15th International Conference on Muon Spin Rotation, Relaxation and Resonance

μSR2020

29th August - 2nd September 2022
Parma, Italy

Abstract Book

https://indico.stfc.ac.uk/e/muSR2020

International Society for µSR Spectroscopy ISMS
Comune di Parma
UNIVERSITÀ DI PARMA
UKRI Science and Technology Facilities Council
ISIS Neutron and Muon Source

Preface

Dear Colleagues,

We take great pleasure in welcoming you to the 15th international conference on Muon Spin Rotation, Relaxation and Resonance, which is taking place at the University of Parma in Italy. Parma is a city famous for its architecture, music, art, prosciutto, cheese and surrounding countryside, and we hope you will have chance to experience some of this during your stay.

When we bid to host μSR2020 in 2017, little did we realise just how challenging it would be to deliver this edition of the conference series! Normally taking place every three years, this meeting has been repeatedly delayed due to the onset of the COVID-19 pandemic and the global turmoil that followed. A special 'μSR2020 science day' was held in December 2021 as a means of keeping the community together, which was a great success. But, as we have all no doubt found during the pandemic, this is no substitute for human interactions. We are therefore delighted to finally be able to hold this meeting in-person to bring our community together again, and extremely grateful for your strong support, with over 180 people registered and almost 220 abstracts submitted.

The conference has been jointly organised by the muon groups at the University of Parma and at the ISIS muon source at the Rutherford Appleton Laboratory in the UK. We particularly want to thank our sponsors: Fondazione MonteParma, CAEN-Nuclear Instruments, 5Pascal-Edwards, Nippongases, Nature Reviews Physics, SOL, Quantum Design, IEEE, Rhode-Schwarz and Leiden Cryogenics, who have generously supported this meeting.

This year's conference starts off on Sunday with a 'Student day' with a difference. While we're starting with a short tutorial session, the bulk of the day is given over to the students themselves, to share their research with their peers through a series of short informal talks. There will even be a prize for the best talk!

The programme continues through the week with talks reflecting all aspects of the μSR technique. We particularly want to thank our invited speakers for their contributions, but want to extend this thanks to everyone contributing to the science programme. We hope it'll prove informative and provoke discussion in equal measure, inspiring new ideas and experiments.

Roberto De Renzi and Adrian Hillier
Joint Conference Chairs
University of Parma and STFC-ISIS

About

Topics

EM Energy Materials

FR Facility Reports

MC Molecular Chemistry and Chemical Physics

NT New Techniques

X New Techniques (Muonic X-Rays)

SEMI Semiconductors

SC Site Calculations

SL Spin Liquids and Related Phenomena

SCE Strongly Correlated Electron Systems

SU Superconductivity

Invited Speakers

Catia Arbizzani, Università di Bologna, Italy
Bruce Gaulin, McMaster University, Canada
Giacomo Ghiringhelli, Politecnico of Milano, Italy
Reizo Kato, RIKEN, Japan
Ioan Pop, Karlsruhe Institute of Technology, Germany
Jorge Quintanilla, University of Kent, UK
Roberta Sessoli, University of Florence and INSTM, Italy
Reiner Zorn, Forschungszentrum Juelich, Germany

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Andrea Vacchi, Udine University, Italy
Isao Watanabe, RIKEN-RAL, Japan
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Koji Yokoyama, STFC-RAL, UK

Sponsors

The µSR2020 organising committee would like to pay a special thanks to the following sponsors:

- 5Pascal-Edwards
- CAEN-Nuclear Instruments
- Fondazione Monteparma
- IEEE
- Leiden Cryogenics
- Nippongases
- Nature Reviews Physics
- Quantum Design
- Rohde & Schwarz
- SOL

Abstract book created on August 25, 2022 by John Wilkinson using the AMCOS package in LaTeX.

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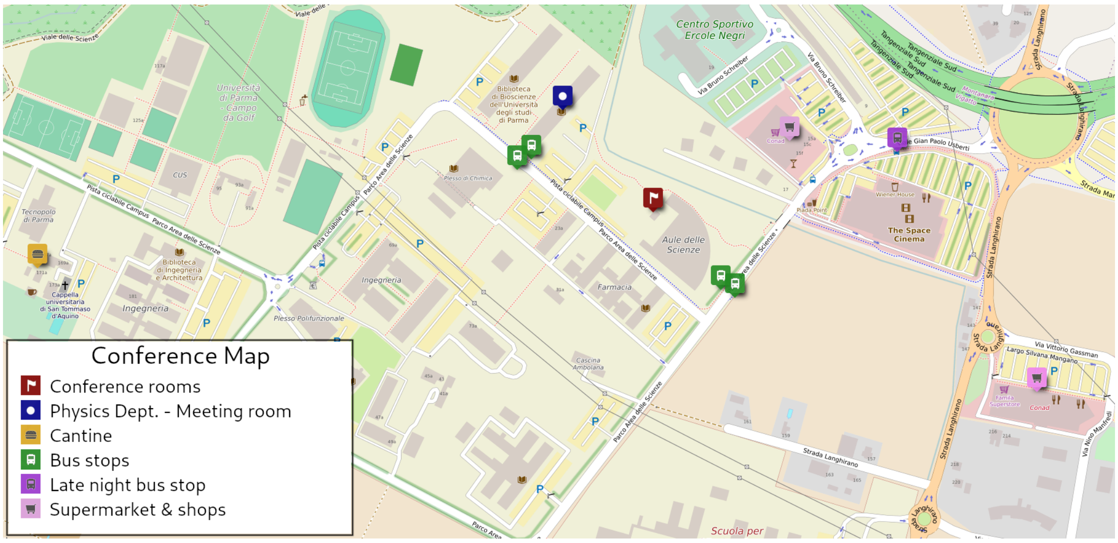
Conference Maps

Map of University

Map of the campus, showing the locations of the key buildings hosting the conference.



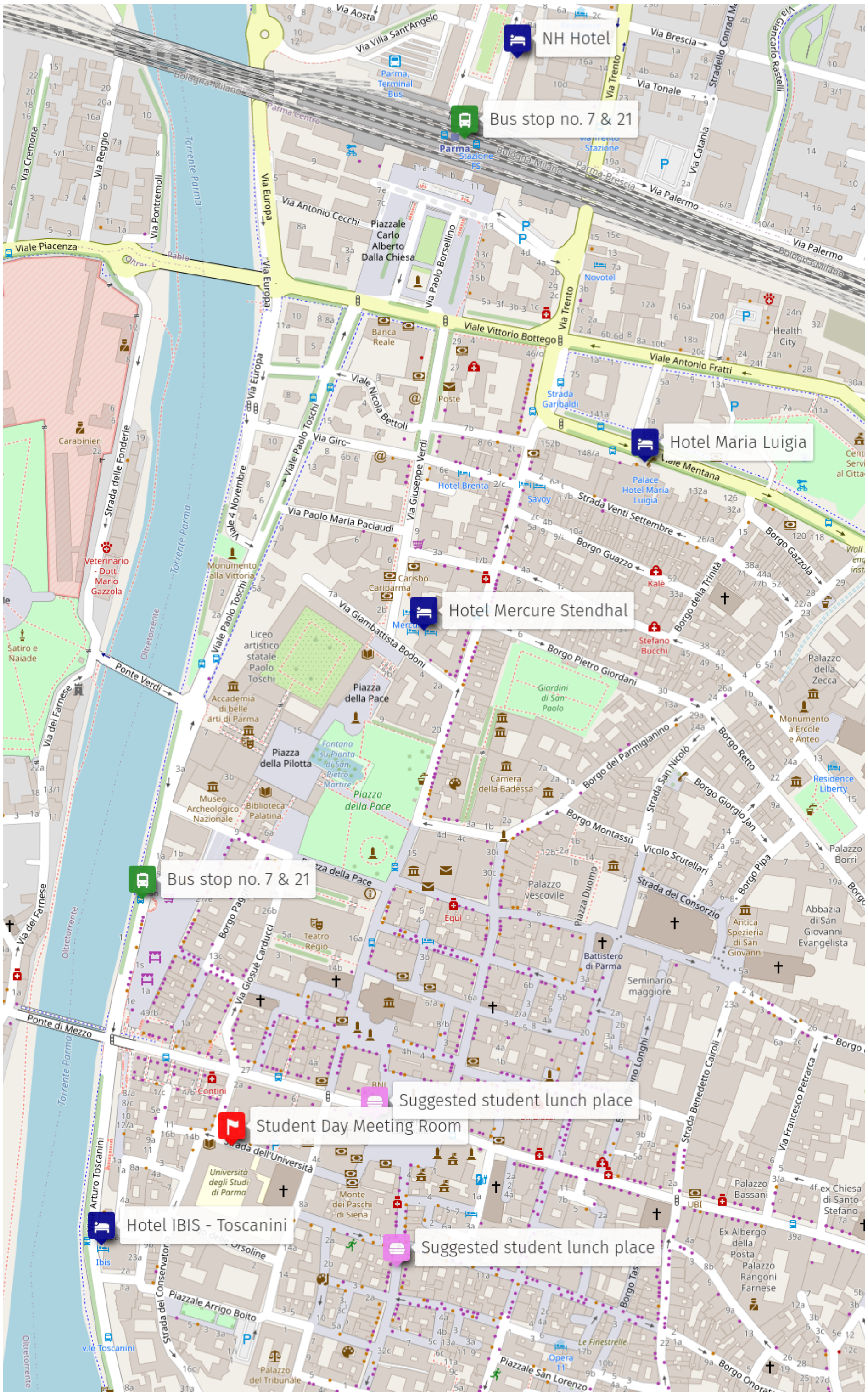
Bus information

The lines reaching the campus are numbers 7 and 21, and the journey to the venue takes approximately twenty minutes. You can find the timetables at https://www.tep.pr.it or with Google Maps.

There are more stops close to the city center and along the river Parma than those reported in the map. You can find them here:

- Line 21: https://www.tep.pr.it/linea/21
- Line 7: https://www.tep.pr.it/linea/7

Map of Parma


NH Hotel
Bus stop no. 7 & 21
Hotel Maria Luigia
Hotel Mercure Stendhal
Bus stop no. 7 & 21
Suggested student lunch place
Student Day Meeting Room
Hotel IBIS - Toscanini
Suggested student lunch place

Information for Presenters

Invited Talks

These have been allocated a 40 minute slot in the programme, which includes time for questions. We suggest allowing 5 minutes for questions.

Contributed Orals

These have been allocated a 20 minute slot in the programme, which includes time for questions. We suggest allowing 5 minutes for questions.

Student Day Presentations

The abstracts for the oral presentations taking place on the Student Day (Sunday 28th August) are listed in this book.

Students are encouraged to also present a poster of their work during the main conference session. Check in the section 'Posters' to find out which poster session you have been allocated.

All speakers: If you wish to use your own computer for your slides, you must ensure that it can connect to HDMI. We will unfortunately not be able to provide an adapter.

Posters

Poster boards are sized 2m (vertical) x 1.2m, to accept at least A0 portrait. Posters should be displayed on the poster boards according to allocated session, whether that be Monday, Tuesday, or Thursday. These poster allocations are listed in this abstract book, in the section 'Posters' (click here if viewing online). Please check your Programme Code and use the corresponding board.

All posters, especially virtual posters for those who are unable to attend, can be uploaded to Padlet for a virtual poster session.

Posters connected with the Facility Updates session on Tuesday afternoon can be displayed all week.

Virtual Sessions

Overview

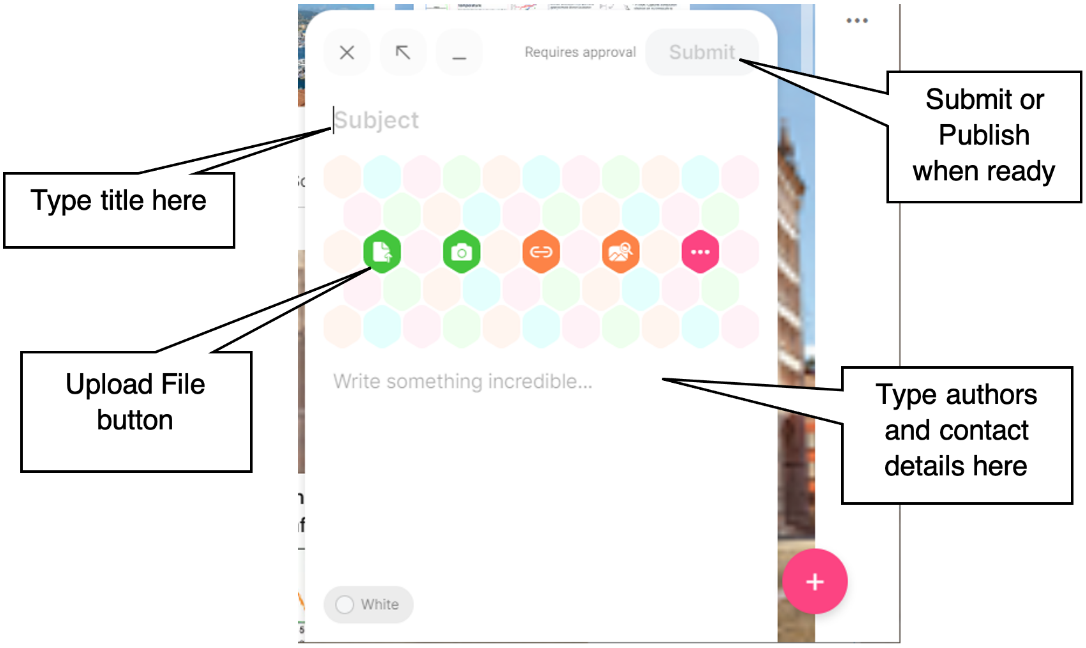
- We are using the Padlet website to host the virtual poster session, and to host the slides from the talks. This will be active during the conference and for at least the following 2 weeks.
- In addition to uploading your poster, you should provide contact details for the presenting author (email recommended) and optionally a link for an online discussion (Zoom or similar).
- Please specify time(s) when you will be available for the discussion – typically this would be the week after the conference.
- In-person poster presenters and speakers are also encouraged to upload their poster or slides for the benefit of those joining the conference virtually.
- We encourage you to upload your contributions as soon as possible to give people plenty of time to browse the material, which is available to all as soon as it is uploaded
- PDF or PowerPoint files are preferred. PDF is better for posters as the online viewer lets you zoom in. The site can also accept image files for posters (jpg, png, etc).
- Please try to answer email questions promptly. If there are "frequently asked questions" then you could put an explanation in the comments attached to your poster.

Instructions

- Padlets have been created corresponding to the various conference sessions as follows:
  - Virtual poster session: https://padlet.com/musr2020/VirtualPosters
  - Poster session 1 (Monday): https://padlet.com/musr2020/PosterSession1
  - Poster session 2 (Tuesday): https://padlet.com/musr2020/PosterSession2
  - Poster session 3 (Thursday): https://padlet.com/musr2020/PosterSession3
  - Facility posters: https://padlet.com/musr2020/FacilityPosters
  - Slides from talks: https://padlet.com/musr2020/Talks
- Click on the relevant link and it will open the page for the session. There may

be a few posters already there.

- Although it's not necessary to create your own account on the Padlet site, we recommend you do as this gives you the option of going back and editing your contribution, for example uploading a new version of the slides.
- Click on the "+" at the bottom right. You get the pop up window shown below:



To helo others identify your contribution, please do the following:

1. Type the 'Programme Code' of your contribution (e.g. 'P-VIR-1', 'O-1', etc) followed by your poster/talk title in the subject box at the top.

2. In the text box below please put:

    - Author names (put the presenting author in bold: drag to select the text and click "B" in the pop up which appears)
    - Contact email for author and discussions
    - *Optional:* Zoom link and time for an online discussion if offered. Be sure to specify the time zone!

3. Click the "Upload file" button and browse to the file on your computer. Click "Open".

4. Once it has uploaded, and a thumbnail has appeared, click “Publish” or “Submit” at the top right.

5. The poster should appear on the main window. Don’t worry about the ordering, we’ll arrange them if required.

6. If you see a message “Awaiting moderation” it means we’ve enabled moderation on the site and will need to check before publishing it.

Viewing the online contributions

- Contributions can be viewed using the same links as used for uploading.

- Click on the image in a contribution to open it full size in the browser window, or click on “...” at the top right and select “Open post”. If it is a PDF you can zoom in with the “+” and “-” buttons and use the scroll bars. For PowerPoint talks, use the “<” and “>” at the bottom or click on the slide to advance.

- The pane at the right (if you used the “Open post” button) shows the poster title, authors and any other information such as the link for an online discussion. It’s also possible to leave comments, if enabled. Note that the presenting author is not automatically informed that comments have been left, so it’s best to use email for questions.

- You can go straight to the next or previous contribution using the “>” and “<” buttons at the top right. Alternatively, click “x” at the top left to go back to the overview page.

Conference Proceedings

Papers will be peer reviewed and published online in the IOP publication: Journal of Physics: Conference Series.

Author guidelines for preparing the pdf files for submission (including templates for LaTeX and Microsoft Word) can be found here.

To help give a uniform feel to the proceedings we strongly encourage authors to prepare manuscripts using LaTeX.

There is no length limit, but around six pages would be suggested, with appropriateness of length being one of the considerations for reviewers.

The online publication will be covered by a Gold open access Creative Commons Attribution (CC BY) licence: Click here for more information.

Papers can be submitted by visiting the Morressier website: https://www.morressier.com/call-for-papers/62f28fe56328740012ed10f6.

Paper submissions close on 5th September.

Conference Excursion

Wednesday 31st August, 14:15 - 19:00.
Visiting Rocca San Vitale di Fontanellato, Villa Magnani, with a glimpse of the Castle of Torrechiara

The bus leaves from Campus at 14:15, with the guided tour of Rocca di Fontanellato starting 14:45. The bus will then continue to Villa Magnani in Mamiano (17:00), passing by the Castle of Torrechiara on the way back to the hotels, that we reach at 19:00. This will be followed by the conference dinner at 20:00, by Trattoria Il Cortile (details of the location and menu are on the next page).

Fontanellato

The Rocca of Fontanellato (1124)
built by order of Oberto I
Pallavicino.

Mamiano

Hidden gems in a Parma Villa:
Filippo Lippi, Cezanne, De Chirico
Morandiand more,
in the setting of a beautiful park.

The Rocca contains a notable
Fresco of Diana and Actaeon by
Francesco Mazzola, il
Parmigianino.

The art collection

Luigi Magnani,
the eclectic
collector, filled
his country
house with five
centuries of
masterpieces.

Torrechiara

On the way
back, the
Castle of
Torrechiara

Conference Dinner

The conference dinner will take place at Società Parmense Lettura e Conversazione (Centro Culturale), Strada Madedonio Melloni, 4, 43121 Parma. Click here to see this in Google Maps.

The menu is as follows (options for special diets will be available):

Appetizers

Le Delizie di Parma mixed cold cuts
(Parma Ham aged 24 months, Culatello Dop, Salame di Felino, Cooked spalla of San Secondo, Parmesan cheese)
Artisan Raw vegetables & Hot Fried Pie Chunks

First course

Tortelli of the Tradition seasoned with melted butter and Parmesan
Risotto alla Giuseppe Verdi with Culatello, Asparagus and Porcini Mushrooms

Second course

Meat with side dishes
Leg of veal with fine herbs
Baked Potatoes and Grilled Vegetables

Dessert

Fresh fruit tart
-
Coffee
-
Alisea spring water
-
Tip. Sparkling White Wine Malvasia dei Colli doc Az. Lamoretti
Tip. Angelico Red Wine (Cabernet - Merlot - Barbera)
Az. Palazzo
Alternatively, sparkling Lambrusco Il Cortile in combination

Programme

Registration is open from 16:00–20:00 on Sunday 28th and 09:00–14:00 on Monday 29th August

CT: Contributed Talk, IT: Invited Talk, YP: Yamazaki Prize, TL: Tutorial lecture

Student day: Sunday 28th August

The entirety of this day will take place at the University Central Palace, via Università 12, Parma

09:30–09:35	**Introduction – Roberto De Renzi, University of Parma**		
	Tutorials		
9:35–10:00	TL	**Francis Pratt** STFC-ISIS	Introduction to muon spin spectroscopy
10:00–10:25	TL	**Leandro Liborio** STFC-SCD	Computational techniques to support muon science
10:25–10:50	TL	**Thomas Prokscha** PSI	Instrumentation for muon spectroscopy
10:50–11:00	**Discussion**		
11:00–11:30	**Coffee Break**		
	Student talks I		
11:30–11:45	CT	**Jonah Adelman** University of British Columbia	Nuclear magnetic resonance of ^{8}Li ions implanted in ZnO
11:45–12:00	CT	**Hank Wu** University of Oxford	A wolf in sheep's clothing? Muon-induced magnetism in quantum spin ice

12:00–12:15	CT	**Yoko Kimura** Osaka University	Negative muon spin relaxation in water and ice
12:15–12:30	CT	**Muhammad Isah** University of Parma	Calculating muon sites and couplings from a high-throughput modelling perspective
12:30–13:45	**Lunch**		

Student talks II

13:45–14:00	CT	**Marta-Villa De Toro Sanchez** TRIUMF and U. of Edinburgh	Development and test of a TDC and amplifier circuit for a multi-channel positron detector
14:00–14:15	CT	**Yuqing Ge** Chalmers University of Technology	Inducing Quantum Criticality in $CrCl_3$ Under Pressure
14:15–14:30	CT	**Changsheng Chen** Fudan University, China	Possible p-wave parity in Cr-based superconductor $Pr_3Cr_{10-x}N_{11}$
14:30–14:45	CT	**George Gill** University of Oxford and STFC-ISIS	Data analysis for µSR experiments with negative muons
14:45–15:15	**Break**		

Student talks III

15:15–15:30	CT	**Maria Mendes Martins** PSI	Profiling defect and charge carrier density in the SiO_2/4H-SiC interface with Low-Energy Muons
15:30–15:45	CT	**Takato Sugisaki** Osaka University	Development of magnetic resonance imaging (MRI) system using beta-NMR technique
15:45–16:00	CT	**Anshu Kataria** Indian Institute of Materials Structure Science	Time-reversal symmetry breaking in nonsymmorphic type-I superconductor $YbSb_2$
16:00–16:15	CT	**Mae Abedi** Simon Fraser University	Anomalous electrical transport in frustrated intermetallic $RCuAs_2$: the role of spin
18:00–20:00	**Welcome Reception**		

