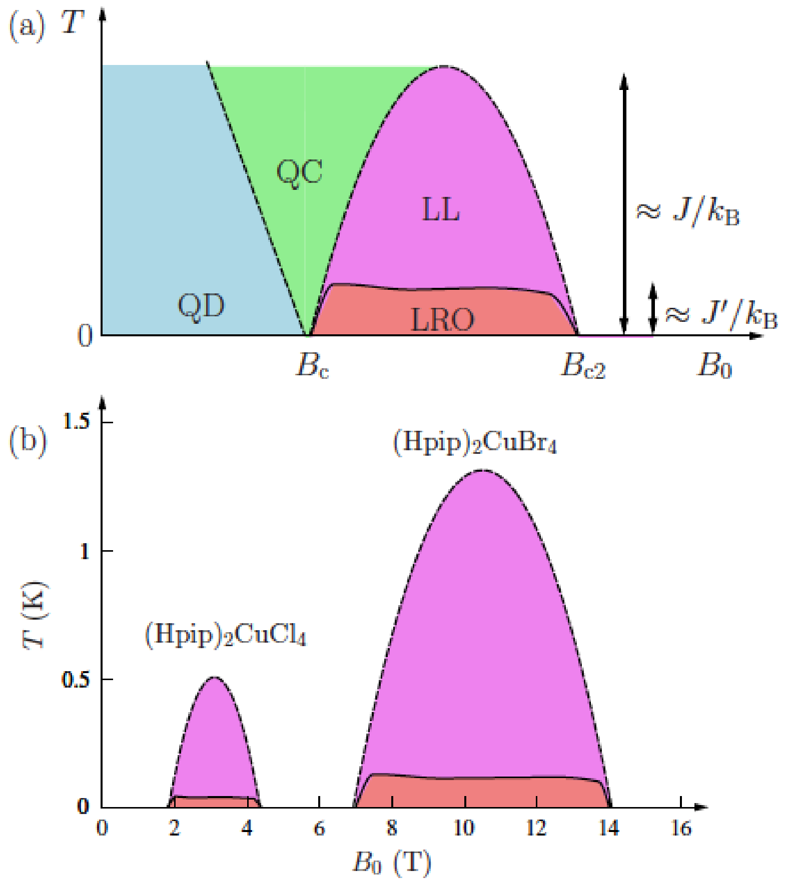
Outline

- Knowledge of the muon site can help us interpret μ^+SR results
- I will present two sets of muon site calculations on systems closely related to our experimental programme: the molecular spin ladder compound $(Hpip)_2CuBr_4$ and the skyrmion-hosting semiconductors GaV_4S_8 and GaV_4Se_8
- Both sets of calculations aim to address particular features of our μ^+SR data

Spin ladders



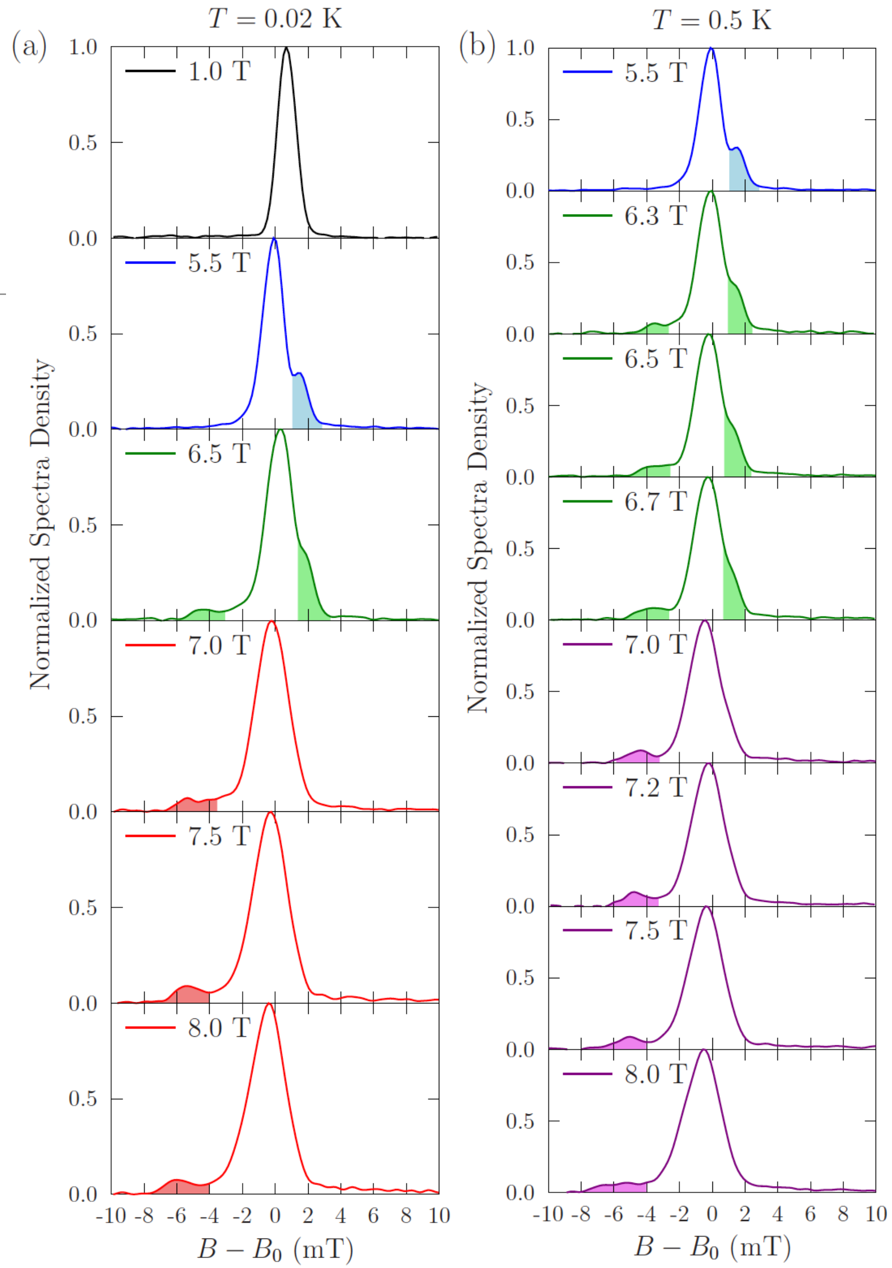
S Ward *et al., J. Phys. Condens. Matter*, **25** 014004 (2013)