Monday 29th August

09:00–09:20	**Opening Remarks**		
9:20–10:20	YP	**Stephen Blundell** University of Oxford	Yamazaki Prize Lecture – The quantum muon
10:20–10:40	**Break**		
	Spin liquids and related phenomena I		
10:40–11:00	CT	**Matjaž Gomilšek** Josef Stefan Institute	Role of Many-Body Quantum Effects in µSR Measurements
11:00–11:20	CT	**Francis Pratt** STFC-ISIS	Studying spin diffusion and quantum entanglement with LF-μSR
11:20–11:40	CT	**Jonathan Frassineti** University of Bologna	Exploting magnetic interactions in Kitaev anti-ferromagnet Na_2PrO_3
11:40–12:20	IV	**Giacomo Ghiringhelli** Politecnico di Milano	What high resolution RIXS can tell us of cuprates (and of other quantum materials)
	Strongly correlated electron systems I		
12:20–12:40	CT	**Tom Lancaster** Durham University	Insights into skyrmion-hosting materials from implanted muons
12:40–13:00	CT	**Andrew W. MacFarlane** University of British Columbia	Studying the evolution of the metallic state in $LaNiO_3$ from a single crystal to superlattices with β-detected NMR
13:00–14:00	**Lunch**		
	Superconductivity I		
14:00–14:40	IV	**Jorge Quintanilla** University of Kent	Unsupervised machine learning of muon experiments – why?
14:40–15:00	CT	**Zurab Guguchia** PSI	Time-reversal symmetry-breaking charge order in a kagome superconductor

15:00–15:20	CT	**Hans-Henning Klauss** T. U. Dresden	Two-component superconductivity in Sr_2RuO_4 studied by uniaxial and hydrostatic pressure μSR
15:20–15:40	CT	**Jeff Sonier** Simon Fraser University	Ubiquitous Spin Freezing in Spin-Triplet Superconductor UTe_2
15:40–16:00	**Break**		

Muonic X-rays

16:00–16:20	CT	**Matteo Cataldo** STFC-ISIS	Negative muons for the characterization of thin layers in Cultural Heritage artefacts
16:20–16:40	CT	**Izumi Umegaki** Toyota Central R&D Labs	Non-destructive operando measurements of muonic x-rays on Li-ion battery
16:40–17:00	CT	**Motonobu Tampo** KEK	Developments on muonic X-ray measurement system for historical-cultural heritage samples in Japan Proton Accelerator Research Complex (J-PARC)
17:00–17:20	CT	**Sayani Biswas** PSI	Muon-Induced X-ray Emission (MIXE) at PSI
17:20–19:00	**Monday Poster Session**		

Tuesday 30th August

09:00–09:40	IV	**Roberta Sesssoli** University of Florence	Opportunities and challenges of molecular spins in quantum nanoscience

Molecular chemistry and chemical physics I

09:40–10:00	CT	**Alessandro Lascialfari** University of Pavia	Spin dynamics of V-based molecular magnets with integer spin values
10:00–10:20	CT	**Giacomo Prando** University of Pavia	Ultrafast molecular rotors in metal-organic frameworks: a combined ^{1}H-NMR and μSR study
10:20–10:40	**Break**		
10:40–11:20	IV	**Catia Arbizzani** University of Bologna	Challenges in next generation batteries for accelerating decarbonization
11:20–11:30	**Sponsor event: Quantum Design**		

Energy Materials

11:30–11:50	CT	**Daniele Pontiroli** University of Parma	H_2 storage mechanism in fullerides studied with μSR
11:50–12:10	CT	**Helena Vieira Alberto** University of Coimbra	Low energy muon study of the p-n interface in chalcopyrite solar cells
12:10–12:30	CT	**Jun Sugiyama** CROSS Neutron Science and Technology Center	Negative muon spin rotation and relaxation for energy materials
12:30–12:50	CT	**Stephan Eijt** Delft University of Technology	New insights into the photochromism of yttrium oxyhydride thin films from in-situ muon spin rotation (MuSR) and positron annihilation spectroscopy (PAS) studies
12:50–13:10	CT	**Martin Mansson** KTH	Ion Diffusion in Na-ion Battery Cathode Material $Na_{0.5}Mg_xNi_{0.17-x}Mn_{0.83}O_2$

13:10–14:20	**Lunch**		
13:40–14:20	**ISMS Executive Meeting (Hybrid)**		

Facility Updates (Hybrid)

14:20–14:35	FU	**Koichiro Shimomura** J-PARC	Present status of J-PARC MUSE
14:35–14:50	FU	**Sydney Kreitzman** TRIUMF	TRIUMF Centre for Molecular and Materials Science Facility Overview
14:50–15:05	FU	**Yu Bao** CSNS	Progress on muon source project at CSNS
15:05–15:15	**Sponsor Event: CAEN-Nuclear Instruments**		
15:15–15:30	FU	**Wonjun Lee** RAON	Status of μSR facility in RAON
15:30–15:50	**Break**		
15:50–16:05	FU	**Thomas Prokscha** PSI	Status of the Swiss Muon Source at PSI
16:05–16:20	FU	**Peter Baker and Isao Watanabe** STFC-ISIS and RIKEN	ISIS Facility Report
16:20–16:30	**Discussion**		
16:30–16:45	**Tributes to Fred Gygax and Jun Kondo**		
16:45–17:20	**ISMS General Assembly**		
17:20–19:00	**Tuesday Poster Session**		

Wednesday 31st August – *Hybrid day*

All talks on this day will be hybrid

Strongly correlated electron systems II

09:00–09:20	CT	**Martin Dehn** University of British Columbia	Discovery of Hidden Charge-Neutral Muon Centers in Magnetic Materials: Implications and Applications
09:20–09:40	CT	**Pierre Dalmas de Reotier** University of Grenoble Alpes	From μSR spectra to the magnetic interaction energy parameters: the MnSi helimagnet as a test case

Site calculations I

09:40–10:00	CT	**John Wilkinson** University of Oxford/STFC-ISIS	Quantum Information: How does it µve through fluorides?
10:00–10:20	CT	**Ifeanyi John Onuorah** University of Parma	Insights into the magnetic ground state of Fe_2P from μSR, NMR and DFT perspectives
10:20–10:40	**Break**		

Site calculations II

10:40–11:00	CT	**Leandro Liborio** STFC-SCD	MuSpinSim: spin dynamics calculations for muon science
11:00–11:20	CT	**Pietro Bonfà** University of Parma	Entanglement between muon and $I > 1/2$ nuclear spins as a probe of charge environment
11:20–11:40	CT	**Benjamin Huddart** Durham University	What can we learn from muon stopping site analysis?
11:40–12:20	IV	**Bruce Gaulin** McMaster University	Dipolar-Octupolar Quantum Spin Liquids in Ce-based Pyrochlores

Spin liquids and related phenomena II

12:20–12:40	CT	**Rajesh Tripathi** STFC-ISIS	Quantum critical spin-liquid behavior in $S = 1/2$ quasikagome lattice $CeRh_{1-x}Pd_xSn$ investigated using muon spin relaxation

12:40–13:00	CT	**Sourav K. Dey and Ryosuke Kadono** KEK IMSS	Quantum spin liquid behavior in geometrically frustrated Mo pyrochlore antiferromagnet $Lu_2Mo_2O_{5-y}N_2$
13:00–13:10	**Conference Photo**		
13:10–14:00	**Lunch**		
14:00–19:00	**Conference Excursion**		
20:00–23:00	**Conference Banquet**		

Thursday 1st September

09:00–09:40	IV	**Reizo Kato** RIKEN	Low-energy Excitations in Quantum Spin Liquid Derived from Molecular Mott Insulator

Spin liquids and related phenomena III

09:40–10:00	CT	**Philippe Mendels** Université Paris (Sacaly)	Universal fluctuating regime in triangular chromate pure Heisenberg S=3/2 antiferromagnets
10:00–10:20	CT	**Sarah Dunsiger** TRIUMF/Simon Fraser University	Searching for spin liquids in buckled compounds
10:20–10:40	**Break**		
10:40–11:20	IV	**Ioan Pop** Karlsruhe Institute of Technology	Muons and Quantum Computing Hardware: Challenges and Opportunities

Superconductivity

11:20–11:40	CT	**Amit Keren** Technion-Israel Institute of Technology	Phase transition from a magnetic-field-free stiffness meter and LEM viewpoints
11:40–12:00	CT	**Debarchan Das** PSI	Unconventional pressure dependence of the superfluid density in topological superconductor α-PdBi2
12:00–12:20	CT	**Tadashi Adachi** Sophia University	μSR Study of the Relationship between the Magnetism, Superconductivity and Electronic Nematicity in Iron-Chalcogenide Thin Films
12:20–12:40	CT	**Ritu Gupta** Geneva University	Complex nature of charge order and superconductivity interplay in correlated kagome superconductor CsV_3Sb_5
12:40–13:00	CT	**Gianrico Lamura** CNR-SPIN	Is the Abrikosov's vortex-model still valid in nematic superconductors?
13:00-14:20	**Lunch**		

Semiconductors

14:20–14:40	CT	**Rui Vilao** University of Coimbra	Muonium reaction in semiconductors and insulators: the role of the transition state
14:40–15:00	CT	**Jonas A. Krieger** Max Planck Institute of Microstructure Physics	Muonium states in semiconducting transition metal dichalcogenides
15:00–15:20	CT	**Kenji Kojima** University of British Columbia	Probing hydrogen sites and negative hyperfine parameter in semiconducting BaSi2 by muon spin rotation
15:20–15:40	CT	**Koji Yokoyama** STFC-ISIS	Carrier lifetimes in high-lifetime silicon wafers and irradiation induced recombination centres
15:40–16:00	CT	**Ryosuke Kadono and Masatoshi Hiraishi** KEK IMSS	Ambipolar Property of Isolated Hydrogen in Oxide Materials Revealed by Muon
16:00–16:20	**Break**		

New Techniques

16:20–16:40	CT	**Xiaojie Ni** PSI	Impact of Growth Conditions on the $CH_3NH_3PbI_3$ Perovskite Solar Cells, Studied by Low-Energy μSR
16:40–17:00	CT	**Andrin Doll** PSI	Coherent microwave control of muonium
17:00–17:20	CT	**Patrick Strasser** KEK	Status of the New Muonic Helium Atom HFS Measurements at J-PARC MUSE
17:20–19:00	**Thursday Poster Session**		

Friday 2nd September

09:00–09:40	IV	**Reiner Zorn** Forschungszentrum Juelich	Microscopic Dynamics of Structural Glasses Investigated by Quasielastic Neutron Scattering

Molecular chemistry and chemical physics II

09:40–10:00	CT	**Derek Fujimoto** University of British Columbia	First depth-resolved beta-NMR measurements of 1-ethyl-3-methylimidazolium acetate
10:00–10:20	CT	**Joseph Wright** University of East Anglia	Probing the [FeFe]-hydrogenase subsite using muon spectroscopy
10:20–10:40	**Break**		
10:40–11:00	CT	**Victoria Karner** TRIUMF	Advances in biochemical applications of β-detected NMR
11:00–11:20	CT	**Amba Datt Pant** IMSS KEK	New insight into μSR in water

Strongly correlated electron systems III

11:20–11:40	CT	**Zaher Salman** PSI	Beta detected NMR of ^{8}Li in 2H molybdenum ditelluride
11:40–12:00	CT	**Charles Mielke III** PSI	Intriguing Topological Kagome Magnetism of $TbMn_6Sn_6$
12:00–12:20	IV	**Tom Lancaster** Durham University	Conference Summary (Hybrid)
12:20–13:10	**Prize Giving, Best Student Day Talk, IEEE Chapter Presentation, and Closing Ceremony (Hybrid)**		

Presentation Abstracts

Student Day

Nuclear magnetic resonance of ^{8}Li ions implanted in ZnO

CT

SEMI

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with
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N. Ohashi, National Institute for Materials Science, Japan
V. Karner, C. Levy, I. McKenzie, G. D. Morris, M. Pearson, E. Thoeng, R. Li, M. Stachura, TRIUMF, Canada
S. Dunsiger, TRIUMF / Simon Fraer University, Canada
K. M. Kojima, TRIUMF and SBQMI, University of British Columbia, Canada
R. M. L. McFadden, W. A. MacFarlane, D. Fujimoto, J. Ticknor, University of British Columbia, Canada

ZnO is a wide direct bandgap (3.4 eV) semiconductor with promising electronic properties potentially useful in room temperature optoelectronic and spintronic devices. It can be used as a dilute magnetic semiconductor by tuning intrinsic or extrinsic magnetic defects while ZnO also demonstrates many unique surface effects such as a photogenerated metallic state. Imperative to utilizing these unique properties is understanding and controlling point defects in its hexagonal wurtzite structure that may lead to stable hole doping. We implanted a low energy (20-25 keV) beam of hyperpolarized spin-2 ^{8}Li ions and used β-detected nuclear magnetic resonance (β-NMR) to understand the stability, structure, and magnetic state of Li defects in ZnO [Adelman et al., arXiv:2109.08637v1]. Closely related to μSR used to characterize isolated hydrogen impurities in ZnO, β-NMR allows complementary investigations of light isotope dopants in the ultradilute limit.

Using ^{8}Li simultaneously as the defect and probe, distinct Li sites are detected by measuring the coupling of the nuclear electric quadrupole moment to the asymmetric electronic charge distribution surrounding the ^{8}Li nucleus. From 7.6 to 400 K, we find ionized shallow donor interstitial Li is exceptionally stable, verifying its role in self-compensation of the acceptor (Zn) substitutional. Like the interstitial, the substitutional defect shows no resolved hyperfine field above 210 K, indicating it is a shallow acceptor. By pulsing the ^{8}Li beam, the spin-lattice relaxation is measured and indicates above 300 K the onset of correlated local motion of interacting defects. This is supported by resonance spectra collected with a CW frequency comb that enhances the amplitude of well-resolved quadrupolar multiplets and confirms a site change transition from disordered interstitial Li to the substitutional. The quadrupole hyperfine interaction exhibiting a $T^{3/2}$ temperature dependence typical of non-cubic metals is also discussed.

A wolf in sheep's clothing? Muon-induced magnetism in quantum spin ice

CT

SCE

H. Wu, Oxford University, UK
with
S. J. Blundell, Oxford University, UK

Compounds of the form $\mathrm{A_2X_2O_7}$ with the pyrochlore structures can exhibit classical or quantum spin ice behaviour if the crystal field environment of the $\mathrm{AO_8}$ arrangement leads to the [111] easy-axis anisotropy. When Pr occupies the A-site, there is a low-lying electronic doublet and $\mathrm{Pr_2X_2O_7}$ compounds are found to be quantum spin ices[1]. Pr^{3+} is a non-Kramers ion and the presence of the muon can distort nearby $\mathrm{PrO_8}$ units and split the doublet ground states[2], resulting in an enhancement of the Pr nuclear moment due to hyperfine coupling with the electronic moments[3]. We explore this effect using a theoretical model that takes account of the important interactions and compare our simulations with μSR data on samples of $\mathrm{Pr_2X_2O_7}$ (X = Sn, Hf, Zr) and new experimental data on $\mathrm{Pr_2ScTaO_7}$, a candidate system that simultaneously realises spin ice and charge ice structures.

References

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[3] B. Bleaney,*Physica***69**, 317 (1973)

Negative muon spin relaxation in water and ice

CT

MC

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with
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K. Kubo, ICU
P. Amba Datt, K. Shimomura, A. Koda, S. Takeshita, KEK

Muons are the main component of cosmic ray particles on the earth, and most of the cosmic ray muons are injected into water or ice, which occupy more than 70% of the earth's surface. When negative muons (μ^-) stop in H_2O, they are mainly trapped by oxygen nuclei and form muonic oxygen atoms Oμ^-, and about 15% of Oμ^- atoms finally change to stable nitrogen isotopes ^{14}N or ^{15}N via the neutron emission after the muon capture process. The nitrogen isotopes produced by such a process may be chemically active due to their high recoil energy and may form various nitrogen compounds through reactions with water molecules. In this situation, μ^-SR spectroscopy is suitable for studying the behavior of such active nitrogen in H_2O, since Oμ^- atoms also act chemically as nitrogen. In the present study, we measured μ^-SR spectra in water and ice to approach what kind of nitrogen compounds are formed by cosmic-ray negative muons, and how they affect the surrounding chemical environment.

Experiments were carried out at the D1 beamline in the Materials and Life Science Experimental Facility (MLF) of J-PARC. H_2O and D_2O samples were irradiated with a negative muon beam (47 MeV/c, double pulse), and ZF and LF-μ^-SR spectra were measured. The result shows that the relaxation due to the nuclear dipolar field is observed in solid H_2O and D_2O at 200 K. The field distribution widths were deduced to be Δ_H=0.27 μs^{-1} and Δ_D=0.066 μs^{-1}, for H_2O and D_2O respectively. The relationship between these two values is well explained by the difference in the spins and magnetic moments of proton and deuteron.

In this conference, we will discuss possible chemical states based on the present results.

CT

SC

Calculating muon sites and couplings from a high-throughput modelling perspective

M. M. Isah, University of Parma, Italy
with
I. J. Onuorah, P. Bonfà, R. De Renzi, University of Parma, Italy

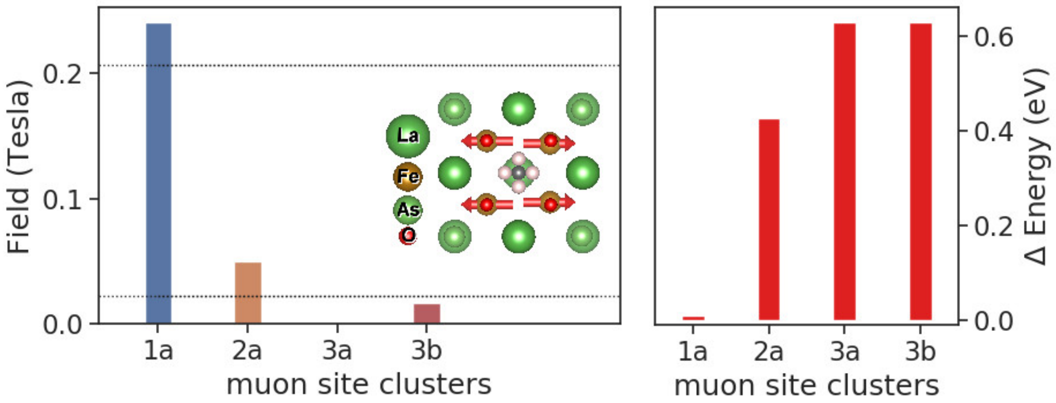

Figure 1: Typical workflow results: In this case for LaFeAsO [2]

In muon spin spectroscopy, the knowledge of muon implantation sites and hyperfine couplings is of importance to the analysis of the experimental data. Over the past decade there has been significant progress in calculating muon sites using first-principles methods such as density functional theory (DFT) [1,2]. However, the protocols required for muon calculations are both resource and task intensive. They are performed sequentially in steps with strenuous human intervention required to track, coordinate and analyse these calculations. The recent advent of the DFT-based high-throughput (HT) approach and the development of dedicated frameworks has opened the possibility of performing this type of sequential large-scale calculations in an efficient way. Here, we present our efforts towards the design and implementation of workflows within the AiiDA integrated platform for high-throughput DFT-based muon calculations aimed at i) the design of a user-friendly approach available to every muon user; ii) benchmarking the scope of sustainable DFT calculations. We started from identifying material selection criteria to exclude the well-known harder cases. We have benchmarked the workflow at its current stage over 16 magnetic compounds. Our preliminary benchmark results demonstrated the feasibility of this plan and have further allowed us to understand the workflow capabilities, its limitations and the likely improvements to be considered for more accurate results of the calculated muon properties. These improvements include; taking into account the muon charge states and spotting the right compromise between sustainable and accurate treatment of electronic correlation effects.

References

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Development and test of a TDC and amplifier circuit for a multi-channel positron detector.

CT

NT

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K. M. Kojima, TRIUMF and University of British Columbia, Canada
T. Ishida , Osaka Metropolitan University, Japan
M. Shoji, M. Miyahara , R. Honda, M. M. Tanaka, KEK, Japan

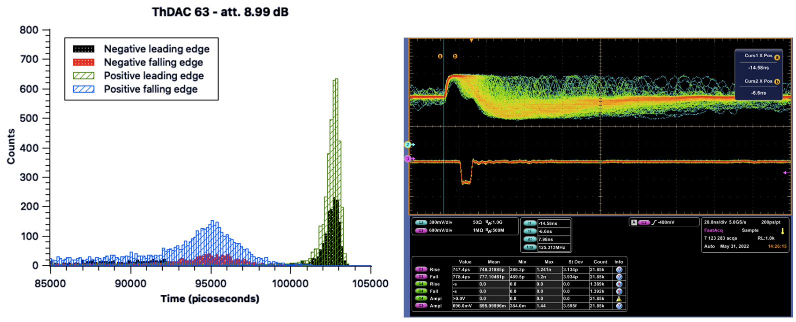

Figure 1

In a continuous beam muon facility positrons are detected by relatively large plastic scintillators without position sensitivity. An idea has been proposed to make these positron detectors multi-channel and able to track the positron trajectories. This will ultimately enable 2-dimensional magnetic imaging of the sample with the µSR technique. To attain this "muon microscope" idea, large numbers of independent photosensors with high-timing resolution will be necessary.

Our group at KEK has developed an amplifier-shaper-discriminator (ASD) circuit named FGATI with 16 channels per chip and a high-resolution time to digital converter, called HR-TDC with a timing resolution on the order of picoseconds. Silicon photomultipliers (SiPMs) from Hamamatsu (MPPC) are employed to give electric pulses for the optical input [1-2]. We have been testing this new set-up at TRIUMF with a pulsed laser to understand the efficiency, transient response, timing resolution, and the data acquisition to a computer. We are now successfully detecting the rising and falling edge timing as well as the time-over-threshold (TOT) of the laser pulses.

The tested circuit will be a basis for the light detection and time recording from scintillation fiber arrays to be used for the multi-channel positron detectors. Multiple layers of such detectors will establish tracking the positron trajectory and aid with the development of the "muon microscope".

This work is partially supported by a Grant-in-Aid for Scientific Research (No.JP21H04666) from Japan Society for the Promotion of Science (JSPS).

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CT

SL

Inducing Quantum Criticality in $CrCl_3$ Under Pressure

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D. Andreica, Babes-Bolyai University, Romania
H. Ohta, Doshisha University, Japan
J. Sugiyama, CROSS and Japan Atomic Energy Agency Japan
R. Gupta, R. Khasanov, Laboratory for Muon Spin Spectroscopy, Paul Scherrer Institute, Switzerland

Accelerated by the discovery of graphene, research on two-dimensional (2D) materials have attracted tremendous attention both from fundamental and applied sciences. Among the large number of 2D materials, chromium trihalides CrX3 (X = Cl, Br, I) van der Waals (vdW) magnets have also raised a large interest due to the existence of many magnetic subtleties that cannot be explained by their magnetic and/or structural transitions.