T. Lancaster *et al*., arXiv:1806.09402 (2018)

Muon induced effects?

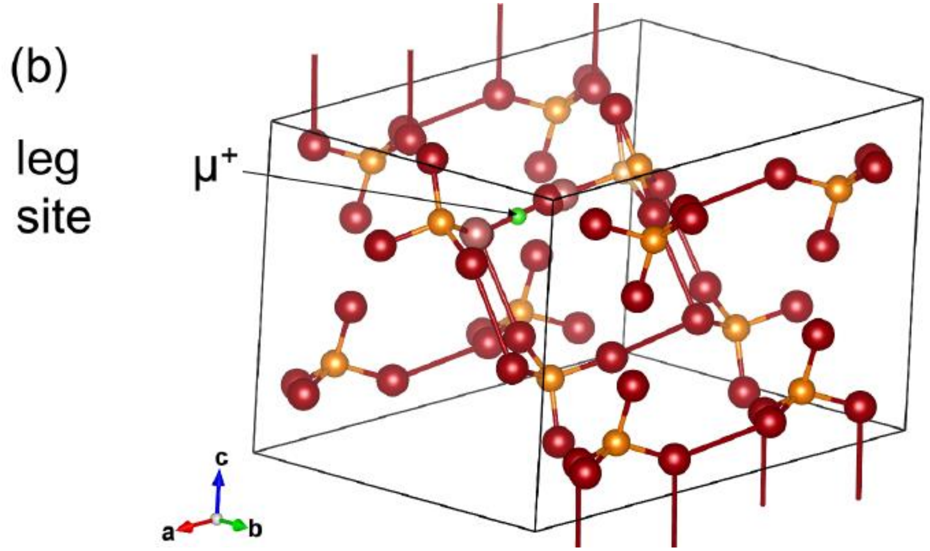
- No local magnetisation expected in quantum disordered (QD) region.
- Small local perturbation made by muon could result in a positive local field.
- Could lead to peak on positive side of B_0 in TF frequency spectra.

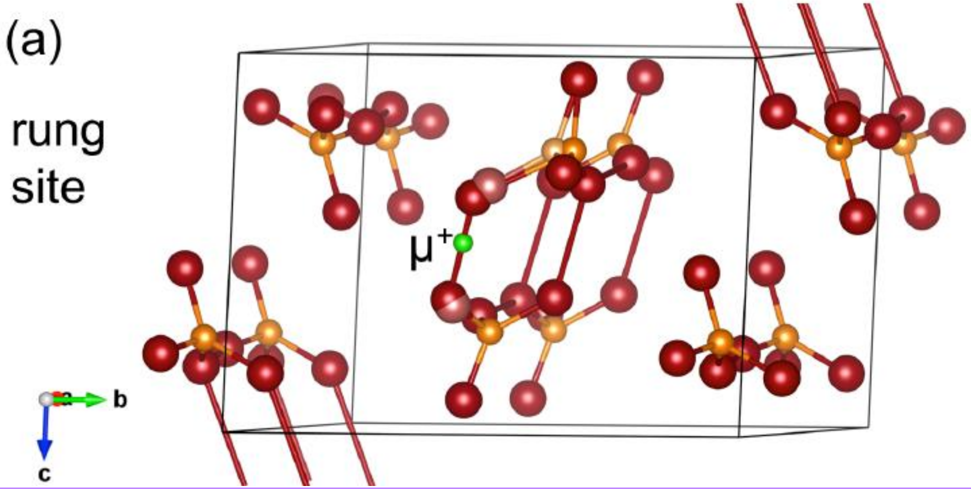


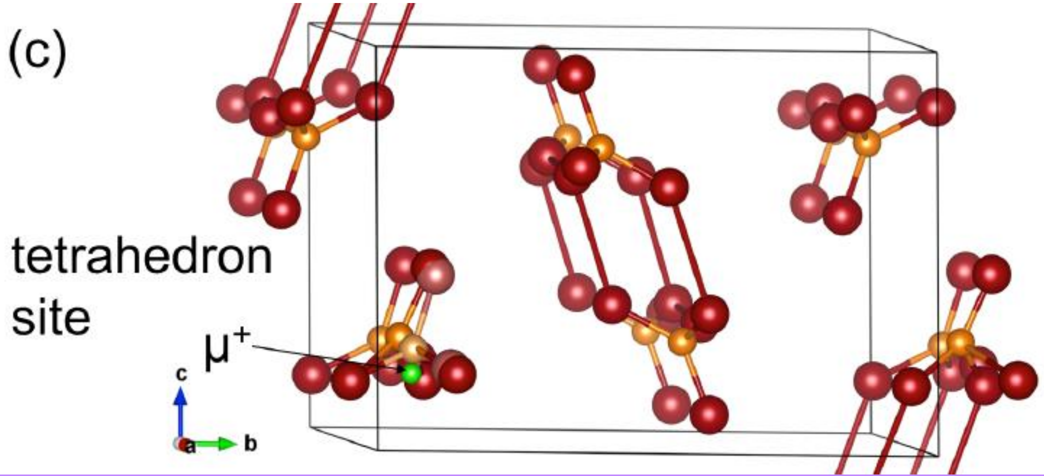
T. Lancaster *et al.*, arXiv:1806.09402 (2018)

Calculated muon sites

- Muon sites calculated from structural relaxations using DFT
- Obtain many stable stopping sites, group into three classes
- Two of these involve the formation of a Br-μ^+-Br bond, muon pulls Br atoms towards it