Numerous studies were performed on CrI3, but only a few have been reported so far on its analogue CrCl3. The 2D vdW CrCl3 compound is stabilized under a rhombohedral symmetry, consisting of 2D Cr layers arranged in a honeycomb web fashion and surrounded by octahedrally coordinated Cl, with weak vdW inter-layers coupling. The layer structure and inter-layer coupling make CrCl3 an ideal system to study under external stimuli such as pressure or magnetic field, where new intriguing states of matter can be unveiled. With such expectations, studies of CrCl3 under room temperature, high pressure have been reported[1]. However, its spin dynamics at low-temperature and high-pressure regime remain unexplored.

In this study, we present the results of our recent muon spin rotation (MuSR) investigations performed on hydrostatically pressured CrCl3. Our previous MuSR results at ambient pressure revealed successive transitions from paramagnetic to short-ranged-order-ferromagnetic then to antiferromagnetic states with strong spin dynamics as the temperature decreases[2]. When applying pressure, we observed that the magnetic ground state is gradually suppressed. A linear extrapolation points toward the suppression of magnetism at about p_c= 30 kbar indicating the possible existence of a quantum critical point at p_c.[3]

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Possible p-wave parity in Cr-based superconductor $Pr_3Cr_{10-x}N_{11}$

CT

SU

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Superconductivity with a critical temperature $T_C \sim$ 5.25 K was recently reported in the Cr-based superconductor $Pr_3Cr_{10-x}N_{11}$. The large upper critical field $H_{C2} \sim$ 20 T, and the strong correlation between $3d$ electrons derived from specific heat, suggest the unconventional superconductivity nature of this compound. We performed muon-spin rotation/relaxation (μSR) measurements on a high-quality polycrystalline of $Pr_3Cr_{10-x}N_{11}$ down to 0.027 K, and specific heat measurements under different magnetic fields up to 9 Tesla. Our μSR data indicate that time-reversal symmetry is broken in the superconducting state of $Pr_3Cr_{10-x}N_{11}$, and the superconducting energy gap is consistent with a p-wave model, which is also supported by the specific heat data.

CT

NT

Data analysis for µSR experiments with negative muons.

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F. L. Pratt, STFC-ISIS Neutron and Muon Source, UK
S. J. Blundell, University of Oxford

Negative muons are often overlooked compared to their positive counterpart, partly due to the loss of around $\frac{5}{6}$ of the μ^- spin polarisation when a μ^- cascades down to the 1s muonic ground state after being captured by a nucleus. One needs to count for around 36 times as long to get statistics comparable to that of a μ^+SR experiment. However, there has been a recent revival of μ^-SR experiments, particularly in the study of hydrogen storage and battery materials [1,2]. When stopped in a material of atomic number Z, μ^- forms a muonic atom and cascades down to its ground state. The muon Bohr radius is 200 times smaller than the electron Bohr radius, and so this probe behaves like an ultra-dilute atom of apparent nuclear charge $Z-1$. The μ^- will be strongly hyperfine coupled to the nuclear spin of the capture atom, but if that nuclear spin is zero, such as an oxygen in MnO, the only coupling will be to the nuclear dipolar fields in a region very close to that capture nucleus. Because of these difficulties new analysis techniques have been developed in WiMDA [3] for the fitting of μ^-SR data, and we have adapted the DFT+μ^+ technique for the case of a negative muon. Both of these new techniques have been applied to MnO where the dipole field simulations show a large field at the oxygen site, and DFT+μ^- calculations show a Jahn-Teller-like distortion around the negative muon.

References

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Profiling defect and charge carrier density in the SiO_2/4H-SiC interface with Low-Energy Muons

CT

SEMI

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with
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Silicon carbide (4H-SiC) is a wide-bandgap semiconductor with promising applications in high-power and high-frequency devices. An advantage of SiC is that it is the only compound semiconductor that has the ability to form native silicon dioxide (SiO_2). The performance of SiC-based devices relies heavily on interface effects. However, characterization of oxidation-induced defects - both in the oxide and the semiconductor - is still challenging.

Low-energy muon spin spectroscopy (LE-μSR) can probe regions very close to the surface and interface up to a depth of 160 nm in SiO_2/SiC structures and is sensitive to charge carrier and defect concentrations.

We have studied SiO_2/SiC interfacial systems with thermally grown and deposited oxides using LE-μSR. The thermal SiO_2 has higher structural order, as indicated by the undisturbed muonium (Mu^0) formation. However, the oxidation process leads to strain in the oxide and to band-bending at the SiC-side of the interface, which affects the SiC faces differently: i) at the (0001) Si-face the results can be explained by the depletion of electrons at the interface and ii) at the $(000\bar{1})$ C-face a carbon-rich n-type region contributes to the increase of the diamagnetic fraction due to Mu^- formation.

Further investigations have been conducted to understand the passivation effects of state-of-the-art post-oxidation annealing (POA) processes on the SiO_2/SiC interface. Particularly, POA in an NO environment leads to an increase in charge carrier concentration near the interface, likely due to N acting as a dopant, which can be quantified based on the measured diamagnetic fraction.

CT

NT

Development of magnetic resonance imaging (MRI) system using beta-NMR technique

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with
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A. Kitagawa, S. Sato, QST, Japan
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D. Nishimura, H. Takahashi, Tokyo City University, Japan
A. Yano, University of Tsukuba, Japan

Today, the technology of magnetic resonance imaging (MRI) has been established and it is essential in the medical field. MRI is the method of making an in-situ image by utilizing nuclear magnetic resonance (NMR). However, the MRI technique has rarely been put to practical use for elements other than hydrogen because of the sensitivity issue. On the other hand, the technique of beta-ray-detecting NMR (beta-NMR) makes it possible to observe NMR for various elements with extremely high sensitivity by measuring the asymmetry of the beta-ray emission from polarized radioisotopes (RIs). By utilizing beta-NMR, we aim to create a 3-dimensional (3D) MRI system. We have developed a detector set with plastic scintillation fibers, which enables us to track back the trajectory of beta-rays. Moreover, by seeking the beta-ray asymmetry at each position in the sample, we can create a magnetic resonance image. We conducted experiments using a spin-polarized $^{12}\mathrm{B}(I = 1, T_{1/2} = 20\ \mathrm{ms})$ beam at HIMAC heavy-ion synchrotron facility of the National Institutes for Quantum Science and Technology. We obtained the data from various samples of mixtures as well as simple substances. We have successfully obtained a 1D image of the beta-ray asymmetry for $^{12}\mathrm{B}$ in Si. The data analysis for 3D imaging are now in progress.

It is expected that this new technique will be applied to non-destructive and non-contact testing related to various fields such as medical and materials science.

In this conference, we will present our new results of the analyses. We will also show some idea that a combination of beta-NMR and mu-SR will expand this technique.

Time-reversal symmetry breaking in nonsymmorphic type-I superconductor $YbSb_2$

CT

SU

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with
R. P. Singh, T. Agarwal, Indian Institute of Science Education and Research Bhopal, India
J. A. T. Barker, A. Hillier, STFC-ISIS Neutron and Muon Source, UK

The interplay of superconductivity with nontrivial topological phases exhibit the fascinating topological superconductivity, which has attracted widespan attention from observing quasiparticle like Majorana fermions to its application in fault-tolerant quantum computation [1,2]. It is proposed that the topological superconductivity can be realized in compounds having topological surface states and superconductivity [3]. Only a few superconducting materials with nontrivial topological states have been discovered, and their superconducting ground state/pairing mechanism can not be adequately understood. Therefore, searching and studying the superconducting ground state of materials having nontrivial topological states is vital.

Here, we present the evidence of time-reversal symmetry breaking (TRSB) in the nonsymmorphic type-I superconductor $YbSb_2$, having a distorted Sb square net crystal structure similar to the other topological system ZrSiS [4,5]. The microscopic muon spin relaxation and rotation investigation confirm the fully gapped type-I superconductivity with broken time-reversal symmetry in its superconducting ground state. This indicates that the nonsymmorphic RSb_2 superconductors are an interesting class of materials that exhibit unconventional superconductivity with fascinating properties and warrant great potential for future studies.

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CT

SCE

Anomalous electrical transport in frustrated intermetallic $RCuAs_2$: the role of spin

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K. Curvelo, McMaster University, Canada
G. D. Morris, TRIUMF, Canada
S. Dunsiger, TRIUMF and Simon Fraser University, Canada
I. St.-Martin, University of British Columbia, Canada

The Kondo effect was a longstanding theoretical puzzle, describing the scattering of conduction electrons in a metal due to dilute, localised d- or f -electron magnetic impurities and resulting in a characteristic minimum in electrical resistivity with temperature. Extended to a lattice of magnetic impurities, the Kondo effect likely explains the formation of so called heavy Fermion systems and Kondo insulators in intermetallic compounds, especially those involving rare earth elements like Ce, Pr and Yb. The hybrisation of the 4f electron states with the conduction band and resultant screening of local moments, required for Fermi liquid behavior in the Kondo lattice, competes with interactions between localised moments. The diversity in the low temperature properties of heavy Fermion metals, as well as their highly tunable nature (with magnetic field, pressure, chemical substitution), make these systems invaluable in the investigation of the emergent properties of highly correlated quantum materials.

Counterintuitively, in a class of ternary intermetallic compounds of the type $RCuAs_2$ (R = rare earth) [1], the rare earths like Sm, Gd, Tb, and Dy with strictly localised 4f character, where the Kondo effect is not anticipated, also exhibit a pronounced minimum in resistivity well above their respective magnetic ordering temperatures. Even more surprisingly, no such minimum is observed for Pr, Nd, and even Yb based members of this series. Recent theoretical predictions suggest geometric magnetic frustration plays a role [2]. More generally, frustration is thought to be an important additional tuning parameter in the Kondo lattice model. A muon spin relaxation investigation of these materials is discussed, shedding light on the role of magnetic fluctuations in determining the electronic transport in heavy Fermion materials.

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Monday 29th August

YP

SL

The quantum muon

S. J. Blundell, University of Oxford, UK

The key physical process at the heart of the muon-spin rotation (μSR) technique is that the spin of the positive muon precesses in a local magnetic field, a process that can be modelled either classically (torque on a magnetic dipole) or quantum mechanically (interference between components in a superposition). However, some aspects of the muon's interaction with its environment bring out features which are purely quantum mechanical and have no classical analogue. Understanding this requires an accurate modelling of the muon site, only possible with modern electronic structure (DFT+μ) methods. I will review a variety of examples of muon experiments on organic, molecular and inorganic systems which will highlight some important qualities of this viewpoint and demonstrate the utitlity of "the quantum muon".

Role of Many-Body Quantum Effects in μSR Measurements

CT

NT

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with
S. Clark, T. Lancaster, Durham University, UK
F. L. Pratt, S. P. Cottrell, STFC-ISIS, Rutherford Appleton Laboratory, UK

For unambiguous interpretation of experimental μSR data, a thorough understanding of quantum zero-point motion (ZPM) of muons in materials is essential. Namely, while ZPM of light nuclei like hydrogen and lithium is known to play a pivotal role in the structure and dynamics of many important classes of materials [1,2], quantum effects of muons in solids can be even stronger due to the lower mass of muons (1/9 the mass of a proton) and can qualitatively change the measured μSR signal [3,4].

There has been much interest in using ab initio computation of muon stopping sites in materials to aid in the interpretation of μSR measurements. However, most computational techniques employed have either neglected quantum muon ZPM, or applied poorly controlled approximations to it with little clarity around the limits of their applicability. To address this, we have developed a unified description of light-particle ZPM in materials [4], clarifying the roles many-body quantum entanglement and anharmonicity play in determining the true ZPM regime. As proof of concept we applied these insights to our precision μSR quadrupolar level-crossing measurements on solid nitrogen, α–N_2, where they allowed us to significantly improve the accuracy of the extracted ^{14}N nuclear quadrupolar coupling constant. This represents the first improvement in its accuracy in over 45 years, despite the ubiquity of solid nitrogen in nature, and a validation of our unified description of light-particle ZPM.

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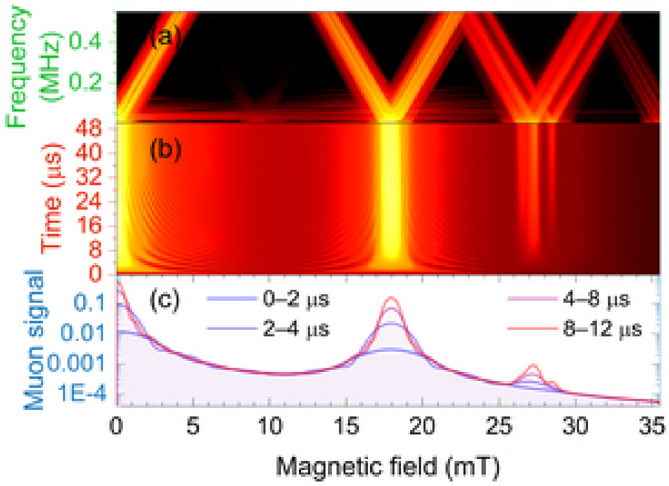

Figure 1: Quadrupolar level crossing resonance spectra of quantum muons in solid nitrogen.

Studying spin diffusion and quantum entanglement with LF-μSR

CT

SL

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with
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S. Manas-Valero, E. Coronado, University of Valencia, Spain
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LF-μSR studies of spin diffusion started with mobile solitons [1] and polarons [2] in conducting polymers. Spin 1/2 antiferromagnetic chains can also support diffusive spin excitations in a certain parameter range of the XXZ model [3], showing either diffusive [4] or ballistic transport [5]. Recent LF-μSR studies of layered triangular lattice quantum spin liquid materials such as 1T-TaS_2 [6] and $YbZnGaO_4$ [7] have shown spin dynamics that is extremely well described by a 2D spin diffusion model, fitting much better than previously proposed models for spin correlations. In $YbZnGaO_4$ the diffusion rate shows a clear crossover between classical and quantum regimes as T falls below the exchange coupling J. That the spin diffusion approach works well in the high T classical region might be expected, but it is found that it also works equally well in the low T quantum region. This allows a T dependent length scale to be derived from the data that can be assigned to a quantum entanglement length ξ. Another entanglement measure, the Quantum Fisher Information F_Q [8] can also be obtained from the LF-μSR data and compared with ξ.

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SL

Exploting magnetic interactions in Kitaev anti-ferromagnet Na_2PrO_3

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Our goal is to analyze the magnetic properties of the Kitaev material Na_2PrO_3 by comparing Neutron Scattering (NS) and Muon Spin Spectroscopy (µSR) experiments, with the addition of ab initio calculations. Alkali-metal lanthanide oxides are an exciting field of study due to their frustrated geometry and possibly anisotropic magnetic interactions, as shown in Fig. 1.

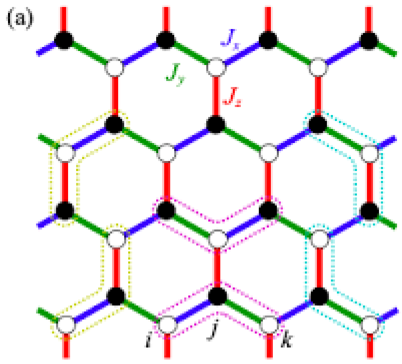

Figure 1: Schematic diagram of Kitaev honeycomb lattice, with anisotropic bond interactions J_x, J_y, J_z.

In this class of materials, also known as Kitaev materials, the SOC energy is comparable to that induced by crystal-field excitations (CEF), and the small spatial extent of f-electron orbitals promotes anisotropic Kitaev terms. Na_2PrO_3 crystallizes with a monoclinic unit cell, where edge-sharing PrO_6 octahedra forms a honeycomb lattice. The effective paramagnetic moment is 0.99 µB, less than the free Pr^{4+} ion moment (2.54 µB), and the origin of its small value is still under debate. In addition, it displays a magnetic ordering transition at T_N = 4.6 K. Previous powder diffraction measurements could not detect any signs of magnetic ordering, despite evidence in specific heat and magnetometry measurements. Moreover, preliminary magnetic neutron diffraction results do not reveal any clear magnetic Bragg peaks, probably due to the low value of Na_2PrO_3 effective paramagnetic moment.

The principal question that motivated our work was to try to explain the small effective paramagnetic moment, considering the presence of the magnetic ordering. Thanks to the muon's extreme sensitivity to small-moment magnetism, here µSR is highly relevant. From this, Na_2PrO_3 shows coherent oscillations of the muon asymmetry below T_N, reflecting the presence of an anti-ferromagnetic (AFM) ordering. In comparison with experimental data, combined ab initio calculations and dipolar simulations were performed in order to elucidate the nature of AFM ordering inside this material and to try to explain the small value of the effective paramagnetic moment.

What high resolution RIXS can tell us of cuprates (and of other quantum materials)

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IV

SU

Resonant Inelastic X-rays Scattering (RIXS) is an energy loss spectroscopy made with x rays whose energy is tuned to a suitable absorption edge. When the instrumental resolution is good enough, RIXS spectra provide information on the energy, dispersion and symmetry of local and collective excitations, such as ligand field excitations, magnons and paramagnons, phonons, particle-hole pairs, charge density fluctuations and order. RIXS is a powerful complement of more traditional techniques like inelastic neutron scattering, Raman scattering, electron energy loss spectroscopy.

The rich physics of cuprates is very effectively captured by high resolution RIXS experiments made at Cu L3 and O K edges. This fortunate conjuncture has boosted the development of better and better instrumentation at synchrotrons and has served as one of the scientific cases for RIXS at XFELs. The field is expanding and experiments are leading to more insightful results, where the different degrees of freedom are organically studied.

After introducing the technique, I will provide a survey of results on cuprate parent compounds [1] and superconductors [2,3] and on infinite layer nickelates [4], which share several properties with high Tc superconductors.

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CT

SCE

Insights into skymion-hosting materials from implanted muons

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Low-dimensional magnetism continues to be of great theoretical and experimental interest, as reduced dimensionality supports strong fluctuations that can result in novel states and excitations. One theme in this field is the understanding of magnetism in reduced dimensions using notions from topology. Examples include topological objects such as walls, vortices and skyrmions, which can potentially exist in the spin textures of a range of systems. In recent years, the experimental discovery of skyrmions in magnetic materials and of their self-organization into a skyrmion lattice, together with their potential for use as high density, low-energy sensors and magnetic storage, has made the investigation of such magnetic topological objects particularly important [1].

Here we report insights gained from our muon-spin spectroscopy (μ^+SR) investigations of materials with topological excitations, including: (i) order and dynamics in $GaV_4S_{8-y}Se_y$, a system hosting Néel skyrmions in which μ^+SR shows how their stability is enhanced through chemical substitution and the application of pressure [2]; (ii) the skyrmion-hosting multilayer system Ta/[CoFeB/MgO/Ta]$_{16}$, where low-energy μ^+SR uniquely reveals changes in the magnetic structure with depth into the multilayer stack; (iii) $Cr_{1/3}NbS_2$, which hosts topological soliton excitations, and where we show that the magnetism is determined directly by features in the electronic bandstructure [3]. These investigations demonstrate how the combination of μ^+SR, magnetometry and electronic structure calculations, both to determine muon sites and more generally, can be used to achieve additional insights into the underlying magnetic behaviour.

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Studying the evolution of the metallic state in $LaNiO_3$ from a single crystal to superlattices with β-detected NMR

CT

SCE

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The rare-earth nickelates ($RNiO_3$) are a prototypical example of a metal-insulator transition. Among the $RNiO_3$, $LaNiO_3$ is unique in remaining metallic, although highly correlated. Interestingly, superlattices with insulating interlayers of $LaAlO_3$, can be driven insulating and antiferromagnetic if they are thin enough [1]. We have used ^{8}Li β-detected NMR (β-NMR), to study $LaNiO_3$ as a single crystal, thin film, and in superlattices with $LaAlO_3$. We observe biexponential spin-lattice relaxation which we attribute to electronic phase separation [2,3]. In the single crystal and bulk-like thin film, both phases appear metallic [2]. However, in the ultrathin layers of the superlattices, the behaviour of one of the phases appears magnetic at low temperature [3].

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IV

SU

Unsupervised machine learning of muons experiments – why?

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Zero-field muon spin relaxation experiments probe directly the intrinsic magnetic fields that arise spontaneously in a given material. The full understanding of such experiments requires a microscopic description of the material under investigation, including its electronic state and the complex interactions between the muon and the material's electronic and structural degrees of freedom. However, paradoxically, such experiments can also yield crucial information about poorly-understood systems, well before we know enough about them for such detailed modelling. In this talk I will ask two questions: “How is this possible?” and “Can we do it better?” To address the first question I will review the particular cases of $LaNiC_2$ and $LaNiGa_2$, two closely related superconductors where the case for an exotic, time-reversal symmetry breaking pairing state is now well established, with muons experiments having played the key role. I will describe how we got to this point, emphasising the prudent use of phenomenological fitting functions and group-theoretical analyses. I will argue that while such approach cannot substitute detailed microscopic modelling (which has to have the final word) it can be crucial to get us to the point where the latter becomes feasible. I will then address the second question, specifically asking whether there is room for improvement in the way we tackle muons data phenomenologically. I will introduce the concept of unsupervised machine learning, using Principal Component Analysis and Auto-encoders as paradigmatic examples. I will propose that unsupervised machine learning can be used to find compact descriptions of muons data, helping with detection of phase transitions and material classification, without requiring either a microscopic theory or phenomenological fitting functions. I will illustrate this with muons data on real magnetic and superconducting materials and introduce simple software tools that can be used to carry out similar analyses.

Time-reversal symmetry-breaking charge order in a kagome superconductor

CT

SU

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The kagome lattice, the most prominent structural motif in quantum physics, benefits from inherent nontrivial geometry to host diverse quantum phases, ranging from spin-liquid phases, topological matter to intertwined orders, and most rarely unconventional superconductivity. Recently, charge sensitive probes have suggested that the kagome superconductors AV3Sb5 (A = K, Rb, Cs) [1] exhibit unconventional chiral charge order. However, direct evidence for the time-reversal symmetry-breaking of the charge order remained elusive. We utilized muon spin relaxation to probe the kagome charge order and superconductivity in (K,Rb)V3Sb5 [2,3]. We observe a striking enhancement of the internal field width sensed by the muon ensemble, which takes place just below the charge ordering temperature and persists into the superconducting state. Remarkably, the muon spin relaxation rate below the charge ordering temperature is substantially enhanced by applying an external magnetic field. We further show [3] that the superconducting state displays a reduced superfluid density, which can be attributed to the competition with the novel charge order. Upon applying pressure, the charge-order transitions are suppressed, the superfluid density increases, and the superconducting state progressively evolves from nodal to nodeless. Our results point to the rich interplay and accessible tunability between unconventional superconductivity and time-reversal symmetry-breaking charge orders in the correlated kagome lattice, offering new insights into the microscopic mechanisms involved in both orders.