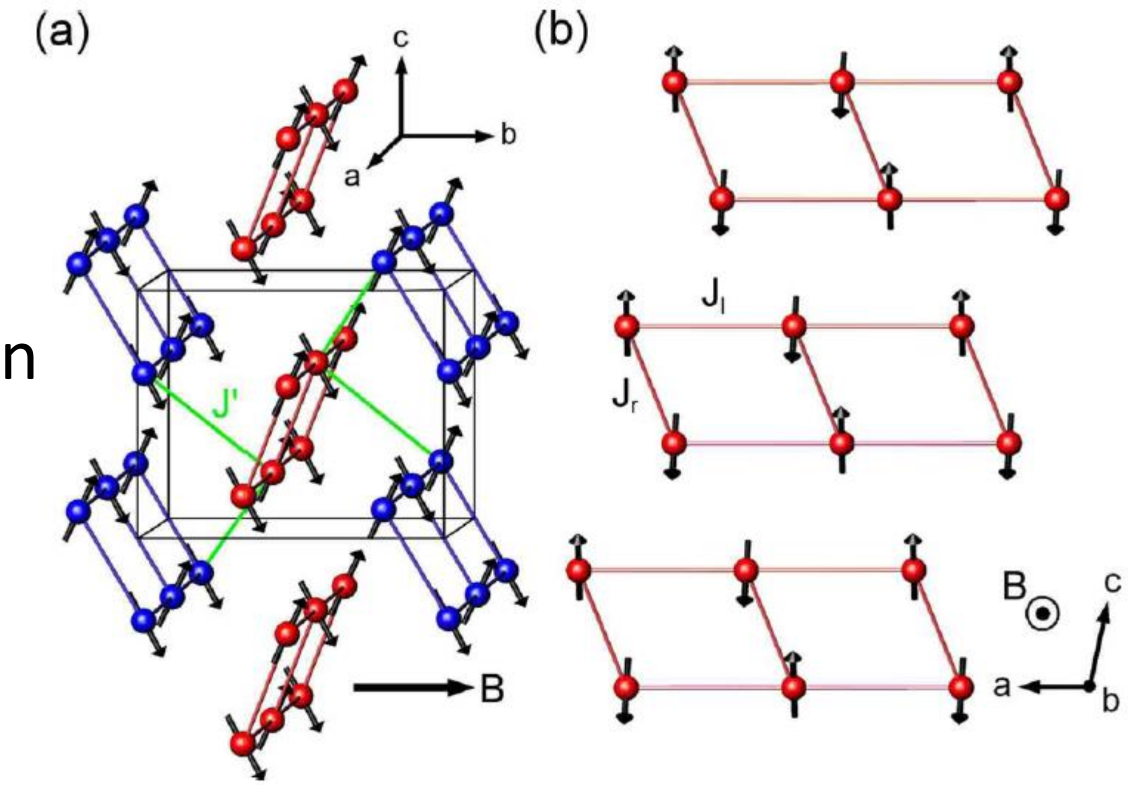




Dipolar field calculations

$$\mathbf{B}_{\text{dipole}}(\mathbf{r}_\mu) = \sum_i \frac{\mu_0}{4\pi r^3}\left[3(\boldsymbol{\mu}_i \cdot \hat{\mathbf{r}})\hat{\mathbf{r}} - \boldsymbol{\mu}_i\right]$$

- Classical magnetic moments located on Cu ions
- Three configurations: FM, AFM and canted AFM
- Fields averaged for sites within each class



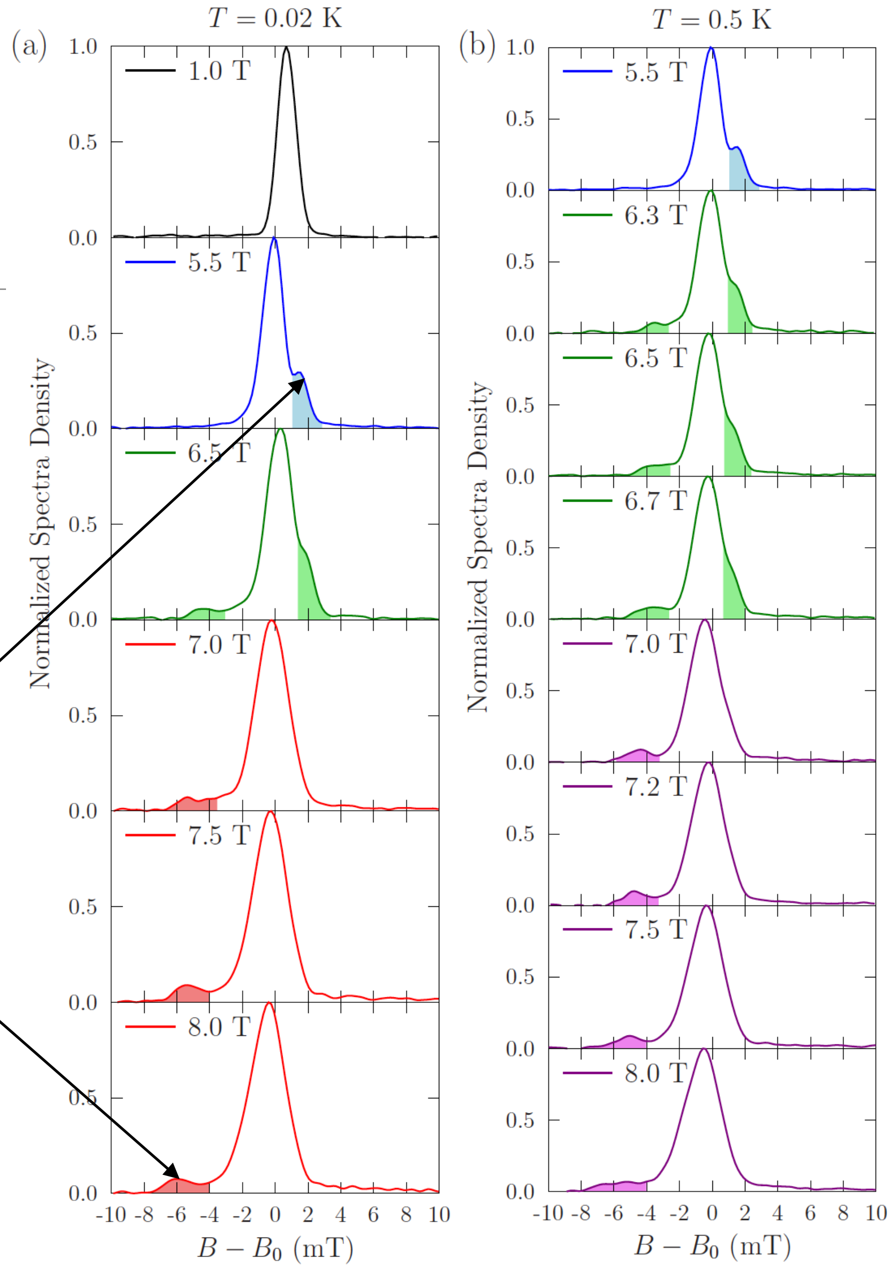
B. Thielemann et al. *Phys. Rev. B* **79**, 020408 (R) (2009)

Dipolar fields and site assignment

- We calculate the component of the local field at the muon along the b axis
- Fields shown below in mT / μ_B

Site	FM	AFM	Canted AFM	0.41 $B_{||}$
Rung	2.0	±5.6	-2.1, 5.2	0.9, 2.1
Leg	-22	±2.7	-19,-15	-7.7, -6.3
Tetrahedron	-64	±34	-71,-27	-33, -11

- The final column gives the expected TF shift for the known ordered magnetic structure



T. Lancaster *et al.*, arXiv:1806.09402 (2018)

Discussion

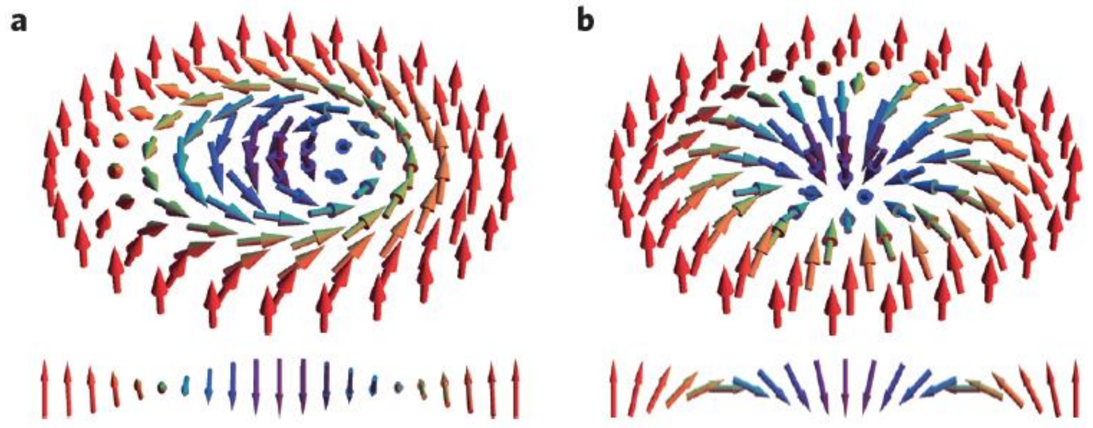
- Impurity-induced AF order is a known property of chain systems, but it is not obvious why the features should only appear in certain parts of the phase diagram

Possible explanations:

- Presence of muon in rung site could cause distortion that reduces size of spin gap
- Interaction between muon-induced moments and QD and LL/LRO phases could lead to fast spin fluctuations and remove static component of field at respective muon sites in each of these phases

Magnetic skyrmions

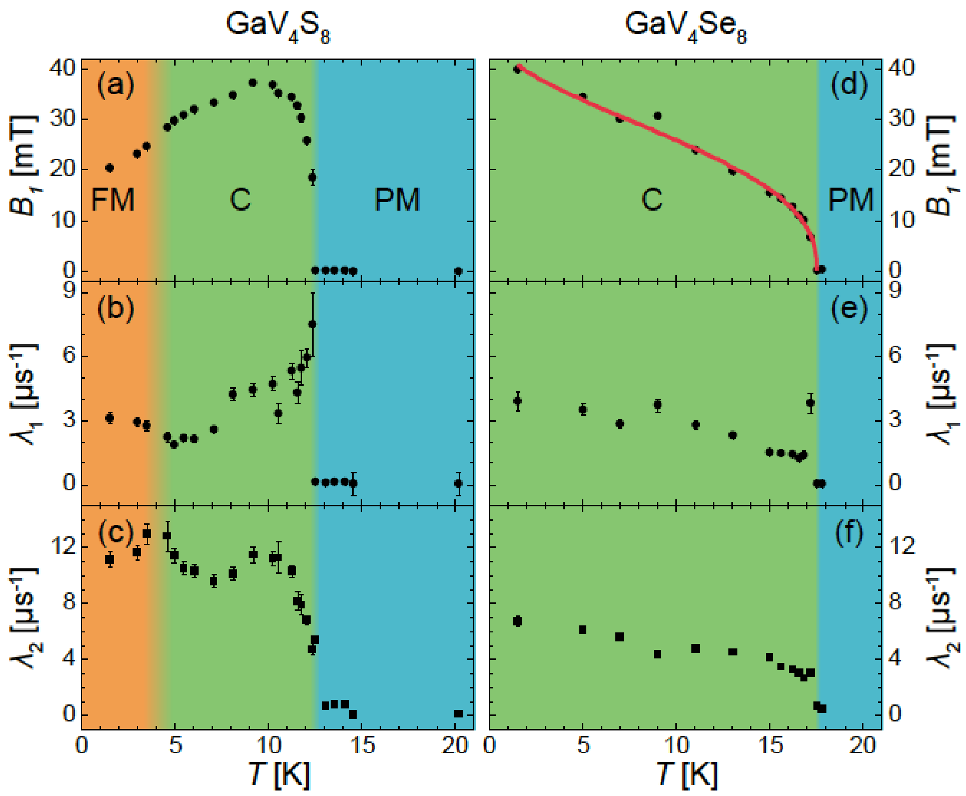
- In non-centrosymmetric crystals energy to form ferromagnetic domains walls can be negative, leads to formation of a skyrmion lattice (SkL)
- Analogy to vortex lattice in type-II superconductors makes μ^+SR a promising technique to study these systems
- Length scales associated with SkL significantly larger than unit cell
- Muons effectively randomly sample SkL