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SU

Two-component superconductivity in Sr_2RuO_4 studied by uniaxial and hydrostatic pressure μSR

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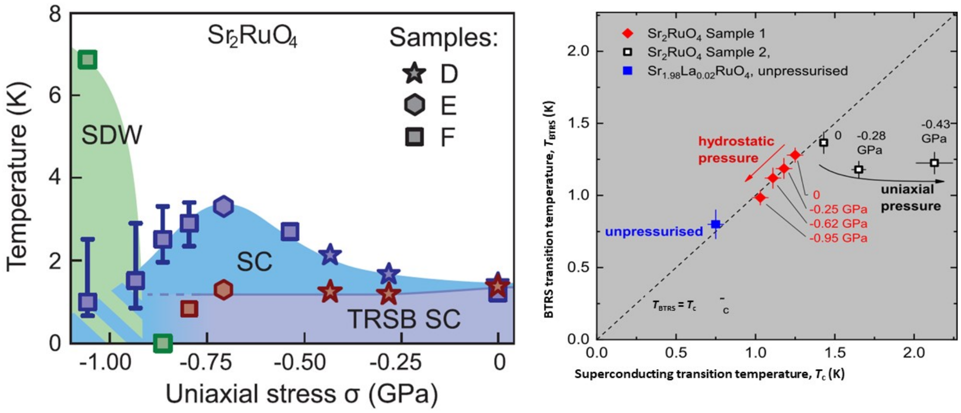

Figure 1: (Left) Electronic phase diagram of Sr_2RuO_4 versus uniaxial pressure applied along the <100> direction [3]. (Right) TRSB transition temperature versus superconducting transition temperature of Sr_2RuO_4 under hydrostatic and uniaxial pressure and La impurity doping [4].

After two decades of research, the symmetry of the superconducting state in Sr_2RuO_4 is still under strong debate. The long time favoured spin-triplet px + i py state is ruled out by recent NMR experiments [1]. However, in general time-reversal-symmetry breaking (TRSB) superconductivity indicates complex two-component order parameters. Probing Sr_2RuO_4 under uniaxial pressure offers the possibility to lift the degeneracy between such components [2]. One key prediction for Sr_2RuO_4, a splitting of the superconducting and TRSB transitions under uniaxial pressure has not been observed so far. Here, we report results of muon spin relaxation (μSR) measurements on Sr_2RuO_4 placed under uniaxial stress [3]. We observed a large pressure-induced splitting between the onset temperatures of superconductivity (T_c) and TRSB (T_{TRSB}). Moreover, at high stress beyond the van Hove singularity, a new spin density wave ordered phase is observed.

To distinguish between a symmetry protected chiral state (d+id) and non-chiral accidentally degenerated order parameters (d+ig, f+ig) we also report μSR studies under symmetry conserving hydrostatic pressure. In these experiment no splitting between T_c and T_{TRSB} is observed (4). In this talk we discuss the implications on the superconducting order parameter in Sr_2RuO_4.

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CT

SU

Ubiquitous Spin Freezing in Spin-Triplet Superconductor UTe_2

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S. J. Blundell, University of Oxford, UK
P. Rosa, S. Thomas, Los Alamos National Laboratory, USA
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The novel superconductor UTe_2 is a rare material wherein electrons form Cooper pairs in a unique spin-triplet state with potential topological properties. Theoretically, spin-triplet superconductivity in UTe_2 may be explained in terms of pairing mediated by either ferromagnetic or antiferromagnetic fluctuations, but experimentally the magnetic properties of UTe_2 remain enigmatic. Here we report on a μSR study of independently grown UTe_2 single crystals that exhibit either a single or double phase transition in the specific heat near the onset of superconductivity. In the absence of an applied magnetic field, we observe an inhomogeneous distribution of magnetic fields in a sizeable volume fraction of all samples studied. The growth in the volume of the magnetic regions is halted by the onset of superconductivity at the critical temperature T_c. Upon further cooling, slow fluctuations of the local fields persist until a disordered spin frozen state appears below about one tenth of T_c. The μSR results are consistent with the formation of magnetic clusters in UTe_2 due to the influence of disorder on long-range electronic correlations or geometrical magnetic frustration associated with the ladder-like U sublattice structure. Our findings suggest that inhomogeneous magnetic clusters are responsible for the ubiquitous residual linear term and low-temperature upturn in the temperature dependence of the specific heat in UTe_2 below T_c. The omnipresent magnetic inhomogeneity may also have implications for the interpretation of other low-temperature experimental observations in the superconducting state of UTe_2.

Negative muons for the characterization of thin layers in Cultural Heritage artefacts

CT

X

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Muonic X-ray Emission Spectroscopy (µXES) is a novel technique based on the detection of high-energy X-rays emitted after the interaction of a negative muon beam with matter. Thanks to the multi-elemental range, a negligible self-absorption effect of the x-rays and very low residual activity left in the sample after irradiation, the technique has been applied to a wide range of studies, with special attention to cultural heritage artefacts. In addition, the technique offers the possibility to perform depth profile studies. By tuning the energy of the incident muon beam, indeed, it is possible to investigate the different layers that constitute a sample. Here we report preliminary results of the analysis on two fire-gilded surfaces, in which the gold layer was supposed to be around 10 microns. In particular, in this work, the technique is coupled with a Monte Carlo based simulation software. Simulations are a powerful tool for improving the data analysis and the interpretation: for µXES especially, by exploiting a simulation software like SRIM or GEANT4, it is possible to assess the thickness of a given layer. To perform a depth profile characterization, the samples were analysed at different beam energies (or momentum). Each of the resulting x-ray spectra was then analysed and gaussian fitted with a data analysis software. Then, the normalised area values were plotted against the momentum to obtain a profile of the variation of the elements as the penetration depth of the beam increased. The output of the simulations was compared with the experimental data and a remarkably good agreement was reached. The results of the work are promising and with this approach, it will be possible to enhance the capability offered by the technique both in terms of data analysis and data interpretation.

CT

X

Non-destructive operando measurements of muonic x-rays on Li-ion battery

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We have developed an elemental analysis technique with muonic x-ray on a Li-ion battery, taking advantages of muon and muonic x-rays, that is, accessibility of negative muons and high energy of muonic x-rays[1,2]. Especially, intense negative muon with low momentum at J-PARC enables us to investigate electrodes in Li-ion battery. There is no non-destructive method to observe Li directly deep inside the Li-ion battery. Elemental analysis with muonic x-rays has great advantages for that.

We have recently performed operando measurements of muonic x-rays on aLi-ion battery at J-PARC for the first time. By this technique, we have demonstrated the intercalation of Li in a cathode during charging and discharging. Also, we found that we can detect metallic Li deposition on a negative electrode using a difference in capture rates between metallic Li and C_6Li[3]. Using this technique, observing an increase in the metallic Li deposition during high-rate charge/discharge cycles is expected to be realized.

We will show the progress in operando measurements of muonic x-rays to study Li-ion batteries at J-PARC.

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Developments on muonic X-ray measurement system for historical-cultural heritage samples in Japan Proton Accelerator Research Complex (J-PARC)

CT

X

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Negative muon elemental analysis, which can measure elemental compositional distribution in the depth direction from 100 nm to several centimeters in a cm-order area with a depth resolution on the order of extmu cm, is a revolutionary technology that enables nondestructive analysis of samples that previously could only be cut and analyzed in cross-section. In recent years, this technique has begun to be applied to historical cultural heritage, and has already been carried out on Japanese archaeological heritage, beginning to provide new insights into Japanese archaeological research. In this talk, we will report on the development of a negative muon X-ray measurement system for elemental analysis of historical cultural heritage at the KEK Muon Science Laboratory (MSL) in the Japan Proton Accelerator Research Complex (J-PARC). At MSL, machine time is very limited and fast measurement of archaeological samples is required. Therefore, we are developing a system to measure negative muon X-rays from archaeological samples at high speed. For this purpose, it is essential to improve the detection efficiency of the detector. Since the analysis of negative muon X-rays requires obtaining energy spectra over a wide energy range with high resolution, high-purity germanium semiconductor detectors (HP Ge) are used; for the pulsed muon source at J-PARC, the Ge detector can detect only one photon or less per pulse. Hence, the use of multiple Ge detectors is essential to obtain high detection efficiency. In addition, to obtain a high signal-to-noise ratio (S/N), noise sources must be identified and suppressed. By increasing the number of detectors and suppressing noise sources, we have succeeded in increasing detection efficiency by about 10 times compared to conventional systems.

CT

X

Muon-Induced X-ray Emission (MIXE) at PSI

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The Muon-Induced X-ray Emission (MIXE) technique, first developed in the 1980's mostly for studying fundamental science, has recently seen a wide usage in the field of applied sciences, which includes archaeology, battery research, meteorites, ancient paintings etc. Probing deep inside the material (up to a few mm) and being non-destructive, this technique is sensitive to all the elements of the periodic table, except hydrogen. The continuous muon source at Paul Scherrer Institute (PSI) along with the newly in-house made instrument is one of the most powerful setups for an efficient usage of this technique.

We present here recent developments of this dedicated detector setup for MIXE at PSI, used at the πE1 beamline, which can deliver negative muon rates between $\sim$1.5 kHz and $\sim$100 kHz for a momentum range between 20 MeV/c and 45 MeV/c, respectively. This setup presently consists of 11 HPGe detectors, with an overall absolute efficiency of $\sim$5% and a resolution of $\sim$1 keV (FWHM) for muonic X-ray energies at $\sim$100 keV. In addition to the HPGe detectors, there are two scintillator detectors, utilized to detect the muon entrance time and as veto counter. By making use of the continuous-wave character of the PSI beam, a clear distinction between X-rays, produced during the muon cascade, and γ-rays produced after the capture of the muon by the nucleus, is possible hence providing a second route for the elemental and isotopic determination.

This setup enables the determination of the quantitative elemental composition within $\sim$1 h of DAQ time. A proof-of-principle experiment, using a simple three-layered sandwich sample has been recently published [1]. Several other experiments on precious objects from archaeology and meteorites along with operando battery samples have been performed and the analysis is in progress.

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Tuesday 30th August

Opportunities and challenges of molecular spins in quantum nanoscience

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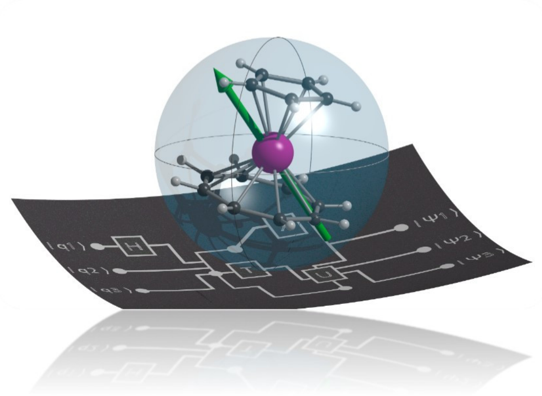

Figure 1

Implementation of advanced Quantum Technologies might benefit from the remarkable quantum properties shown by molecular spin systems based on the coordination bond. The versatility of the molecular approach combined with rational design has recently boosted the operativity temperature of molecules acting as bits of memory, otherwise known as Single-Molecule Magnets, or the coherence time of molecular spin qubits. The richness and tunability of the spectrum of spin levels make them particularly suitable for quantum error correction, while spin-spin interaction can be tuned to realize quantum gates and quantum simulators. Molecules can also be processed to be deposited on surfaces, allowing the realization of hybrid nanostructures. However, achieving the control of single molecules is also challenging, requiring to couple the electric field, which can be confined at the molecular scale, with the spin degrees of freedom of the molecule. Investigation of the spin dynamics at the level of the monolayer requires developing innovative tools and muon spin resonance might be an important resource.

Spin dynamics of V-based molecular magnets with integer spin values

CT

MC

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In the present work, we investigate the spin dynamics of one-dimensional spin-integer molecular nanomagnets $((CH_3)_2NH_2)V_7MF_8(O_2CtBu)_{162}C_7H_8$, with M=Ni/Mn, in short V_7M [1,2,3], by means of magnetization, susceptibility and MuSR measurements. These heterometallic nanomagnets contain seven vanadium ions (s=1) and one Ni^{2+} (s=1) or Mn^{2+} (s=5/2) ion, arranged in the form of regular rings. The theoretical studies of rings with a finite number of integer spins indicate a gapped ground state and a significant deviation from the Landé rule, valid for semi-integer spins [4,5]. On the other hand, the infinite spin-integer chain exhibits a topological Haldane gap between the ground state and the first excited state [6]. As confirmed by experimental data, the ground state of V_7Ni and V_7Mn is expected to be antiferromagnetic, similarly to the molecular nanomagnet V_7Zn [1,2,7], and the exchange coupling constants among the nearest neighbour magnetic ions are estimated to be of the order of a few Kelvin degrees. Susceptibility and magnetization measurements at low temperatures display anisotropy effects when an external magnetic field is applied. The muon longitudinal relaxation rate λ vs temperature, at magnetic fields $\mu_0 H \geq$ 500 G, in the range $1.5 \leq T \leq 100K$, follows a heuristic Bloembergen-Purcell-Pound model [8]. No effect related to a topological gap is evinced.

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CT

MC

Ultrafast molecular rotors in metal-organic frameworks: a combined ^{1}H-NMR and μSR study

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Typically, the solid state is not well suited to sustaining fast molecular motion - however, in recent years a variety of molecular machines, switches and rotors have been successfully engineered within porous crystals and on surfaces. Here, we report on a combined ^{1}H-NMR [1] and μSR [2] study of fast-rotating molecular rotors within the bicyclopentane-dicarboxylate struts of a zinc-based metal-organic framework. Here, the carboxylate groups anchored to the metal clusters act as an axle while the bicyclic units are free to rotate. The three-fold bipyramidal symmetry of the rotator conflicts with the four-fold symmetry of the struts, frustrating the formation of stable conformations and favouring the continuous, unidirectional, ultrafast rotation of the bicyclic units down to cryogenic temperatures. As a remarkable consequence, the fast-motions regime for the ^{1}H-NMR spin-lattice relaxation rate is maintained down to at least 2 K, as confirmed by its dependence on temperature and magnetic field. These results are confirmed by zero-field and longitudinal-field μSR experiments and, in particular, by the dependence of the longitudinal relaxation rate on temperature. At the same time, the experimental evidences suggest several implantation sites for the muons, among which one directly onto the rotating moiety. Muons thermalized in this latter site generate clear oscillations in the depolarization (shown in the picture) resulting from the dipolar interaction with the ^{1}H nuclear moments on the rotors. We evidence a highly unusual dependence of these oscillations on temperature, suggesting a complex influence of the rotations on the muon implantation and diffusion.

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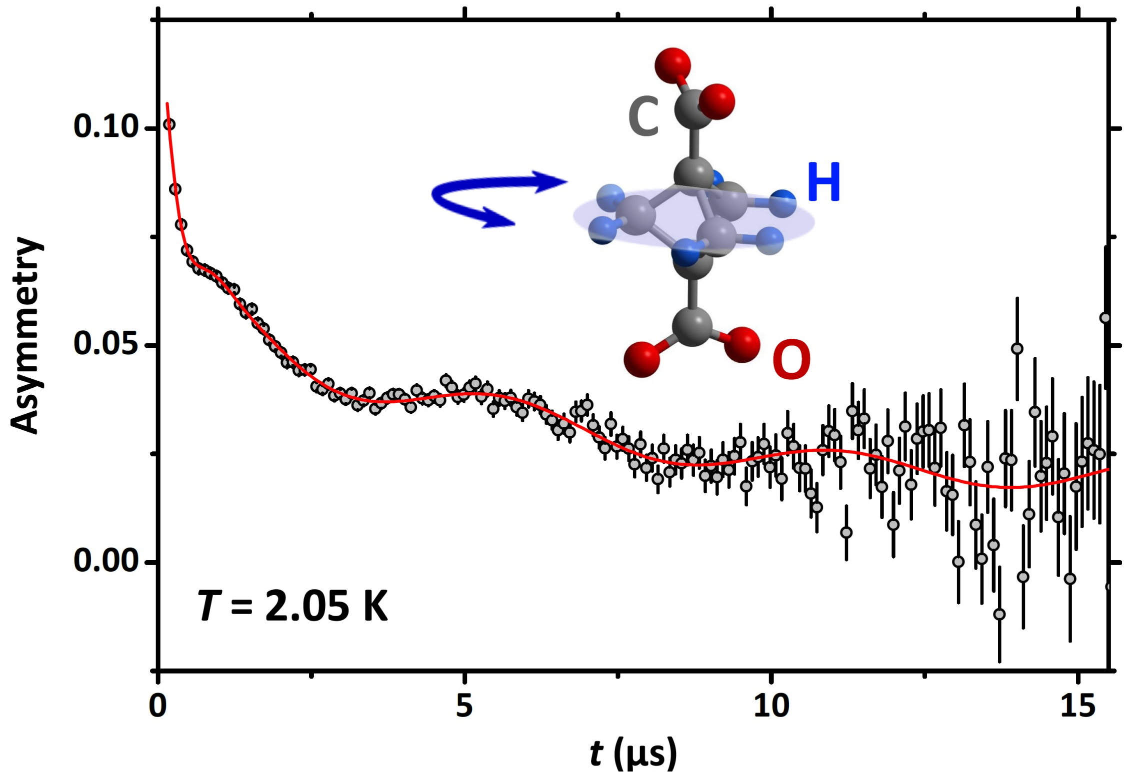

Figure 1: Evidence of a H-μ-like state on the rotating moiety at low temperatures.

IV

EM

Challenges in next generation batteries for accelerating decarbonization

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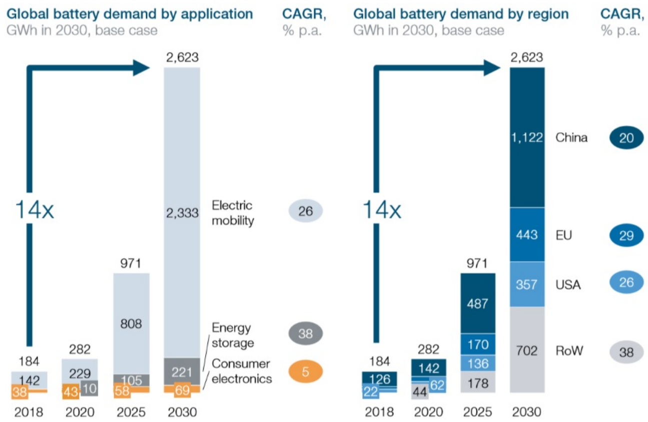

Figure 1: Expected growth in global battery demand by application (left) and region (right) [4]

Batteries are a key-technology for accelerating decarbonization. The benefits of the development of advanced batteries are enormous: broader energy access, specifically for off-grid communities, the transport electrification that reduce the dependency from fossil fuels and the harmful local emission of nanoparticulates, better utilization of intermittent energy sources [1]. Europe has decided to invest significantly in numerous projects and initiatives: the European Commission (EC) launched the European Battery Alliance in October 2017 to build a competitive manufacturing value chain in Europe for the creation of sustainable and fully recyclable cells and batteries [2, 3]. The EC funded the long-term research initiative Battery2030+ [4], thus guaranteeing accelerated support for research and innovation of advanced lithium-ion batteries and disruptive technologies such as Li metal solid state batteries, and the technologic platform Batteries Europe, which will coordinate the efforts and the resources of private and public partners to implement the research activities.

While Li-ion batteries will continue to play a major role in the energy storage, new and disruptive ideas are needed for the creation of sustainable batteries which pave the way to European competitiveness during the transition to a climate-neutral society.

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H2 storage mechanism in fullerides studied with μSR

CT

EM

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When positive muons (μ+) are implanted in insulating materials, they capture electrons to form muonium (Mu), a light isotope of H. This process makes muon spin resonance technique (μ SR) suitable for studying H interaction with matter, for example in hydrogen storage (HS) materials.

Among carbon-based materials, recently metal intercalated fullerides demonstrated to be promising for HS, representing de-facto a novel class of HS compounds: in particular, it has been shown that both lithium and sodium cluster intercalated fullerides can reversibly absorb relevant amount of hydrogen (up to 5 wt

In this work we show how uSR helped us to shed light on the hydrogenation process of these systems. In detail, we performed a μSR investigation of Li6C60 and Na10C60, either as-prepared or after hydrogenation, on the EMU and ARGUS beamlines, at ISIS-RAL. Interestingly, we found that in these compounds the formation of muonium is not inhibited, thanks to the presence of the intercalated partly ionized alkali clusters. Muonium was found to react with C60 to form adduct radicals, appearing as a missing fraction in the muon spin signal. This phenomenon is dependent on temperature and is invariably enhanced on cooling for all the investigated samples.

Such findings indicated that in these systems C60 hydrogenation is already feasible at cryogenic temperatures, with an efficiency even larger than at high T, while the high T needed for hydrogen storage in fullerides is only required to overcome the alkali metals mediated H2 dissociation barrier. Following this hint, we managed to further enhance the hydrogen absorption by co-intercalating transition metals nanoparticles (Pt, Pd) in the fullerides interstices.

CT

EM

Low energy muon study of the p-n interface in chalcopyrite solar cells

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The slow muons technique provides a quantitative approach to characterize the effect of various cover layers on the passivation of bulk defects near the p-n junction of solar cells [1]. Several cover layers on top of the chalcopyrite Cu(In,Ga)Se2 (CIGS) semiconductor absorber were investigated in this work, namely CdS, ZnSnO, Al2O3 and SiO2.

The figure shows the depth profile of a measurement on a CdS/CIGS sample. The diamagnetic fraction is used as an indication of the perturbation of the lattice at the site of the muon. The lower part of the figure shows the model depth profile obtained after deconvolution of the experimental data with the range distribution function. The dip in the diamagnetic fraction near the interface indicates that the lattice is more perturbed in this near-interface region than further inward in the sample. We find that CdS provides the best defect passivation; the oxide materials are less effective.

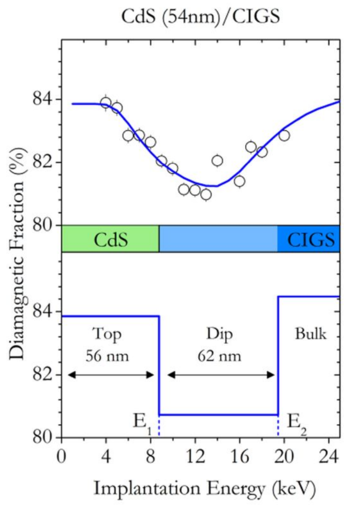

Figure 1: Depth profile of the diamagnetic fraction for CdS/CIGS. The lower part displays the model function used in the fit.

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Negative muon spin rotation and relaxation for energy materials

CT

EM

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A positive muon spin rotation and relaxation (μ^+SR) has been widely used for assorted materials to study a microscopic internal magnetic field. However, the counterpart technique, μ^-SR, is less common mainly due to a small asymmetry of the μ^-SR signal, typically 1/6 to that of μ^+SR, caused by the loss of the spin polarization during a capture process of μ^- by nuclei. This means that 36 times higher statistics are needed for μ^-SR measurements to achieve a reliability comparable with the one of μ^+SR. Fortunately, recent developments of the intense pulsed muon beam together with a multi-detectors counting system enable the measurement of the μ^-SR spectrum within a reasonable amount of beamtime. As a result, we have developed a new tool to detect internal magnetic fields from a fixed view point, since the muonic atom (the bound state between μ^- and an element of the target material) should be stable up to the decomposition temperature of target materials. This is particularly important for research on energy materials, in which various atoms and/or ions are diffusing and such species could affect the local stability of the implanted μ^+ at the interstitial site. Here, we summarize our μ^-SR results on hydrogen storage material MgH_2 [1], cathode materials of ion batteries $LiMnPO_4$ [2] and $Li[Ni_{1/2}Mn_{3/2}]O_4$ [3], and an anode material $Li_4Ti_5O_{12}$ [4].

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CT

EM

New insights into the photochromism of yttrium oxyhydride thin films from in-situ muon spin rotation (MuSR) and positron annihilation spectroscopy (PAS) studies

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Thin films of rare-earth metal oxyhydrides, such as yttrium oxyhydrides ($YH_{3-2x}O_x$), show a pronounced photochromic effect where the transparency of the films decreases reversibly over a large range of sub-bandgap wavelengths upon exposure to UV light. This makes these materials suitable candidates for applications in smart windows. However, the exact mechanism behind the photochromic effect is unknown. We investigated the behavior of $YH_{3-2x}O_x$ thin films, with different O:H ratios, under dark and illuminated conditions using in-situ muon spin relaxation, employing low energy muons at the LEM spectrometer. Transverse Field (TF) measurements, complemented by ZF and LF experiments, revealed that the muonium (Mu^0) formation, inferred from the missing fraction in the TF depolarization curves, increases with increased O:H ratio corresponding to a larger semiconductor band gap. The temperature dependence of the muonium fraction was well described by a transition-state model, where Mu^0 formation and gradual Mu^+ recovery takes place, accompanied by the formation of a Mu^+-O^{2-} complex and a polaron at the Y cation. The activation energy ($E_{A,dia}$) associated with Mu^+ recovery is dependent on lattice relaxation and is lower for thin films of higher H content ($E_{A,dia} = 29$–45 meV). In-situ illumination further reduces this energy barrier for all measured oxyhydrides, suggesting that the photochromic effect involves a reversible structural rearrangement during photodarkening. In the light of our muon spin rotation studies, we discuss several proposals for the identity of the light-absorbing species generated by the electron-hole pairs created upon UV illumination, such as the formation of metallic domains by H^- diffusion, hydroxide formation, color centers, and dihydrogen formation. We complement our discussion with recent findings from in-situ positron annihilation studies on similar films, that suggest that hydrogen vacancies are formed, as well as metallic domains that may play an important role in the mechanism of the photochromic effect.

Ion Diffusion in Na-ion Battery Cathode Material $Na_{0.5}Mg_xNi_{0.17-x}Mn_{0.83}O_2$

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CT

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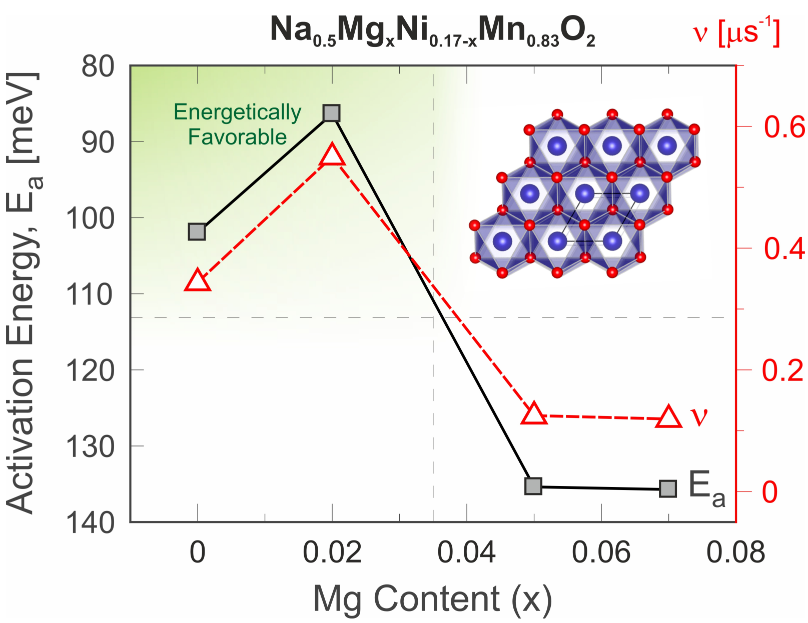

Figure 1

While Li-ion batteries are considered the main candidate for mobile applications, compounds based on lithium's heavier cousin, sodium (Na) have also started to receive a lot of attention lately as candidates for future batteries. One reason is that the Li-reserves are limited and if large scale energy storage become a reality in our future sustainable society, we might have to consider alternatives to the Li-ion technology [1]. During last decade, an increasing number of new Na-battery materials with improved performance have been discovered and the general interest for sodium-based energy storage have increased tremendously. Among the cathode materials the 2D layered P2 – $Na_{2/3}Ni_{1/3}Mn_{2/3}O_2$ compound [2,3] has shown promising storage capacity and operating voltages above 3.5 V. Unfortunately, this material displayed very poor cyclability i.e. short battery life times, directly related to structural transition during the charge cycles. A potential remedy was found by partly substituting Ni for Mg. The resulting $Na_{0.67}Ni_{0.3-x}Mg_xMn_{0.7}O_2$ compound [4] also displayed improved Na-ion diffusion rates. In this study we have investigated the Na-ion self-diffusion by means of muon spin rotation (μ^+SR) [5,6] for the compound series $0 \leq x \leq 0.07$. We surprisingly find that even a very small amount of Mg substitution (x = 0.02) results in the best cycling stability and highest Na-ion mobility [7].

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Present status of J-PARC MUSE

CT

FR

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J-PARC MUSE is responsible for the inter-university user program and the operation, maintenance, and construction of the muon beamlines, namely D-line, S-line, U-line, and H-line, along with the muon source at MLF.

At D-line, which provides the world's most intense pulsed negative and positive muon beams, various scientific studies, including those on industrial applications, archeology, and fundamental physics, have been performed. In FY2021, non-destructive analysis was carried out on samples brought back by Hayabusa2 from the asteroid Ryugu, which are thought to preserve the elemental composition of the solar system in its primordial state.

Stable operations have been achieved in S1 area of S-line for µSR. In addition, a group at Okayama University constructed a new experimental area, S2, in FY2020 for muonium 1s-2s measurement.

U-line, uses electrostatic lenses to focus low-energy muons obtained by laser ionization of thermal muonium to produce energy-variable and high time-resolution ultra-slow pulsed muon beams for various experiments. A muon spin spectrometer for materials science research using the µSR method has been installed in the U1A area, and is being upgraded and upgraded for the start of the inter-university user program. The spectrometer is located on a high-voltage stage and the depth of penetration into the sample can be controlled in the range from sub-keV to 30 keV.

The H line is a high-intensity muon beamline where experiments such as high-statistics fundamental physics experiments and transmission muon microscopy are planned. The first beam observed in the H1 experimental area, the first branch, in January 2022.

At present, the beam commissioning is being carried out in collaboration with several research groups that plan to conduct experiments at the H-line.

TRIUMF Centre for Molecular and Materials Science Facility Overview

CT

FR

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This document briefly describes the mission, governnace, operations, infrastructure and future directions of TRIUMF's CMMS. The current muon and beta-detected NMR experimental facilites are revisted and the status of a number of pending beamline projects and spectrometer instalations are introduced.

Progress on Muon Source Project at CSNS

CT

FR

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A Muon station for sciEnce, technoLOgy and inDustrY (MELODY) has been listed in the CSNS II upgrade plan, and the infrastructure construction is scheduled to start by the end of 2022. Up to 5Hz of proton pulses will be extracted from the RCS ring to a stand-alone target station. One surface muon and one decay muon beamline are designed to provide multi-terminals for applications. In this report, we describe the design of MELODY and prospect for future applications.

CT

FR

Status of μSR facility in RAON

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with
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Rare Isotope Science Project (RISP) launched in 2011 to build the Rare isotope Accelerator complex for ON-line experiment for rare isotope science (RAON), ends the 1st stage of which completes one of two main accelerators (low-energy superconducting linac, SCL). Since 2019, μSR facility has been designed and constructed, composed of muon production target chamber, transport beamline, beam dump, except spectrometer. In this talk, we report the current status of μSR facility in RAON as an applicative facility of RAON and a tool for investigating materials.

Status of the Swiss Muon Source at PSI

CT

FR

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The Laboratory for Muon Spin Spectroscopy (LMU) at PSI develops and operates the six muon instruments of the Swiss Muon Source (Sμ;S). We give an overview of the current status, with an update on the commissioning of the new FLAME instrument and the upgrade plan of the μE4 beamline to increase the rate of low-energy muons by 50% in 2025. Furthermore, a new experimental facility is under development: the Muon-Induced-Xray-Emission (MIXE) instrument using negative muons for non-destructive, depth-selective elemental analysis of archeological artefacts, extraterrestrial samples and for operando studies of devices.

On a longer term, PSI is planning the major upgrade project IMPACT of the High-Intensity Proton Accelerator (HIPA). IMPACT ("Isotope and Muon Production using Advanced Cyclotron and Target technologies") aims for the production of radioactive isotopes for cancer diagnosis and therapy, and the installation of HIMB, the two "High Intensity Muon Beams". HIMB involves the replacement of the existing target M and the two beamlines πM1 and πM3 by a new target H with two very high-intensity surface muon beamlines μH2 and μH3 with muon rates up to 10^{10}/s. This will offer unique new possibilities for muon applications [1]. Installation of this major facility upgrade is foreseen in a 1.5 years shutdown in 2027/2028. The project proposal is currently being under evaluation.

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CT

FR

ISIS Facility Report

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There are five muon instruments and two further experimental areas at ISIS including RIKEN-RAL, able to deliver both surface and decay muons appropriate for different experiments. Since June 2021 the whole muon facility has been in an extended shutdown as significant work has taken place on the accelerator, the muon collimator, and the Target Station 1 neutron target. We now expect muon beams to be restored late in 2022, with the full user programme restarting in February 2023.

The major muon group project is the Super-MuSR instrument upgrade, which is expected to be funded within the £90m Endeavour programme. This promises to bring a step-change in capability, with a highly pixelated detector and novel acquisition electronics increasing the counting rate up to 20x, and a pulse slicer and spin rotators increasing the available frequency range up to 10x. This will provide a bridge between the capabilities of pulsed and continuous muon sources. Particular benefits will be seen by experiments that require data at long times after muon implantation, in-operando device measurements, and parametric studies. Other projects within the group have included refurbishing the HiFi magnet, adding positron degraders to EMU to improve performance, improving the laser capabilities on HiFi, and improving our sample environment equipment.

During the shutdown there has been a full refurbishment of the RIKEN-RAL beamlines, which is being carried out as part of the transition of the facility to ISIS ownership. As well as replacing obsolete services and beamline equipment, the sample environment suite has been updated, with new cryostats, 3He inserts, and dilution fridge inserts, to be compatible with the equipment recently acquired for the other beamlines, improving reliability, redundancy, and capability. RIKEN-RAL is in high demand with the elemental analysis science programme and the FAMU proton Zemach radius now running alongside the condensed matter programme.

Wednesday 31st August

CT

SCE

Discovery of Hidden Charge-Neutral Muon Centers in Magnetic Materials: Implications and Applications

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Spin polarized muons are widely known as an extremely sensitive local probe of magnetism. Additionally, positively charged muons implanted into semiconductors and insulators often bind an electron to form a charge-neutral muon-electron bound state frequently referred to as a muonium center. While studied extensively in non-magnetic semiconductors and insulators as light analogues of corresponding hydrogen centers, charge-neutral muon states are rarely considered relevant in magnetic materials. Apart from the singular exception of antiferromagnetic MnF_2[1], no long-lived charge-neutral centers had been identified in magnetically ordered materials up-to-date.

Here, we present strong evidence that charge-neutral muon centers *do* exist in magnetic compounds. Detailed new μSR investigations of the antiferromagnets Cr_2O_3[2], Fe_2O_3[3] and MnF_2, in conjunction with density-functional-theory calculations, reveal that charge-neutral muon states are present in magnetic materials and can form with different electronic structures, analogous to the variety of muonium centers found in non-magnetic materials.

Crucially, we find that in magnetic materials, charge-neutral muon states do not display any signatures conventionally associated with muonium centers, making it difficult to distinguish them from the often assumed positive charge state. We demonstrate that the presence of the additional charge alters the local electronic and magnetic structure, affecting the μSR signal and its relationship with the intrinsic magnetic properties. Since the muon is used extensively as a sensitive magnetic probe, it is imperative to understand under what conditions charge-neutral states are formed in magnetic materials, and what impact they have on the observed μSR frequencies and damping rates.

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From μSR spectra to the magnetic interaction energy parameters: the MnSi helimagnet as a test case

CT

SCE

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For several decades the intermetallic compound MnSi has fascinated the community for different aspects of its physical and magnetic properties. Among these properties is the exotic temperature-magnetic field phase diagram. While this diagram was first established in the 1970s, the exact nature of one of the phases was only identified in 2009 as a lattice of magnetic skyrmions, i.e. a topological magnetic texture.

In this contribution we present recent developments in the interpretation of the muon response of MnSi in the helimagnetic and conical phases, respectively observed in zero and finite fields. These developments are based on a computation of the asymmetry spectrum in terms of the incommensurate magnetic structure parameters and the muon site and coupling.

In a first step we show the magnitude m of the magnetic moment in the helical phase, the temperature dependence of which has attracted little attention in the literature, to decay as T^2 from its low temperature value. We interpret this decay as the result of spin waves excitations. The slope of m vs T^2 determines the two dominant energy contributions in the traditional expression used for magnetic energy of the system.

In a second step, instead of the previously mentioned continuous field model, we consider a microscopic model for the energy, accounting for the presence of four magnetic Mn sites in the crystal unit cell and the symmetry elements of the $P2_13$ space group in which MnSi crystallizes. The minimization of the energy is obtained for structures that somewhat deviate from the regular helical and conical phases. This result is consistently confirmed by fits to the asymmetry spectra which provide a quantitative determination of the microscopic model parameters. Directions for future developments are presented.

CT

SC

Quantum Information: How does it μve through fluorides?

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with
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The unitary evolution of a quantum system preserves its coherence, but interactions between the system and its environment result in decoherence, a process in which the quantum information stored in the system becomes degraded. A spin-polarized positively charged muon implanted in a fluoride crystal realizes such a coherent quantum system, and the entanglement of muon and nearest-neighbor fluorine nuclear spins gives rise to an oscillatory time dependence of the muon polarization that can be detected and measured. In this talk, we will show that the decohering effect of more distant nuclear spins can be modelled quantitatively, allowing a very detailed description of the decoherence processes coupling the muon-fluorine "system" with its "environment," and allowing us to track the system entropy as the quantum information degrades [1]. Examples of this approach to various fluorides will be presented, using these methods to gain knowledge of the nature of the muon stopping site, distinguish between different crystalline phases of a compound, and identify Frenkel defects [2].

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Insights into the magnetic ground state of Fe_2P from μSR, NMR and DFT perspectives

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Fe_2P alloys have been proposed as promising for applications in magnetocaloric refrigeration due to their first-order magnetic transitions coupled to a magnetoelastic transition, which gives rise to a giant magnetocaloric effect in the vicinity of their Curie temperature [1]. The magnetic structure of Fe_2P has been investigated and known to order ferromagnetically, with magnetic moments along the c-axis. However, these earlier sparse and often very old literature on Fe_2P are characterized by inconsistencies in the quantitative description of the Fe_1 magnetic moment size and the presence of helical states below T_c.

Here, using a combined effort of two spectroscopic techniques, μSR and NMR, in addition to DFT calculations, we have accurately characterized the magnetic ground state of Fe_2P. We perform zero applied field measurements using both experimental techniques below the ferromagnetic transition T_C = 220 K [2]. Our DFT calculations reproduce the experimental results and further allow us to improve their interpretation. We show a detailed characterization of the microscopic coupling between the electrons and P-nuclei or the muon in Fe_2P, which where then utilized to discuss the microscopic origin of the NMR and μSR resonances. Particularly, the computational predictions allow to identify correctly a previously mis-attributed signal from ^{31}P nuclei, an information relevant for future experiments. This work completely characterizes the signal of two technique of election for the characterization of magnetic properties, thus providing an important base for further analysis of different alloy compositions.

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CT

SC

MuSpinSim: spin dynamics calculations for muon science.

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MuSpinSim is a Python software to simulate muon (μSR) experiments. In particular, it simulates the spin dynamics of a system of a muon plus other spins such as electrons and atomic nuclei. MuSpinSim can simulate various common experimental setups used in μSR, such as zero, transverse and longitudinal field experiments; and it can simulate μSR experiments that are resolved in time, field, or temperature. Furthermore, MuSpinSim can account for the effects of hyperfine, dipolar, quadrupolar and Zeeman couplings, as well as simulate quantum systems exchanging energy with the environment with the Lindblad master equation. Finally, MuSpinSim can be used to fit experimental μSR data with simulations that use all of the capabilities described above. The fittings can be run in parallel on multiple cores, which significantly reduces the computational cost of the most expensive tasks. In this work, we present the Python package MuSpinSim with all the utilities it provides to facilitate simulations of μSR experiments, demonstrate the effectiveness of the method with some chosen example systems and show a prototype application of MuonGalaxy, a web-based implementation of MuSpinSim that is based on the Galaxy platform [1].

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

CT

SC

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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 ^{19}F 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.

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CT

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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.

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Dipolar-Octupolar Quantum Spin Liquids in Ce-based Pyrochlores

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In geometrically-frustrated Ce-based pyrochlores, such as $Ce_2Zr_2O_7$, the effective S=1/2 of the Ce3+ crystal field ground state doublet is known to act both as a conventional dipole magnetic moment, and as an octupole. This constrains the form of its near-neighbour Hamiltonian, and allows for different ordered or quantum disordered ground states in this family of materials, where either the dipolar or octupolar nature of the S=1/2 degree of freedom dominates. I will describe recent experiments [1,2], mostly neutron scattering and heat capacity, which show how the nature of the Ce3+ ground state doublet can be revealed, and how a particular form of quantum spin liquid can be identified as the likely ground state in $Ce_2Zr_2O_7$.

CT

SL

Quantum critical spin-liquid behavior in $S = 1/2$ quasikagome lattice $CeRh_{1-x}Pd_xSn$ investigated using muon spin relaxation

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We present the results of muon spin relaxation (μSR) on the Ce-based quasikagome lattice $CeRh_{1-x}Pd_xSn$ (x = 0.1 to 0.5). Our zero-field (ZF) μSR results reveal the absence of both static long-range magnetic order and spin freezing down to 0.05 K in the single crystal sample of $x = 0.1$. The weak temperature-dependent plateaus of the dynamic spin fluctuations below 0.2 K in ZF-μSR together with its longitudinal-field (LF) dependence between 0 and 3 kG indicate the presence of dynamic spin fluctuations persisting even at T = 0.05 K without static magnetic order. On the other hand, the magnetic specific heat divided by temperature C_{4f}/T increases as -log T on cooling below 0.9 K, passes through a broad maximum at 0.13 K and slightly decreases on further cooling. The ac-susceptibility (χ_{ac}) also exhibits a frequency independent broad peak at 0.16 K, which is prominent with an applied field H along the c-direction. We, therefore, argue that such behavior for $x = 0.1$ (namely, a plateau in the spin relaxation rate (λ) below 0.2 K and a linear T-dependence in C_{4f} below 0.13 K) can be attributed to a metallic spin-liquid (SL) ground state near the quantum critical point (QCP) in the frustrated Kondo lattice. The LF-μSR study suggests that the out of kagome plane spin fluctuations are responsible for the SL behavior. The ZF-μSR results for the $x = 0.2$ polycrystalline sample exhibits similar behavior to that of $x = 0.1$. A saturation of λ below 0.2 K suggests a spin-fluctuating SL ground state down to 0.05 K. The ZF-μSR results for the $x = 0.5$ sample are interpreted as a long-range antiferromagnetic (AFM) ground state below T_N = 0.8 K, in which the AFM interaction of the enlarged moments probably overcomes the frustration effect.

Quantum spin liquid behavior in geometrically frustrated Mo pyrochlore antiferromagnet $Lu_2Mo_2O_{5-y}N_2$

CT

SL

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The magnetic ground state of a quantum spin liquid (QSL) candidate compound, $Lu_2Mo_2O_{5-y}N_2$ oxynitride pyrochlore ($S = 1/2$, Mo^{5+}), was investigated by muon spin rotation/relaxation experiment. In contrast to $Lu_2Mo_2O_7$ ($S = 1$, Mo^{4+}) which exhibits a spin glass-like freezing of Mo moments below $T_g \simeq 16$ K, no such spin freezing or long range magnetic order was observed down to 0.3 K. More interestingly, two distinct magnetic domains discerned by spin dynamics were observed below ~13 K; one showing the “sporadic” spin fluctuation similar to that observed in other QSL candidate compounds including the kagome antiferromagnets, and the other showing the fast paramagnetic fluctuation that is only weakly suppressed with decreasing temperature. Their origins are discussed in terms of the bond randomness induced by the partial substitution of O with N and the inhomogeneous Mo valency due to O deficiency ($y > 0$) [1].

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Thursday 1st September

Low-energy Excitations in Quantum Spin Liquid Derived from Molecular Mott Insulator

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A molecular Mott insulator ß'-EtMe$_3$Sb[Pd(dmit)$_2$]$_2$ (dmit = 1,3-Dithiol-2-thione-4,5-dithiolate) is a quantum spin liquid (QSL) candidate. In the crystal with the space group $C2/c$, Pd(dmit)$_2$ anion radicals are strongly dimerized to form a dimer with spin 1/2. The dimers are arranged in an approximately isosceles-triangular lattice, which leads to a frustrated S = 1/2 Heisenberg spin system.