I. Kézsmárki et al. Nat. Mater. **14,** 1116 (2015)

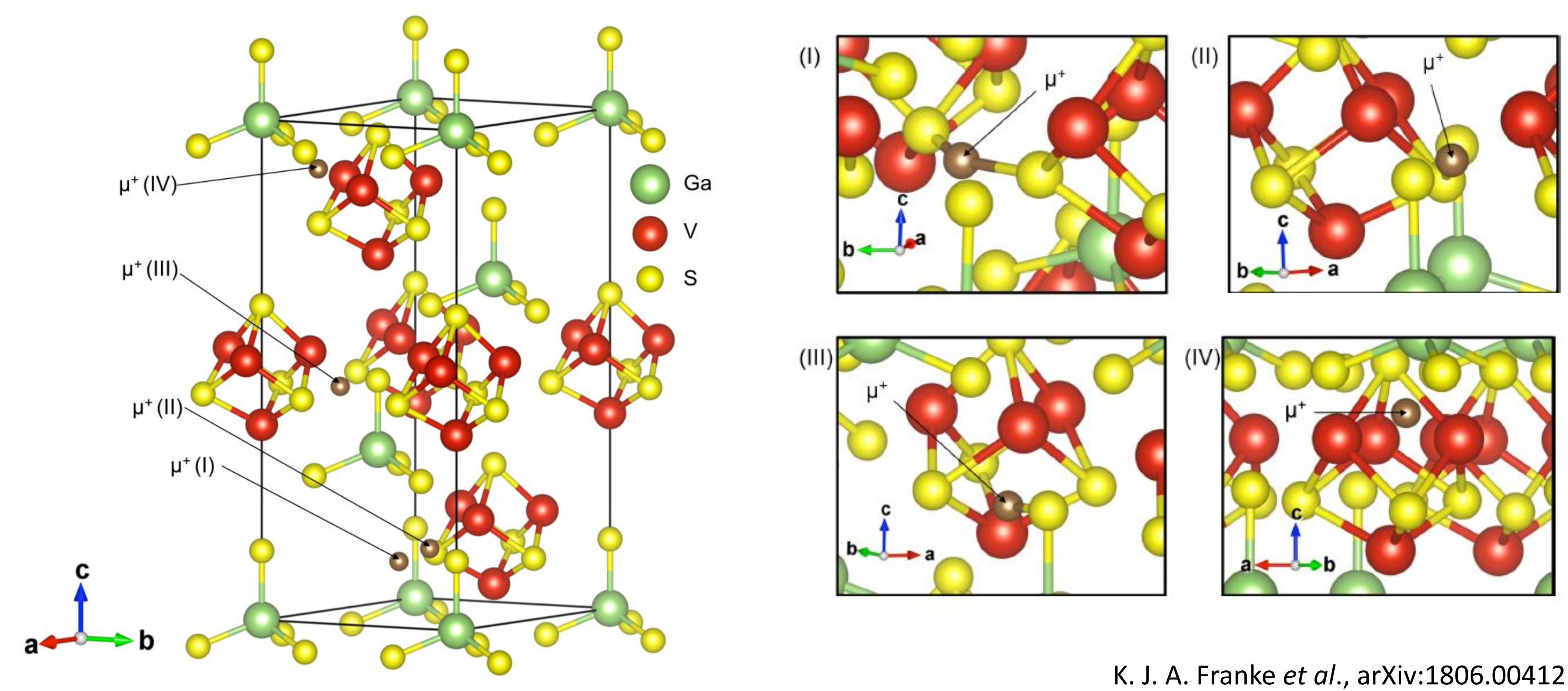
Motivating muon sites

- We investigated members of the series $GaV_4S_{8-y}Se_y$ using μ^+SR, that have been shown to host Néel-type skyrmions.
- LF µSR is sensitive to the SkL phase through the enhanced relaxation due to the emergent dynamics that accompany the SkL
- For ZF measurements, observe unusual temperature dependence of internal field in GaV_4S_8, not seen in GaV_4Se_8. Could this be due to the nature of the muon site?