The system shows no magnetic order down to a very low temperature (19 mK) that corresponds to J/12,000, where J (250 K) is the nearest-neighbor spin interaction energy. The HOMO-LUMO mixing in the dimer unit induces fragmentation of S=1/2 electron spin with strong quantum fluctuation.

Low-energy excitations in the QSL state are open to debate even now. Heat capacity and magnetization indicate gapless fermion-like excitations, while ^{13}C-NMR indicates an existence of a nodal gap. ESR and μSR probed the spinons, revealing their gapless character and an unexpectedly large degree of in-plane anisotropy in the spin dynamics. This anisotropic spin dynamics indicates quasi-one-dimensional diffusive motion in the direction of the weakest magnetic coupling in the triangular lattice.

In 2010, it was reported that thermal conductivity is characterized by its large value and gapless behavior (a finite temperature-linear term). In 2019, however, two other research groups reported opposite data (much smaller value and a vanishingly small temperature-linear term) and the discrepancy in the thermal conductivity measurement data emerges as a serious problem concerning the ground state of QSL. An origin of the discrepancy will be discussed.

I deeply thank all my collaborators, especially, H. Cui, M. Uebe, S. Fujiyama, Y. Oshima, I. Watanabe (RIKEN), Y. Nakazawa (Osaka Univ.), Y. Ishii (Shibaura Institute of Technology) and F. L. Pratt (STFC).

CT

SL

Universal fluctuating regime in triangular chromate pure Heisenberg S=3/2 antiferromagnets

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The series of triangular compounds $ACrO_2$ is a model series for studying the Heisenberg model on S=3/2 (Cr^{3+}: half-filled t_{2g} orbitals) triangular antiferromagnets and the impact of interlayer couplings on the dynamics. For this, we report µSR measurements on α-$HCrO_2$ and $KCrO_2$ [1] which complete former studies on the series of triangular compounds $ACrO_2$, A = Li , Na [2, 3]. Coupled to ^{1}H and ^{39}K nuclear magnetic resonance (NMR), we establish the static character at low-T, as expected for a near neighbour Heisenberg model, yet displaying a broad and remarkable regime with slow fluctuations extending from T_N down to 0.2 T_N. This regime is marked by a maximum in the µSR relaxation rate occuring at 0.7 T_N, associated with an NMR wipe-out.

The scaling of the NMR and µSR data with respect to J or T_N supports a scenario where a crossover from 2D to 3D correlations sets in around 0.7 T_N preceded by a typical 2D regime of the TLHAF which appears to be a hallmark of the TLHAF with ABC stacking. We discuss the role of interlayer frustration which may bear implications to recent spin-liquid candidates with the triangular geometry and exclude a scenario à la Berezinskii-Kostelitz-Touless of vortex-antivortex topological excitations in that regime. In turn, this underlines the crucial need of further neighbour interactions, anisotropy typical of rare earth or even disorder to stabilize a quantum spin liquid state in triangular antiferromagnets such as $YbMgGaO_4$.

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Searching for Spin Liquids in Buckled Compounds

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SL

The phrase 'quantum spin liquid' (QSL) refers to a system in which strong quantum fluctuations prevent long-range magnetic order from being established, even at temperatures well below any interaction energy scale. No spontaneous symmetry breaking is involved, nor a conventional local order parameter. Thus, it is not described using the Landau theory of phase transitions and constitutes a novel phase of matter. These systems exhibit a wealth of exotic phenomena like long-range entanglement and fractional quantum excitations, which are of fundamental interest but also hold great potential for quantum communication and computation.

Magnetic species decorating a two dimensional kagome lattice constitute the most heavily studied QSL candidates. Quantum fluctuations are prevalent due to geometrical magnetic frustration, low coordination number and quasi low dimensionality. Two particularly well-studied experimental realisations are volborthite, where it is believed spatial anisotropy plays an important role and herbertsmithite $ZnCu_3(OH)_6Cl_2$. However, the presence of excess Cu^{2+} replacing the nonmagnetic Zn^{2+} induces randomness in the magnetic exchange coupling, complicating explanations of the experimental observations.

Our focus is the investigation of a series of newly synthesised QSL candidates. The insulating materials $YCu_3(OH)_6O_xCl_{3-x}$ (x = 0, 1/3) display a kapellasite-like structure and no sign of Cu/Y mixing from single crystal x-ray refinements. In the x = 0 compound, the kagome lattice is perfect; in the x = 1/3 compound, it is slightly buckled.

In $Ba_4Ir_3O_{10}$, Ir^{4+}($5d^5$) ions form Ir_3O_{12} trimers of three dimensional face-sharing IrO_6 octahedra, which are vertex-linked, forming wavelike 2D sheets. However, it is proposed that intra-trimer exchange is reduced and the lattice recombines into an array of coupled 1D chains with additional spins. As such, the compound is a candidate Tomonaga-Luttinger liquid (TLL) and presents a novel route to exploring quantum liquid behaviour. A muon spin relaxation investigation of these novel compounds is discussed.

IV

SU

Muons and Quantum Computing Hardware: Challenges and Opportunities

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One might wonder: what do muons have to do with quantum computing? I will argue that environmental muons and ionizing radiation in general represent a source of noise and dissipation which until recently has been underestimated in the quantum devices community. I will present measurements performed in the deep-underground laboratory of Gran Sasso [1] which show a significant improvement in the performance of superconducting quantum hardware thanks to the shielding provided by 1.6 Km of granite. On the other hand, low energy muon beams engineered at dedicated large-scale facilities represent a powerful materials characterization tool, and as such might play a role in the understanding and mitigation of material defects in superconducting and semiconducting quantum hardware.

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Phase transition from a magnetic-field-free stiffness meter and LEMviewpoints

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CT

SU

A new method to measure the superconducting stiffness tensor $\bar{\rho}_s$, without subjecting the sample to magnetic field is applied to $La_{2-x}Sr_xCuO_4$ (LSCO) [1]. The method is based on the London equation $\boldsymbol{J} = -\bar{\rho}_s \boldsymbol{A}$, where $\boldsymbol{J}$ is the current density and $\boldsymbol{A}$ is the vector potential. Using rotor free $\boldsymbol{A}$ and measuring $\boldsymbol{J}$ via the magnetic moment of superconducting rings, we extract $\bar{\rho}_s$ at $T \to T_c$. The technique, named Stiffnessometer is sensitive to very small stiffness, which translates to penetration depth on the order of a few millimeters. We apply this method to two different LSCO rings: one with the current running only in the CuO_2 planes, and another where the current must cross planes. We find different transition temperatures for the two rings, namely, there is a temperature range with two-dimensional stiffness. The same method is also used to measure the coherence length, ξ_0, by increasing $\boldsymbol{A}$ to a point where linear response breaks. Finally, we compare our result with a Low Energy μSR (LEM) experiment performed on the same samples and discuss the advantage and disadvantage of each technique.

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CT

SU

Unconventional pressure dependence of the superfluid density in topological superconductor α-PdBi2

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with
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The Pd-Bi family of compounds has become quite popular system to explore topological superconductivity due to their intrinsic capability to maintain strong spin orbit coupling (SOC). Amongst various members of this family, α-$PdBi_2$ turns out to be very promising due to its superconducting (T_c = 1.7 K) as well as topological properties such as Dirac point at 1.26 eV below the Fermi energy at the zone center, Rashba state near the Fermi energy etc. Notably, the ARPES data display multiple band crossings at the Fermi energy which signals a possible multiple gap superconducting gap structure in this compound. To explore this interesting aspect, we investigated the superconducting properties of the topological superconductor α-PdBi2 at ambient and external pressures up to 1.77 GPa using muon spin rotation (μSR) experiments. The ambient pressure μSR measurements demonstrate a fully gapped s-wave superconducting state in the bulk. The observation of s-wave superconductivity in α-$PdBi_2$ is quite crucial in search for Majorana fermions as it is theoretically predicted that in presence of an in-plane magnetic field, the Majorana zero mode can be realized utilizing the coupling of an s-wave superconductor with a material exhibiting Rashba states. Further, AC magnetic susceptibility and μSR measurements under hydrostatic pressure manifest a continuous suppression of T_c with increasing pressure. We observed a considerable decrease of superfluid density by 20 % upon application of external pressure. Remarkably, the superfluid density follows a linear relation with T_c which was found before in some unconventional topological superconductors and hole doped cuprates. This finding indicates a possible crossover from Bose-Einstein to Bardeen-Cooper-Schrieffer like condensation in α-$PdBi_2$.

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μSR Study of the Relationship between the Magnetism, Superconductivity and Electronic Nematicity in Iron-Chalcogenide Thin Films

CT

SU

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The iron-chalcogenide FeSe exhibits various electronic states such as superconductivity, the so-called electronic nematicity, as well as a magnetic order under hydrostatic pressure. Therefore, this system attracts considerable research attention in an effort to understand the interplay between the different electronic states. In S-substituted thin films of FeSe$_{1-x}$S$_x$ in which positive chemical pressure is induced by the smaller S substitution for larger Se, we formerly found a kink in the temperature dependence of the electrical resistivity at highly S-substituted thin films of $x \geq 0.18$ without the nematic state [1]. The kink has been observed around the magnetic transition temperature T_N in bulk FeSe under pressure [2]. To investigate the possible magnetism in FeSe$_{1-x}$S$_x$ and compare with Te-substituted FeSe$_{1-y}$Te$_y$ in which negative chemical pressure is induced, we performed muon-spin-relaxation (μSR) measurements [3].

Zero-field μSR time spectra of FeSe$_{1-x}$S$_x$ with $x = 0.3$ and 0.4 revealed the formation of a short-range magnetic order at low temperatures. The value of T_N is higher in $x = 0.4$ than in $x = 0.3$, suggesting a S-induced magnetic order in the FeSe$_{1-x}$S$_x$ thin films. For slightly S-substituted $x = 0.1$ with the nematic state, on the other hand, it was found that a long-range magnetic order was formed at low temperatures. As the value of T_N at $x = 0.1$ is higher than that of $x = 0.4$, distinct magnetic states would be formed in the slightly (with nematic) and highly (without nematic) S-substituted FeSe$_{1-x}$S$_x$.

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CT

SU

Complex nature of charge order and superconductivity interplay in correlated kagome superconductor CsV_3Sb_5

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Recent family of Kagome superconductors AV3Sb5 (A = Rb, K, Cs) offers a natural playground to study the interplay between different electronic states such as non-trivial chiral charge order (CO) and unconventional superconductivity [1-5]. This is because of its unique crystal structure that results in flat bands across the Brillouin zone, crossing of linear bands at K-corner, appearance of van Hove singularities at M-edges of the Brillouin zone. CsV3Sb5 is of particular interest compared to Rb and K counterparts due to distinct M-dome shaped two peak behaviors in its superconducting transition temperature Tc vs. pressure phase diagram. The phase diagram is however drawn through transport measurements accessing only macroscopic nature of interplay between CO and SC [6]. Thus, microscopic nature and theoretical understanding of their correlation remains unanswered. We have carried out muon spin relaxation/rotation (µSR) experiments under hydrostatic pressure up to 1.9 GPa. Nearly threefold enhancement in Tc and superfluid density ns at 1.74 GPa compared to their respective ambient pressure values has been observed. Interestingly, ns also displays two peak like feature with pressure. Three different regions of phase diagram manifest distinct linear relationship between Tc and ns. The µSR results and DFT calculations conjointly suggest possible evolution of CO from a superimposed tri-hexagonal Star-of-David phase at low pressures to the staggered tri-hexagonal phase at intermediate pressures [7]. Our studies thus uncover different regions of phase diagram with CO showing varying degree of interplay with SC.

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Is the Abrikosov's vortex-model still valid in nematic superconductors?

CT

SU

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Spontaneous rotational-symmetry breaking (RSB) in the amplitude of the superconducting gap is a necessary condition for "nematic" superconductivity. This was evidenced in the topological superconductor $Cu_xBi_2Se_3$ where, despite the threefold symmetry of its lattice, a twofold symmetry of electronic properties emerged from nuclear magnetic resonance[1], transport[2], and specific-heat[3] measurements, when the applied magnetic field is rotated in the Se planes. This is also the case of $CaSn_3$ semimetal with the cubic $AuCu_3$-type structure: we prove a spontaneous RSB below Tc[4] by magnetotransport- and muon-spectroscopy (µSR) measurements.

Particularly meaningful are the transverse-field (TF)- µSR results in the mixed superconducting phase of $CaSn_3$, where the muon-depolarization rate depends on the magnetic field direction (here, applied along the [110] or [001] crystal directions). The absence of any additional muon depolarization along [110] suggests that an*unconventional vortex lattice* (VL) sets in. Conversely, in the [001] case, a VL encompassing at least 52% of the sample volume indicates the bulk nature of superconductivity.

Similarly, by scanning tunnelling spectroscopy in $Cu_xBi_2Se_3$, vortices exhibit an elliptical shape within stretched VLs for applied fields H orthogonal to the Se planes, whereas "no obvious in-plane vortices" could be observed for H parallel to the Se layers[5].

Such evidence and our current experimental results on $CaSn_3$ seriously question the pertinence of the conventional Abrikosov model to the superconducting mixed state of nematic superconductors since multi-component order parameter superconductors may exhibit unusual vortex structures (fractional and/or non-axial vortices)[6].

Finally, the superfluid density in the (001) planes, extracted from TF-µSR data, shows a fully gapped low-temperature behaviour, with $\Delta(0)$=0.61(7) meV. Additional zero-field µSR results indicate that the superconducting state is time-reversal invariant. This fact and the RSB in a fully-gapped superconductor suggest $CaSn_3$ as*nematic superconductor with an unconventional pairing state in a multidimensional representation*.

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[6] https://doi.org/10.1103/RevModPhys.63.239

Muonium reaction in semiconductors and insulators: the role of the transition state

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A. Weidinger, *Private*

CT

SEMI

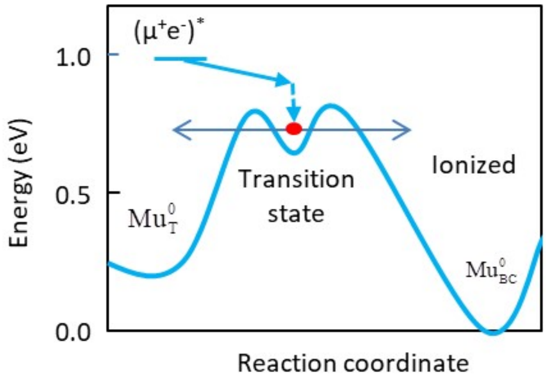

Figure 1: Muonium is trapped at a shallow minimum (transition state) at the top of the diffusion barrier. From there, it can decay thermally activated either to the muonium ground state (e.g. to neutral muonium in tetrahedral configuration) or to a bound configuration (e.g. to neutral or ionized bond-centered muonium).

The model describes the reaction of atom-like muonium with the host lattice at the end of the implantation trajectory. Reactions of the bare muon with the host or prompt formation of the final states are not covered by this model. Since these alternative processes are temperature independent, their maximum contribution can be estimated from the smallest value that occurs at any given temperature. They can be considered as a temperature-independent "background".

At the end of the trajectory, the muonium has just enough kinetic energy to jump across the potential barrier from one interstitial site to the next. At the top of the barrier, muonium is so slow that a strong inelastic interaction, e.g., the excitation of a local stretching mode, can occur and a weakly bound muon-electron configuration, the transition state, is formed (see Fig. 1).

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SEMI

Muonium states in semiconducting transition metal dichalcogenides

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The usual response of muonium to an external magnetic field is dominated by the hyperfine interaction, which causes the observed spectrum to show the transition frequencies between different muonium spin states. However, we have recently discovered an unconventional magnetic muonium state in 2H-$MoTe_2$ where the muonium acts a magnetic impurity, which polarizes the local electronic magnetic moments [1]. For sufficiently small externally applied fields, the "magnetic" muonium effectively behaves as a diamagnetic muon in a local magnetic field. Here, we show experimentally that in 2H-$MoTe_2$ the magnetic muonium coexists with another conventional, non-magnetic muonium state (Fig. 1b). The latter is axially symmetric with a hyperfine coupling of $A_{\|}$=1426(1) MHz and $A_{\perp}$=1368(3) MHz, corresponding to an effective Bohr radius of $\approx$ 0.82 Angstrom. The hyperfine coupling remains fairly constant, as a function of temperature, until the state disappears around the same temperature where the magnetic muonium disappears as well. We employ density functional theory calculations to reveal that this is linked to the presence of two muonium sites in the compound: one within the van der Waals gap that becomes magnetic, and a second one inside the layer, that is conventional. A similar behavior is also observed in 2H-WSe_2 (Fig. 1a), indicating that this is a more general feature of semiconducting transition metal dichalcogenides.

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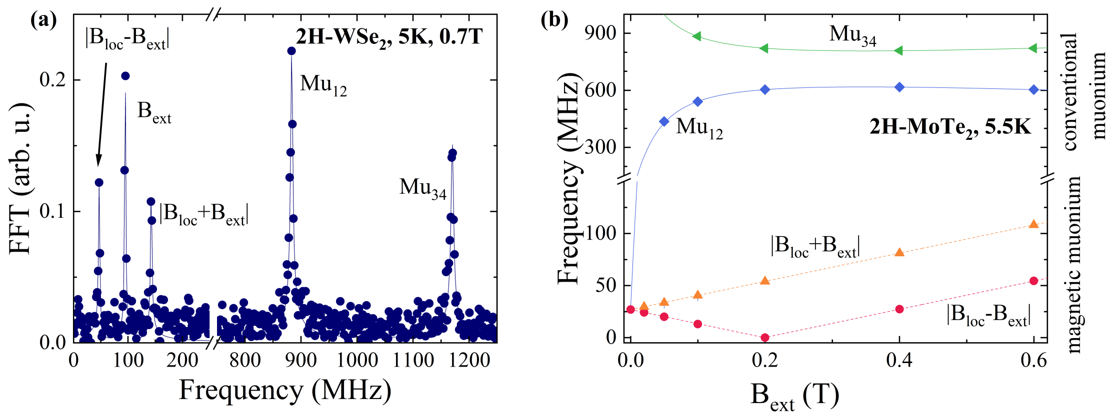

Figure 1: (a) Local field distribution in 2H-WSe_2 at 5K in a 0.7T transverse field. (b) Applied field dependence of the oscillation frequencies in 2H-$MoTe_2$ at 5.5K.

CT

SEMI

Probing hydrogen sites and negative hyperfine parameter in semiconducting BaSi2 by muon spin rotation

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Z. Xu, Y. Yamashita, T. Suemasu, University of Tsukuba, Japan

Hydrogen passivation of defects is commonly used to reduce defects in semiconductors such as GaAs, diamond, and Si. We recently found by experiment that atomic hydrogen is also very effective in significantly increasing a minority-carrier lifetime (> 10 µs) in BaSi2, one of the emerging materials for thin-film solar cell applications. This means that defects no longer act as recombination centers in BaSi2 after hydrogen passivation [1-2]. But three has been no experimental data about the hydrogen site in BaSi2. We employed muons to study the hydrogen state in single-crystalline BaSi2. Distinct neutral muonium state was identified in the high transverse-field measurements. From the temperature dependence, negative hyperfine parameters was suggested. From the angle-dependence of the hyperfine parameter in the magnetic fields applied in the a x b, b x c, and c x a planes, and comparison to the calculations based on density-functional theory (DFT), the hydrogen site in the BaSi2 crystal is proposed.

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Carrier lifetimes in high-lifetime silicon wafers and irradiation induced recombination centres

CT

SEMI

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Photoexcited muon spin spectroscopy (photo-μSR) was used to measure excess charge carrier lifetimes in passivated silicon wafers. Optically generated excess carriers interact with muonium centres via carrier exchange interaction and induce relaxation in the μSR time spectrum. The photo-μSR technique utilises this additional relaxation rate as a measure of the excess carrier density, which in turn enables us to measure carrier lifetime spectra by controlling delays between a muon and laser pulse [1]. In addition, the depth-resolved measurement can characterise carrier kinetics at specific depths within a Si wafer and enables us to separate bulk and surface recombination rates [2]. Based on these developments, we recently applied the technique to passivated Si samples with extremely long effective lifetimes ($>$1 ms) and observed that prolonged muon irradiation resulted in significant degradation of a measured lifetime [3]. Follow-up characterisation measurements, including deep-level transient spectroscopy, strongly suggested that beam damage generated defect-related recombination centres in bulk. Our results demonstrate an extremely rare case in μSR applications, where beam damage to crystalline lattice was clearly detected by virtue of high-lifetime Si wafers and, in turn, low native defect densities.

References

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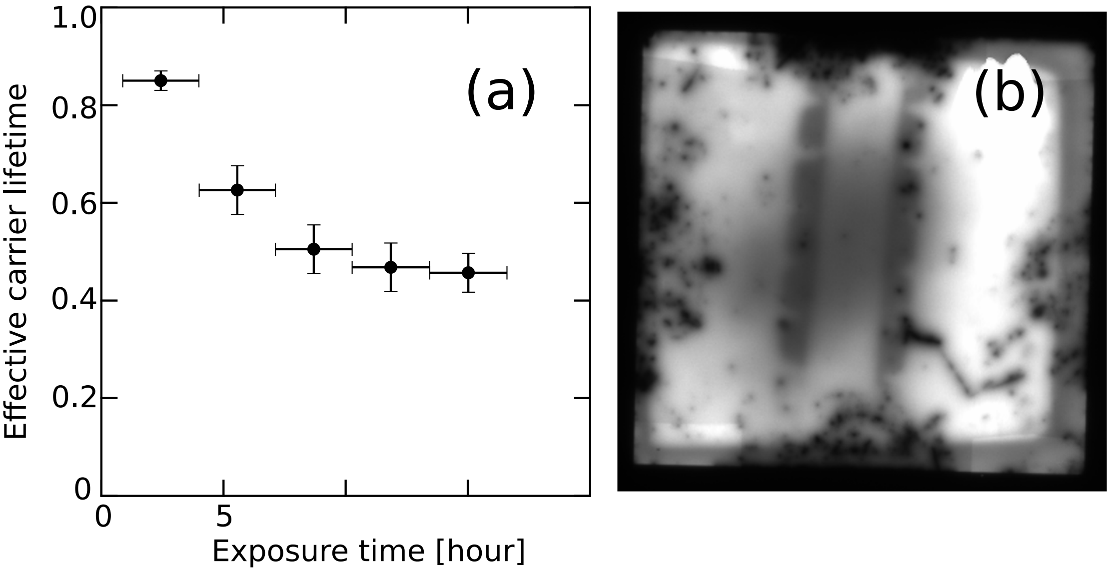

Figure 1: A series of repeat lifetime measurements were performed on a HfO_2 passivated Si sample. (a): Effective carrier lifetimes were measured as a function of beam exposure time. (b): A photoluminescence lifetime image was taken on the sample (5×5 cm^2) after the muon experiment. White parts closer to the edges indicate longer carrier lifetimes. The central black spot with shorter lifetimes corresponds to a region exposed to muon beams.

Ambipolar Property of Isolated Hydrogen in Oxide Materials Revealed by Muon

CT

SEMI

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The study on the electronic state of muon as pseudo-hydrogen (represented by the elemental symbol Mu) by muon spin rotation has long been appreciated as one of the few methods to experimentally access the electronic state of dilute hydrogen (H) in semiconductors and dielectrics. Meanwhile, theoretical predictions on the electronic state of H in these materials by first-principles calculations using density functional theory (DFT) do not always agree with the observed states of Mu. In order to address this long-standing issue, we have re-examined the vast results of previous Mu studies in insulating/semiconducting oxides with special attention to the non-equilibrium character and the ambipolarity of Mu. As a result, we established a semi-quantitative model that enables systematic understanding of the electronic states of Mu in most oxides.

First of all, Mu often occurs simultaneously in a neutral (Mu^0) and a diamagnetic state (Mu^+ or Mu^-) in wide-gap oxides, which is not explained by DFT calculations that predict only diamagnetic states with the polarity determined by the equilibrium charge-transition level ($E^{+/-}$). Our model considers that μ^+ interacts with self-induced excitons upon implantation to form relaxed-excited states corresponding to a donor-like (Mu_D) and/or an acceptor-like (Mu_A) states. Moreover, these states are presumed to accompany the electronic level ($E^{+/0}$ or $E^{-/0}$) predicted by the DFT calculations for H. By considering that the stability of these two states including their valence is determined by i) the relative position of $E^{\pm/0}$ in the energy band structure of the host and ii) a potential barrier associated with the transition between Mu_D and Mu_A, we find that the known experimental results can be explained systematically in accordance with $E^{\pm/0}$. The model also provides new insights into the polaron-like nature of the electronic states associated with shallow donor Mu complexes and the fast diffusion of Mu^0_A.

CT

EM

Impact of Growth Conditions on the $CH_3NH_3PbI_3$ Perovskite Solar Cells, Studied by Low-Energy μSR

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with
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L. Lei, University of Nottingham, UK

Metal halide perovskites (MHPs) have attracted great attention in recent years due to their enormous potential for application in optoelectronic devices. However, the defects at surface/interfaces and grain boundaries of perovskite films, which impede the further enhancement of power conversion efficiency (PCE) and long-term stability of halide perovskite solar cells (PSCs), still need to be fully understood. Here, we studied the impact of different growth conditions on the interface and grain boundaries of $CH_3NH_3PbI_3$ perovskite films by low-energy μSR. Our measurements show that low-energy μSR can become a powerful technique for studying the defect engineering of PSCs.

Coherent microwave control of muonium

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CT

NT

We demonstrate the most fundamental coherent control techniques by excitation of microwave spin transitions in muonium, namely driven Rabi oscillations and Ramsey fringes upon free evolution. Unprecedented performance is achieved by triggering microwave pulses by a single implanted muon, which enables coherent spin manipulation of individual muonium atoms.

As a first example, we suppress extrinsic line broadening with the Ramsey experiment on strongly coupled muonium in SiO_2 (Figure 1). As a second example, we retrieve the electron g-factor of bond-centered muonium in Si using the double electron-muon resonance (DEMUR) technique and decouple the system from its environment by strong driving of the electron-muon double quantum transition.

Overall, we expect that this capability will provide a powerful tool to investigate the effect of the environment on isolated coupled spins, uncover the details of coupled electron-muon systems in matter and validate quantum electrodynamics in the context of (vacuum) muonium spectroscopy.

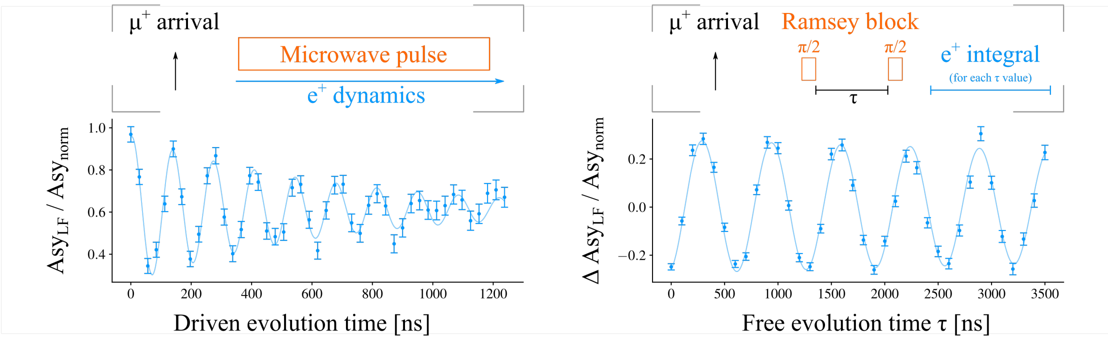

Figure 1: Microwave experiments with muonium formed in SiO_2 at 280 K, showing Rabi oscillations excited by 3.6 GHz microwaves (left) and phase-coherent Ramsey fringes excited by 30 ns pulses (right). The upper schemes depict the timing of the experiment.

CT

NT

Status of the New Muonic Helium Atom HFS Measurements at J-PARC MUSE

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with
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S. Fukumura, S. Kawamura, M. Kitaguchi, T. Okudaira, H. M. Shimizu, H. Tada, Nagoya University, Japan
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S. Seo, The University of Tokyo and RIKEN, Japan

We recently proposed new precision microwave spectroscopy measurements of the ground-state hyperfine structure (HFS) of muonic helium atom [1]. Muonic helium is a hydrogen-like atom composed of a helium atom with one of its electrons replaced by a negative muon. The ground-state HFS, resulting from the interaction of the remaining electron and the negative muon magnetic moment, is very similar to that of muonium but inverted, and the same technique can be used to precisely measure muonic helium HFS. It is a sensitive tool to test three-body atomic system, bound-state quantum electrodynamics theory, and determine fundamental constants of the negative muon magnetic moment and mass. The world most intense pulsed negative muon beam at J-PARC MUSE gives an opportunity to improve previous measurements, and to test further CPT invariance through comparison of the magnetic moments and masses of positive and negative muons.

Test measurements at D-line are in progress utilizing MuSEUM apparatus at zero field. Muonic helium HFS were measured at different helium pressures to determine the pressure shift using methane as an electron donor. The obtained results have already better accuracy than previous measurements [2,3]. Muonium HFS was also measured to investigate the isotopic effect on the pressure shift. We also started investigating a new experimental approach to improve HFS measurements by repolarizing muonic helium atoms using a spin exchange optical pumping (SEOP) technique [4]. If successful, this would drastically improve the measurement accuracy. An overview of the different aspects of these new muonic helium HFS measurements and the latest results will be presented.

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Friday 2nd September

IV
NT

Microscopic Dynamics of Structural Glasses Investigated by Quasielastic Neutron Scattering

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In this presentation I will give a short introduction into quasielastic neutron scattering (QENS) and its application to glass-forming systems. QENS operates on time scales from picoseconds to a microsecond and at the same time has a spatial resolution in the Ångström range. Therefore, it is well suited for the study of molecular and polymeric glass-formers.

The dynamics of glass-formers is still poorly understood, but certain universal features can be found which a theory has to explain. Foremost, there is the α relaxation, which governs what is usually called 'glass transition'. Its temperature-dependence is highly non-Arrhenius and the shape of correlation functions non-exponential. In addition, faster relaxations may be present, among which the universal 'fast β relaxation' in the picosecond range is strongly related to the α relaxation in mode-coupling theory. As the fastest universal process, glasses show an excess of the vibrational density of states above the Debye model in the low frequency range, the so-called 'boson peak'.

All these phenomena can be observed by QENS with the additional information of a length scale. In addition, it is possible to study them in confined glass-formers in order to access their system-size-dependence. Selected QENS experiments will be presented and discussed.

CT

MC

First depth-resolved beta-NMR measurements of 1-ethyl-3-methylimidazolium acetate

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with
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Over the past decade, we have been using beta-detected NMR to examine the properties of amorphous materials. While this has typically focused on polymers, [1] we have recently been interested in ionic liquids (ILs). ILs are binary mixtures: they are composed of two oppositely charged molecular species. They are also liquid at room temperature. Their properties, determined by strong electrostatic forces, make them attractive candidates for the development of next-generation battery technology.

The long-range forces between ions also affect their dynamics, one of our primary interests in amorphous materials. This makes ILs a fascinating comparison to the relatively well-understood case of polymers. As with polymers, many ILs are extremely resistant to crystallization and will instead vitrify upon cooling. In our prior work, we showed that β-NMR was a good probe of bulk IL dynamics and dynamic heterogeneity [2]. In our present experiments, we turn to the question of how the surface modifies these properties, presenting the first depth-resolved β-NMR measurements in 1-ethyl-3-methylimidazolium acetate. This interfacial region is important for understanding how constrained dimensionality affects dynamics, which in turn may affect this IL's effectiveness as a potential electrolyte in batteries or capacitors.

We will show that both the surface and the glass transition have large effects on molecular dynamics, which in many aspects differs greatly from our expectations. In the glassy phase, the surface dynamics appear to be simultaneously faster (i.e., liquid-like) and yet still heterogeneous (i.e., glass-like), an apparent departure from our understanding of "normal" behaviour. Additionally, relaxation becomes faster below the glass transition temperature.

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CT

MC

Probing the [FeFe]-hydrogenase subsite using muon spectroscopy

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S. P. Cottrell, STFC-ISIS, Rutherford Appleton Laboratory, UK

In the drive to replace fossil fuels with sustainable alternatives, achieving the reversible interconversion of protons and dihydrogen is a crucial target. The reaction can be carried out readily using platinum-based systems, but the cost and availability of this precious metal preclude scaling such approaches. In nature, the [FeFe]-hydrogenase enzymes have evolved to perform the very same task at rates that rival platinum electrodes. These systems feature a large protein component in addition to a core bioinorganic unit, the 2Fe2S subsite. To enable us to produce practical catalysts we need to mimic the chemistry carried out by the enzyme: the natural system itself is too large and sensitive for wide-scale use. Thus understanding the chemistry of the 2Fe2S subsite is vital.

Central to the hydrogen chemistry carried out by the subsite is its interaction with protons. Probing the solution kinetics and electrochemisty of model systems allows us to understand key reactivity of iron hydrides on a timescale as short as one second. However, much of the most interesting behaviour of these models occurs on much shorter timescale. For example, the location of the primary protonation sites is still an open question, with terminal and bridging hydrides possible candidates along with the sulphur, carbonyl and cyanide ligands. Muonium, as a ‘light’ analogue of H·, offers the means of studying the structure and dynamics of such chemistry on the nanosecond timescale. The use of the avoided level cross (ALC) technique has now allowed to identify two sites for primarily muonation in this model in the solid stat, with density functional theory (DFT) assignment strongly implicating competing bridging and terminal binding. This unique insight opens up the possibility of new reaction pathways in both models and the enzyme as well as demonstrating the wider importance of muon techniques in studying reactive organometallic systems.

Advances in biochemical applications of β-detected NMR

CT

MC

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Since the implementation of β-detected NMR (β-NMR) at TRIUMF, it has mainly been used to study condensed matter systems ranging from metals to superconductors to topological insulators. In the last few years, there has been a desire to extend the applications of β-NMR to include the study of biochemical problems. For a number of metal ions in our body, such as Mg(II), Zn(II) and Cu(I), the absence of convenient physical and spectroscopic properties limits our ability to characterize their role in health and disease using conventional techniques, such as classical NMR. However, β-NMR has the possibility to help address these gaps in our knowledge by aiding in the elucidation of metal coordination in biomolecules.

In this presentation, I demonstrate that we are able to observe ^{31}Mg binding to the biomolecule adenosine 5'-triphosphate (ATP) in solution. The resonance spectrum shows two distinct peaks which indicates that we observe not one, but two distinct complexes between Mg^{2+} and ATP. We identify these complexes with ^{31}Mg β-NMR complemented by ^{31}P NMR and DFT calculations. This represents the first measurement of a β-NMR probe binding to a biomolecule and is an important milestone in applying β-NMR to the study of biochemical problems[1].

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CT

MC

New insight into μSR in water

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Over the past four decades, muon spin rotation and relaxation technique in water and ice has been reported by several groups [1-4]. Most of the previous studies were focused on muonium chemistry (detection, its relaxation, reaction and frequencies) in water and ice. To deepen the understanding of muon behavior in water and application of μSR to life sciences and hydrated samples, we performed temperature dependent μSR study in water. We found the temperature dependent oscillation in zero-field spectra in ice for the first time and proposed a new model – interaction between four spin-one-half system – to interpret the data. We found two stopping sites (proportion of 35 % and 10 % of incident muons) for muons in hexagonal ice in which the muons in larger fraction (35 %) move towards optimized geometry site with temperature approaching the melting point. The distances of the muon and protons are successfully detected in subatomic scale. This study will be helpful to understand the charge dynamics in materials, for example, ion diffusion in battery materials, proton transfer in hydrated materials, proton transfer in biological membranes and in general transport of other spin-nuclei in solid state materials.

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Beta detected NMR of ^{8}Li in 2H molybdenum ditelluride

CT
SCE

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Layered transition-metal dichalcogenides (TMDs) are proposed as building blocks for van der Waals (vdW) heterostructures. Semiconducting TMDs are further prone to host magnetic impurities, e.g. at defects or interstitials. Here we investigate the behavior of interstitial ^{8}Li$^+$ implanted into 2H-MoTe$_2$ at depths of $\sim$110 nm with β-detected NMR. We find that unlike muons [1], the ^{8}Li$^+$ does not show any signature of induced magnetism. We confirm this result by density functional theory, which identifies the Li stopping site at the 2a Wyckoff position in the vdW gap and shows the absence of Li-induced electronic spin polarization. Both, the spin lattice relaxation (Fig. 1c) and the resonance lines (Fig. 1a) show evidence for Li diffusion or a site change above 200K. The line shape of ^{8}Li$^+$ is found to consist of quadrupolar satellites on top of a broad central peak (Fig. 1a). Therefore, we employ a frequency comb measurement, where four frequencies, $\omega_0 - 3\omega_{\rm comb}$, $\omega_0 - \omega_{\rm comb}$, $\omega_0 + \omega_{\rm comb}$, and $\omega_0 + 3\omega_{\rm comb}$ corresponding to the first-order quadrupolar satellite transitions are excited simultaneously as a function of $\omega_{\rm comb}$. This offers an enhanced sensitivity to the quadrupolarly split portion of the line. Using this method, we find a small decrease of the quadrupolar frequency with increasing temperature (Fig. 1b), showing the typical behavior associated with thermally excited phonons.

References

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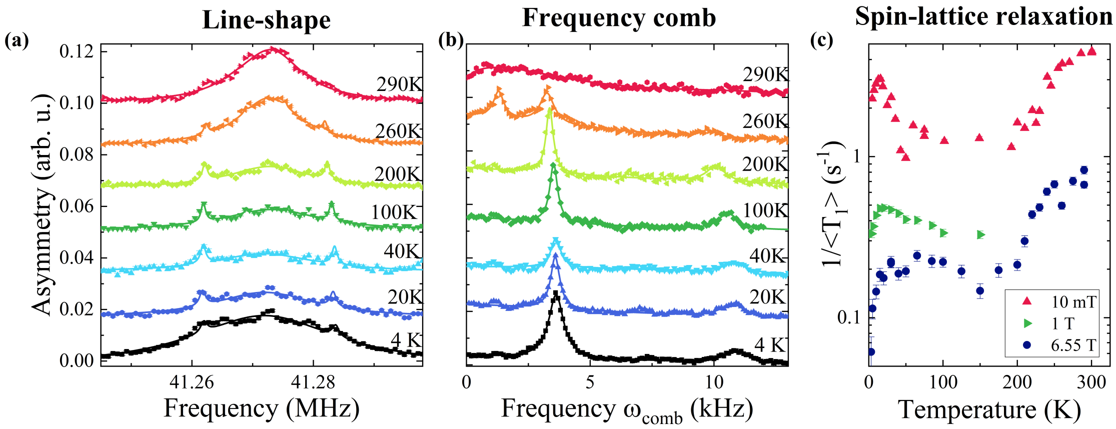

Figure 1: (a) $^8Li^+$ line shape and (b) frequency comb in 2H-$MoTe_2$ at different temperatures, which are offset for clarity. (c) Temperature dependence of the spin lattice relaxation rate at different applied fields.

Intriguing Topological Kagome Magnetism of $TbMn_6Sn_6$

CT

SCE

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Magnetic topological phases of quantum matter are an emerging frontier in physics and material science [1-6], of which kagome magnets appear as a highly promising platform. Here, we explore magnetic correlations in the recently identified topological kagome system $TbMn_6Sn_6$ using μSR, combined with local field analysis and neutron diffraction [1,4]. Our studies identify an out-of-plane ferrimagnetic structure with slow magnetic fluctuations which exhibit a critical slowing down below $T_{C1} \simeq 120$ K and finally freeze into static patches with ideal out-of-plane order below $T_{C1} \simeq 20$ K. The appearance of the static patches sets in at a similar temperature as the appearance of topological transport behaviors. We further show that a hydrostatic pressure of 2.1 GPa stabilizes the static out-of-plane topological ferrimagnetic ground state in the whole volume of the sample. Therefore the exciting perspective arises of a magnetically-induced topological system whose magnetism can be controlled through external control parameters. The present results [4] will stimulate theoretical investigations to obtain a microscopic understanding of the relation between the low-temperature volume-wise magnetic evolution of the static c-axis ferrimagnetic patches and the topological electronic properties in $TbMn_6Sn_6$.

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Tunable anomalous Hall conductivity through volume-wise magnetic competition in a topological kagome magnet

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Magnetic topological phases of quantum matter are an emerging frontier in physics and material science. Along these lines, several kagome magnets have appeared as the most promising platforms. Recently, we explored magnetic correlations in the kagome magnet $Co_3Sn_2S_2$ [1]. Using muon spin-rotation (μSR) and ARPES, we present evidence for competing magnetic orders in the topological kagome lattice of this compound. Our results show that while the sample exhibits an out-of-plane ferromagnetic ground state, an in-plane antiferromagnetic state appears at temperatures above 90 K, eventually attaining a volume fraction of 80% around 170 K, before reaching a non-magnetic state. Strikingly, the reduction of the anomalous Hall conductivity (AHC) above 90 K linearly follows the disappearance of the volume fraction of the ferromagnetic state. We further show that the competition of these magnetic phases is tunable through applying either an external magnetic field or hydrostatic pressure. Our results taken together suggest the thermal and quantum tuning of Berry curvature induced AHC via external tuning of magnetic order. μSR played a crucial role in this study, since it serves as an extremely sensitive local probe for detecting small moments and ordered magnetic volume fractions in the bulk of magnetic materials.

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μSR Study of Superconductivity Above H_{c2}: A Filamentary State in Type-II Superconductors

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The standard interpretation of the phase diagram of type-II superconductors was developed in the 1960s and has since been considered a well-established part of classical superconductivity. In particular, according to the standard picture, in a sample of type-II materials of a planar geometry in a parallel (in-plane) field, superconductivity nucleates at Hc3 approximately twice as big as the upper critical field Hc2. Between these critical fields the superconducting phase exists in a form of a thin surface sheath. Contrarily, in the same sample but in the perpendicular (out-of-plane) field superconductivity nucleates in the bulk at Hc2 and there is no superconductivity above this field. However, upon closer examination a number of fundamental issues arises that leads one to question this standard picture. To address these issues, we studied equilibrium properties of niobium samples near and above the critical field Hc2 in parallel and perpendicular magnetic fields. The samples investigated were very high-quality films and single-crystal disks with the Ginzburg-Landau parameters in the range from 0.8 to 1.3. A set of complementary measurements has been performed, which include bulk muSR, dc magnetometry, electrical transport and scanning Hall-probe microscopy. Contrary to the standard scenario, we observed that a superconducting phase is present in the sample bulk above Hc2 and the field Hc3 is the same in both parallel and perpendicular fields. It will be shown that above Hc2 the superconducting phase forms filaments parallel to the field regardless of the field orientation. Near Hc2 the filaments preserve the hexagonal structure of the preceding vortex lattice of the mixed state, and the filament density continuously falls to zero at Hc3.

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Non-destructive elemental analysis for medical inheritances by muonic X-ray measurement

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X

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Muon induced X-ray emission is a powerful technique for non-destructive elemental analysis for bulk material. This method have developed as practical quantitative analysis at J-PARC, and in present, this method have been applied for various samples, such as archeological artefacts, meteorite and so on. In this paper, we report the results of applying this method to medical heritage in Japan. About 200 years ago, by introducing Western medicine, many formulations in glass bottles have been left since the late Edo period. The analysis for these bottles are important for studying the development of medicine in Japan, but some bottles can not be opened due to aging. In this study, elemental analysis experiment using muons was conducted at J-PARC for a glass bottle that can not be open produced in the early 1900's stored at Osaka University. By adjusting the incident muon energy, the muous selectively stopped inside the glass bottle, and emitted muonic X-rays were measured by germanium semiconductor detectors. The X-ray peaks of muonic mercury and chlorine atoms were clearly observed, and we concluded the formulations was mainly composed of mercury chloride.

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The BAM cell: an electrochemical device for operando ionic diffusion measurements using muon spectroscopy

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Understanding the complex ways that battery materials change on charging and discharging is vital for improving their function in operation, but traditional ex-situ muon measurements have barely scratched the surface of this deep mine of information. Here, we present an electrochemical cell that enables ionic diffusion measurements using muon spectroscopy (µSR) at the ISIS Neutron and Muon Source. Traditional ex-situ powder µSR measurements provide valuable fundamental properties, but they often do not investigate important ionic diffusion pathways which are only established during battery operation as charge is (de)intercalated to/from the structure. Operando experiments have the potential to follow the rate of atomic-scale ionic motion in functioning batteries, allowing the influence of structural phenomena which occur during charging/discharging, such as phase changes or lattice contractions, to be determined. The Battery Analysis by Muon (BAM) cell is described here as a simply assembled, electrochemically reliable device, which provides comparable performances to commercially available equivalent devices and can be used to study a variety of cell chemistries. The cell's suitability for µSR measurements is demonstrated by an example operando experiment on a Li-ion half cell with cathode material NMC811, which produced high quality data from the specimen of interest. This experiment outlined the benefits of µSR to follow ionic diffusivity properties during charging/discharging and uncovered a link between the material phase transitions and the measured field distribution width. Such results facilitate further development of our operando methodology, with a range of future applications of the BAM cell available for exploration.