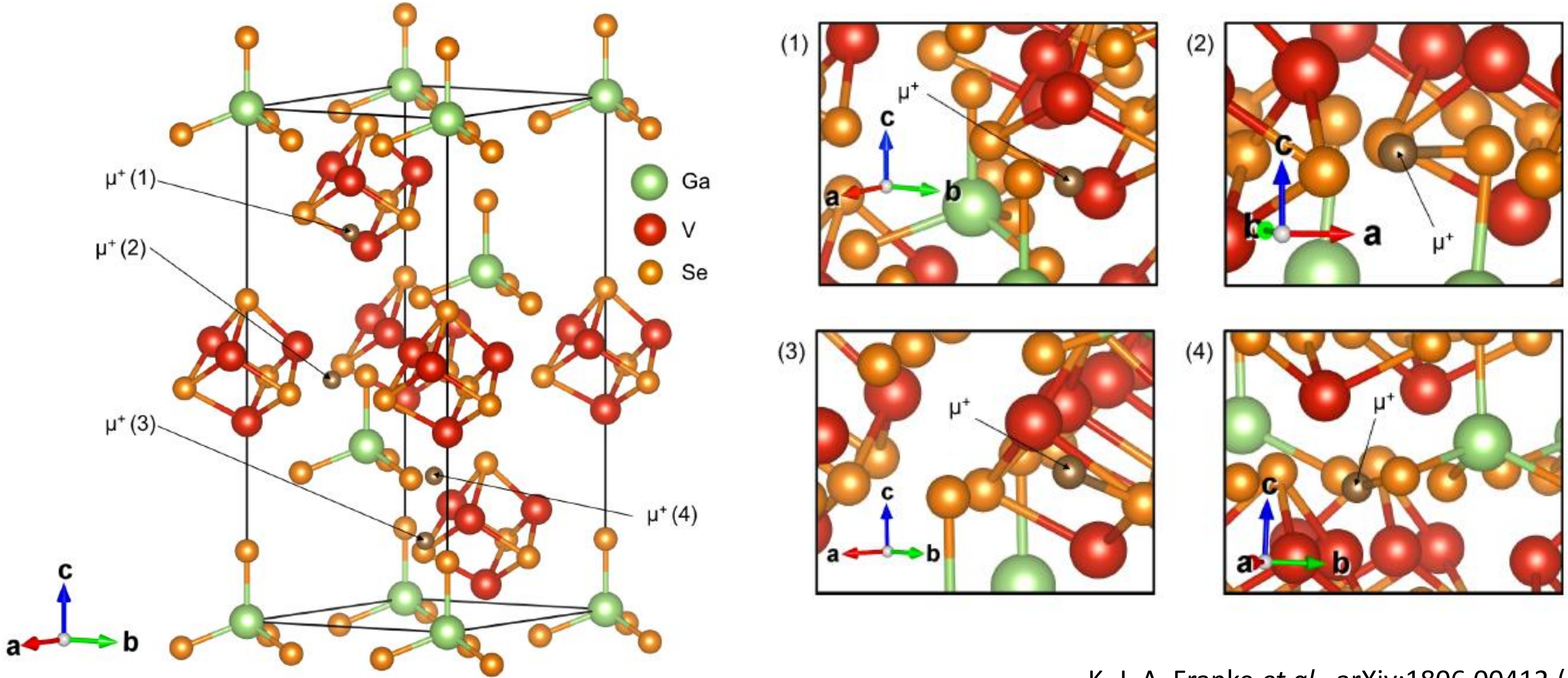
K. J. A. Franke *et al.*, arXiv:1806.00412 (2018)

GaV_4S_8 sites



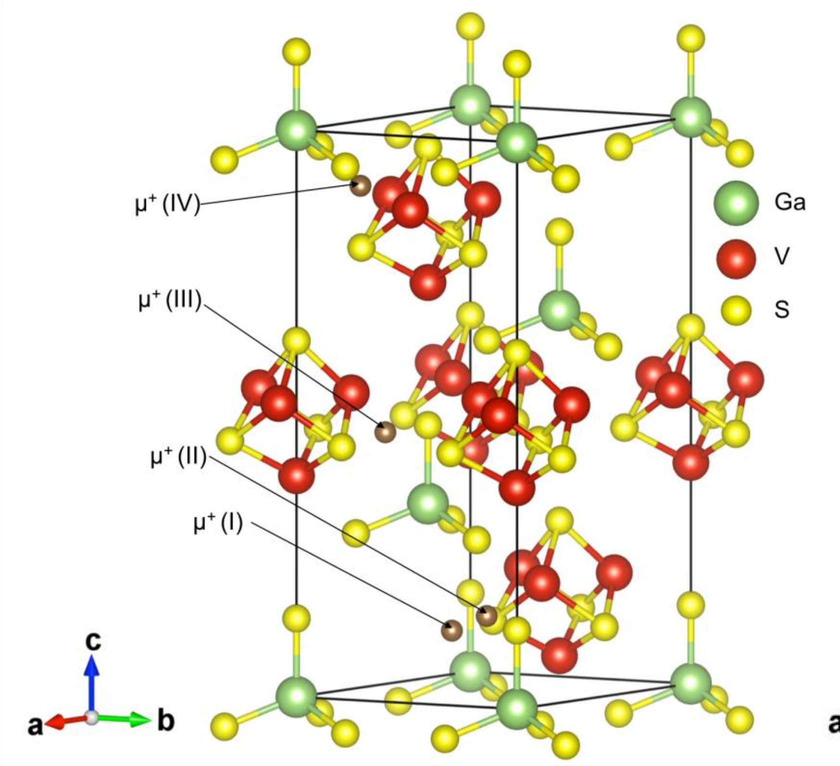
K. J. A. Franke *et al.*, arXiv:1806.00412 (2018)

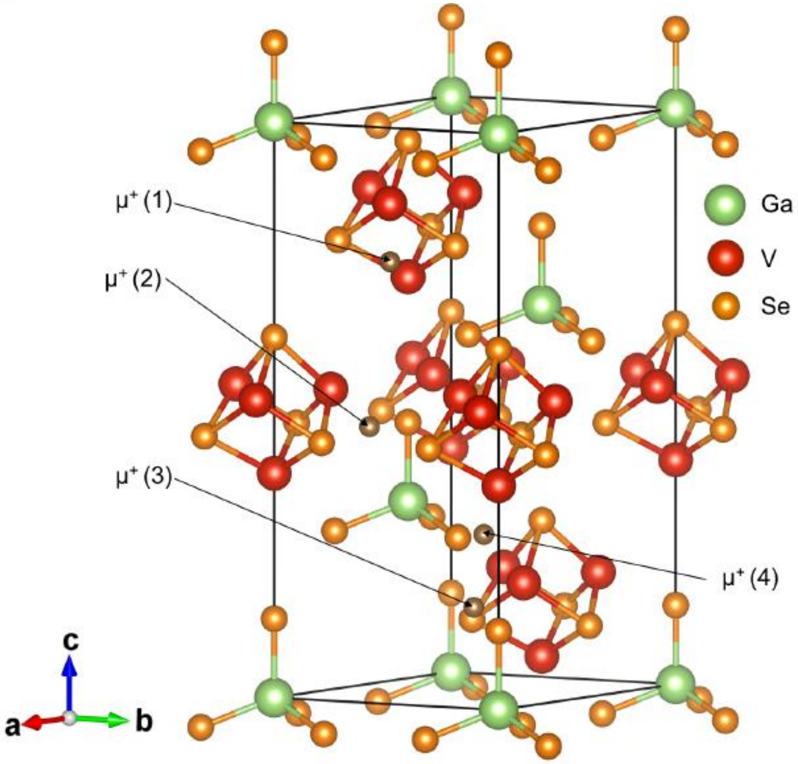
GaV_4Se_8 sites



K. J. A. Franke *et al.*, arXiv:1806.00412 (2018)

Site comparison





- Ordering of similar sites different in two cases
- *d* is distance of muon to nearest S/Se atom

	GaV_4S_8			GaV_4Se_8	
Site	ΔE [eV]	d [Å]	Site	ΔE [eV]	d [Å]
I	0	1.4	4	0.381	1.6
II	0.137	1.5	3	0.190	1.7
III	0.288	1.4	2	0.145	1.7
IV	0.293	2.0	1	0	2.2

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

Discussion

- No significant structural distortions for any of the sites, muon is likely to faithfully probe the magnetism in this system
- It is possible that the lowest energy site is only one occupied, corresponding to two magnetically inequivalent sites due to muons at these sites experience different internal fields as a result of the complex incommensurate magnetic structure.
- The hyperfine contribution at the muon site may play a role
- Hubbard U required to reproduce insulating properties, doesn’t seem to alter muon stopping site

Conclusions

- Muon induced distortions can lead to unusual features in μ^+SR, site calculations can help us understand these.
- For structurally similar systems, the relative stability of stopping sites may be different.
- It is not always necessary to accurately reproduced all of the material properties within DFT to determine the muon stopping site.

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