Search for a space charge layer in thin film battery materials with low-energy muons

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In an all solid state Li-ion battery, it is crucial to reduce ionic resistivity at the interface between the electrode and the electrolyte in order to enhance Li+ mobility across the interface, because Li^+ ions naturally drift across such interface. In particular, recent first principles calculations predict the presence of a space-charge layer (SCL) at the interface because of the difference in the Li^+ chemical potential between the two materials [1], as in the case for the interface between a metal and a semiconductor in electronic devices. However, the presence of SCL has never been experimentally observed. We have therefore initiated series of studies for direct observation of SCL in different cathode battery materials, exploiting the unique depth-resolved features of the LEM-μ^+SR experimental technique.

Our first attempt in a fresh multilayer sample, Cu(10 nm)/Li_3PO_4(50 nm)/$LiCoO_2$(100 nm) on a sapphire substrate, revealed a gradual change in the nuclear magnetic field distribution width, originating from the nuclear fields, as a function of implantation depth even across the interface between Li_3PO_4 and $LiCoO_2$. This implies that the change in the field distribution width at SCL of the sample is too small to be detected by LEM-μ^+SR. Since the SCL is expected to be amplified by charge-discharge reactions, future attempts to observe the space-charge layer will be conducted on multilayer samples after charge and discharge.

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Unconventional superconductivity in topological ruthenium silicides with Kramers and hourglass fermions

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The convergence of two major research strands in modern condensed-matter physics: topological materials and unconventional superconductivity, constitutes a new field of study. Topological materials with Kramers or hourglass fermions represent a special subclass, recently realized in materials lacking inversion symmetry or with a nonsymmorphic space group. At the same time, there is a surge of interest in identifying time-reversal symmetry (TRS) breaking (a key feature of unconventional superconductivity) in this class of materials, as a new routine way to realize topological superconductivity.

By using the muon-spin rotation and relaxation technique, backed by detailed theoretical analyses, we show that TRuSi (*T* = Ti, Nb, Hf, and Ta) noncentrosymmetric materials represent a family of compounds encompassing all the above unique properties [1]. Their bulk normal states behave as three-dimensional Kramers nodal-line semimetals, characterized by a fairly large antisymmetric spin-orbit coupling and by glide-reflection-protected hourglass-like fermions. We also identify surface states near the Fermi level of TRuSi materials More interestingly, NbRuSi and TaRuSi undergo a superconducting transition, which spontaneously breaks TRS below T_c, while surprisingly showing a fully-gapped superconducting ground state. This superconducting ground state is consistent with a unitary (*s* +*ip*) pairing, i.e., with a mixture of spin-singlet and spin-triplet pairings. As such, the TRuSi family provides an ideal platform for investigating the rich interplay between the exotic properties of Kramers nodal-line/hourglass fermions and unconventional superconductivity.

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Unfolding of the depth profiles with universal-range distribution functions

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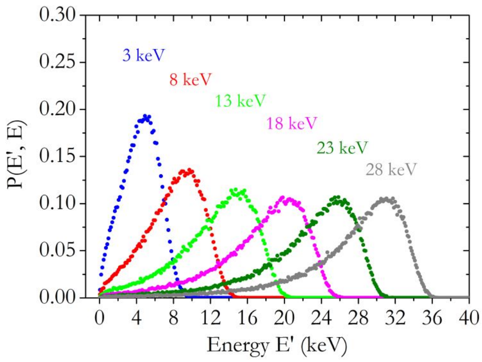

Figure 1: Universal range distributions in energy space for different implantation energies.

The analysis of depth-dependent data of thin-film film semiconductor heterostructures is discussed in this work. The data is obtained by varying muon implantation energy, E, using the Low Energy Muon facility (LEM) at PSI, Switzerland. Since the measurement method has a finite resolution, deconvolution of the measured profile with the resolution function is required. The unfolding can be implemented in the real space (that is in depth variable x), using range distribution function, P(x,E), obtained by Monte Carmo simulations. The unfolding in depth space requires detailed knowledge of the sample which may not be available. It is shown that it is much simpler to start by performing the deconvolution in the implantation energy space and to transform it afterwards into real space. This requires transforming P(x,E), in P(E',E) by an adequate variable change x = f(E'). The best approach is to use the relation between the median and the implantation energy for the coordinate transformation, since it ensures that the range distribution is centered at the implantation energy E. The range distributions in energy space, as derived from the depth distributions in CdS, are depictured in the Fig.1. They are considered nearly universal for all materials.

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Hydrogen impurity in MgO as seen by the muonium analogue

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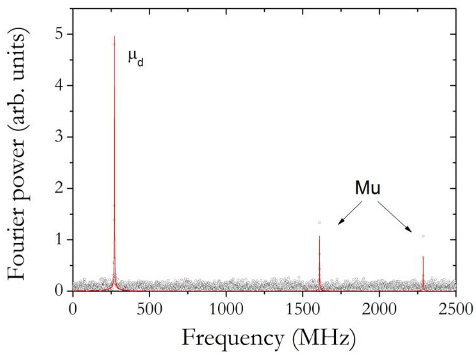

Figure 1: FFT of MuSR spectrum of MgO at T=6K and B=2T.

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.

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Non-destructive Elemental Analysis of Lunar Materials with Negative Muon Beam at J-PARC

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A muonic atom is formed when a muon is captured in an atom system, and characteristic muonic X-ray emission occurs with the muon deexcitation process. The chemical composition of a material can be known based on the intensities of the emitted muonic X-rays. Non-destructive elemental analysis using negative muon beam has been highly developed in the last decade. This method provides a powerful tool to determine the material composition of meteorites without causing damage.

We performed a muon experiment at the D2 muon beamline of the Muon Science Establishment (MUSE) in the Japan Proton Accelerator Research Complex (J-PARC). Three lunar meteorite samples (NWA482, NWA032, DEW12007) were wrapped with 12.5 μm Kapton foil and installed in a stainless steel analysis chamber filled with Helium gas. The total exposure time of muon irradiation with a momentum of 27 MeV/c for each sample was around 10 hours, and the emitted muonic X-rays were observed by six low-energy high-purity germanium semiconductor detectors, which were installed around the samples.

The peaks with energies of 76.7, 89.2, 92.7, 54.8, and 56.4 keV were clearly observed in the energy spectrum and were identified as the muonic X-rays from Si, Al, Fe, Ca, and Mg, respectively. The intensities of these muonic X-rays were determined by data fitting with gauss functions. Because the self-absorption of the sample and the detection efficiency of germanium semiconductor affect the measurement, the corrections based on the Monte-Carlo simulation were also applied in this study.

We successfully defined the chemical comparison of element/Si ratios of three lunar meteorites based on quantitative analysis for muonic X-ray measurement. The observed chemical composition suggests that the DEW12007 (polymict regolith breccia) could be a mixture of basaltic crust (NWA032-like) and anorthositic crust (NWA482-like) in terms of Al, Fe, Ca, and Mg contents.

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Positive muons, electrons, and nanostructures

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In this presentation, I will show where positive muons shine light on nanochemistry uniquely, where they provide complementary information to pulse radiolysis and where the muon laser spectroscopy stand in this complementary world of positive muons and electrons. I will show some of our pulse radiolysis data and our muon spin spectroscopy data obtained from our work on different nanostructures in the solid state and in liquids.

Developments of analysis functions for μSR time spectra which show intermediate shapes between Gaussian and Lorentzian

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How to choose analysis functions is a key matter to deduce the information in physics from the muSR results. For instance, local magnetic fields at the muon site in the paramagnetic state are well known to be coming from surrounding nuclear dipole moments. In this case, the field distribution at the muon site becomes to be the Gaussian distribution [1]. This Gaussian distribution typically occurs when there are independent contributions from many magnetic sources with similar amount of contribution. On the other hand, in case that, one magnetic spin, which is located nearest to the muon, tends to give a dominant contribution, the local field due becomes random and a different field distribution appears at the muon site. For the dilute limit (effectively for concentrations less than 3 5 %), the field distribution becomes to be Lorentzian [2].

In our presentation, we described the crossover field in terms of a convoluted function of Gaussian and Lorentzian. We derived the equation of the three-dimensional (3D) convolution in two ways. The first derivation uses the convolution integral starting directly in the 3D space. The other derivation starts from that of the one-dimensional (1D) convolution and make it to be converted to the 3D form. From the latter, we showed that the equation can be decomposed to a sum of three known convolutions. By applying the Fourier transform to this equation, we achieved the correct relaxation function for the zero-field condition, which was found to be given by a simple analytical equation. In addition, we tried to describe the intermediate analysis function under applied magnetic fields and under dynamic fluctuations based on the development of the zero-field intermediate analysis function. Finally, we applied our developed analysis function to some μSR results to make sure its validity [3].

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Local electronic structure of interstitial hydrogen in MgH_2 inferred from muon

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with
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Metal hydrides have attracted attention as one of the candidate materials that can serve as safe and efficient hydrogen (H) storages. In particular, MgH_2 has great potential as a solid H-storage material because of its high storage capacity of 7.6 wt%. However, its slow hydrogenation and dehydrogenation rates and the high decomposition temperature ($\sim$300°C) are major obstacles to the practical applications. Understanding the microscopic mechanisms of the H-related processes is key to engineering solutions to improve the H-intake/release kinetics and to lower the decomposition temperature. To this end, the information on the electronic state of interstitial H (which exists as an intermediate state in the reaction kinetics) is crucial in gaining insight into the rate-limiting processes.

The preceding studies on the microscopic state of H in MgH_2 have been mainly via computational approaches based on density functional theory (DFT), but there have been few experimental investigations to validate the prediction of DFT calculations. We have introduced muons as pseudo-H into MgH_2, and studied their electronic and dynamical properties in detail to elucidate the corresponding interstitial H states. As a result, we found two species of Mu states showing comparable yields; a paramagnetic state with relatively large hyperfine parameters (0.5-1.7 GHz) that undergoes rapid conversion to diamagnetic states, and a quasistatic diamagnetic state described by the Kubo-Toyabe relaxation function. In this talk, we discuss the correspondence between these Mu states and the predictions from the DFT calculations.

β-NMR studies of the temperature, depth and molecular weight dependence of dynamics in normal and ultrastable polystyrene glasses

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The observation that the glass transition temperature of polystyrene (PS) thin films decreases with decreasing film thickness led to the suggestion that there is a very thin layer near the free surface where the polymer motion is faster than in the bulk. Direct confirmation of enhanced dynamics near the free surface has proved elusive as few techniques can measure how the dynamics varies with distance from the free surface on the nm length scale and those that can either use bulky probes or multilayer films that modify the dynamic gradients. Implanted $^{8}Li^{+}$ is a much less perturbing probe and with β-detected nuclear magnetic resonance (β-NMR) we can measure the depth dependence of the γ relaxation of PS, which involves motion of the phenyl side groups.[1,2,3] The γ relaxation has a double exponential depth dependence from the free surface, with a characteristic length of 6 nm. We have produced ultrastable glass (USG) films of low-molecular weight PS by physical vapor deposition that exhibit properties similar to those of a normal glass (NG) that has been aged for several years. Our β-NMR measurements indicate the bulk γ relaxation is slower in the USG compared with the NG while the opposite is true near the free surface where the γ relaxation is faster in the USG compared with the NG. These trends are more significant for samples with a larger apparent age.

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P

SCE

DFT Investigations on Magnetic Properties with Muon in La_2CuO_4 by Using LSDA+U Functional

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with
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The mother material of the La-based high-Tc superconducting oxides, La_2CuO_4 (LCO), which family of materials possesses a d9 electronic configuration for copper ions, acts as a three-dimensional antiferromagnetic Mott insulator. LCO has been well investigated experimentally and theoretically in the past, but there are still questions on electromagnetic states to be investigated. The on-site Coulomb potential, U, on the Cu site plays a key role for magnetic properties forming the covalent state of electronic orbitals between Cu and O. We are performing first-principles calculations based on the density functional theory (DFT) to investigate the covalent state and discuss experimental results by using muons. One important key issue for this problem is what kind of electronic correlation functional should be chosen for calculations. In our presentation, we report detail DFT calculation results on LCO by using the Local Spin Density Approximation (LSDA) functional with the Vienna ab-initio simulation package (VASP) to investigate structural and magnetic properties of LCO.

The calculated magnetics moment of Cu in the antiferromagnetically ordered state with the spin direction along the b-axis without the muon is 0.491 μ_B, which was agreed upon well with the neutron scattering experiment. We found that the calculated band structure and the density of states indicated that U significantly influenced the hybridization of Cu-3d with O-2p orbitals at the valence and conduction bands influencing the band-gap energy. After adding the muon into the calculation model, it was confirmed that the muon deformed the local crystal structure around the preferable muon position and drastically reduced the magnetic moment of Cu near by the muon changing surrounding electronic states. We are now trying to investigate this situation by using other functionals and will report the results in our presentation.

Magnetic Properties of La_2CuO_4 Nanoparticles

P

SCE

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with
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A nano-size effect on magnetic materials shows novel and causes the magnetic properties different from those observed in a bulk form. The nano-size effect has been well investigated in metals but not yet explored in the high-Tc superconducting oxides. La_2CuO_4 (LCO) is a parental compound of La-based high-T_c superconducting cuprates which have a long-range antiferromagnetic (AF) ordering of Cu spins. LCO nanoparticles were synthesized using the sol-gel method by controlling the time and temperature of a sintering process. It was found from our zero-field µSR on LCO nanoparticles that the magnetic transition temperature drastically decreased with decreasing the particle size. On the other hand, the saturated internal field at the muon site did not change at all, suggesting that the AF spin alignment around the muon in the nanoparticle state is the same as in the bulk sample. We proposed a core-shell model to understand our µSR results. We assumed that the core corresponds to the long-range ordering and a shell correspond to non-ordered regions where Cu spin did not form a static ordering. We are now investigating how to control oxygen deficiencies that affect magnetic interaction in LCO. In our presentation, detailed µSR results and some characterizations of magnetic properties in LCO nanoparticles will be reported.

P

EM

Current Status of Operando-μ^+SR for Battery Materials at J-PARC

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with
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Ion transport in solids is a key feature for the operation of ion batteries. There are two parameters for describing ion transport in battery materials; one is a self-diffusion coefficient (D^J) and the other is a chemical diffusion coefficient (D^C). The former diffusion is caused by thermally activated fluctuation of ions, while the latter diffusion is caused by a flow due to a concentration gradient of ions. Majority of work concerning battery materials, D^C has been measured with an electrochemical technique under a concentration gradient of the ion in a half-cell. D^C is then estimated using the relationship: $D^C = \Theta D^J$, in which Θ denotes a thermodynamic factor.

According to the Cottrell equation, the time evolution of the current of the planer electrode in the half-cell under an ion-concentration-gradient has a relation, $I(t) \propto A_{re}\sqrt{D^C}C$, where A_{re} and C denote the reactive surface area of the electrode and the concentration of the ion. Thus, the obtained value from the electrochemical measurement is not D^C but $D^C A_{re}^2$. Because the correct A_{re} in liquid or solid electrolytes is unknown, it is very difficult to determine D^C. We have thus initiated series of experiments to measure intrinsic D^J of battery materials with μ^+SR [1]. Due to the change in the crystal structure and occupancy of a regular Li site with SOC, D^J is predicted to depend on SOC [2]. Therefore, it is highly desirable to measure D^J as a function of SOC under working condition, namely, an operando μ^+SR. We are attempting to establish such technique in J-PARC, and show the current status.

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Superconductivity nearby quantum critical point in hole-doped organic strange metal κ-(ET)$_4$Hg$_{3-\delta}$Br$_8$

P

SU

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The hole-doped organic superconductor κ-(ET)$_4$Hg$_{3-\delta}$Br$_8$, (κ-HgBr), where δ=11

ET=bis(ethylenedithio)tetrathiafulvalene, has been the key to bridge the knowledge gap between half-filled organics and doped cuprate systems. Nonetheless, the isotropic triangular lattice of ET dimers of κ-HgBr, unlike the square lattice in cuprates, is suspected responsible for its susceptibility which is well scaled with the organic spin liquid insulator κ-(ET)$_2$Cu$_2$(CN)$_3$. However, both κ-HgBr and cuprate have a region at high temperature and high-pressure corresponding to the $strange\ metallic$ state where resistivity exhibits a linear temperature dependence which is non-Fermi-liquid (non-FL) behavior. In κ-HgBr this non-FL region gradually changed to an FL state by pressure [1], like the change of metallic state from optimal to overdoped cuprates. The ^{13}C-NMR concluded that the antiferromagnetic fluctuations contribute to the origin of the non-FL in κ-HgBr [3]. This evidence may locate superconducting κ-HgBr nearby quantum critical point (QCP) in between FL and localized states, where in its non-FL state the incoherent conductivity was observed [1,3].

Our zero-field μ^+SR experiment showed the relaxation rate from around 10 K down to 0.3 K is temperature-independent. This is a high possibility of the superconducting state that preserved time-reversal symmetry. There was almost no change in the 120 Oe of transverse-field-μ^+SR time spectra, at 0.3 K and above the superconducting temperature T_c = 4.6 K, indicating that the London penetration depth is longer than a μm order, while we estimate the lower critical field, $H_{c1} = 25(5)$ Oe. These could be an indication of a strong-coupling superconductor. We will discuss a possible mechanism of preserved time-reversal Cooper pairing formation from strong-coupling non-FL metal with geometrical frustration.

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P

EM

Muon Studies of the Proton Conducting Polymer Nafion

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The fluorinated ionomer Nafion, first discovered by the DuPont company, is a material that provides efficient proton conducting membranes for application in important technological areas such as hydrogen fuel cells. Although many aspects of the polymer have been studied in relation to these applications, the microscopic mechanisms for proton transport in this polymer are still only poorly understood. We have therefore applied implanted muon techniques to the study of Nafion, aiming to to gain information about these mechanisms via the muon acting as a local spin probe. Our results indicate that the muon is highly sensitive to the hydration state of the polymer and to the dynamical processes of the various sub-phases within the material. A three component model is found to describe the data well. This model has one F-μ-F component reflecting muons in the PTFE-like polymer matrix, a second component representing quasi-static environments that are not closely coupled to the F atoms and a third component encompassing highly dynamic proton-coupled environments. The properties have been studied within this modelling framework as a function of temperature and hydration level.

Integration of arts and sciences by using negative muon non-destructive analysis at J-PARC MUSE

P

X

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We have been developing a non-destructive, position-selective, and quantitative multi-elemental analysis method by using negative muons at J-PARC MUSE. Our final goal is to establish a platform of the integration of arts and science, where historical relics can be analyzed non-destructively, by combining quantum beams techniques utilizing muons, neutron or photons.

At the symposium, the current status of the negative muon non-destructive analysis held at J-PARC MUSE, on Japanese old coins (Koban, Cho-gin), bell-shaped bronze vessel of the Yayoi period, and Ogata Koan's sealed medicine etc. will be introduced.

P

MC

The electron transfer channel in the sugar recognition system assembled on nano gold particles

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The recently reported electrochemical sugar recognition system consisting of a nano-sized gold particle (GNP) with a diameter of 10 nm, a ruthenium complex and a pheylboronic acid, attracts much interest because of its high sensitivity for various sugars such as D-glucose or D-fructose. When sugar molecules are attached to the phenylboronic site, the response of electrochemical voltammetry of the Ru site changes, enabling the system to work as a sensitive sugar-sensor [1]. In this recognition process, the change in the electronic state at the boron site caused by sugar must be transferred to the Ru site. However, mechanisms of its transfer as well as the sensitivity amplification are not understood until now [2].

We have utilized the method of labelled electrons with muons and also the proton NMR to find out a channel of the electron transfer from the phenylboronic acid site to the gold nano particle via the one dimensional alkyl chain. If this transfer is driven by diffusive spin channel, characteristic field dependence is expected in the longitudinal spin relaxation rate of muSR and 1H-NMR[3,4]. We have observed significant decrease in the spin relaxation rates with increasing applied longitudinal field between 0.1 and 6 T for muSR and 1H-NMR. The result will be discussed in terms of low dimensional spin diffusion along alkyl chains.

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Investigation of the magnetic topological insulator family ($MnBi_2Te_4$) (Bi_2Te_3)$_n$ by µSR and NMR

P

SCE

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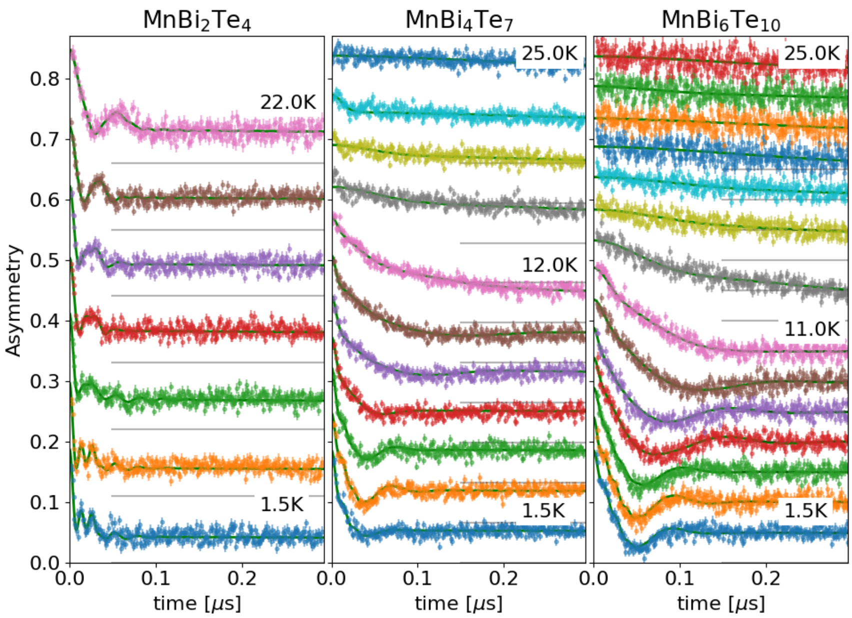

Figure 1: ($MnBi_2Te_4$) (Bi_2Te_3)n Zero Field µSR asymmetries vs. time at different temperatures

Time-reversal symmetry breaking in a topological insulator (TI) opens a surface gap and distinguishes chiral quantum states that could eventually be exploited in electrically controlled spintronic devices. The new approach to this state in a TI is with the intrinsic magnetic proximity of a magnetic insulator that can be achieved with layered van der Waals materials.

($MnBi_2Te_4$) (Bi_2Te_3)n are one of the first such examples, where the increasing number n of TI layers controls the magnetic properties and dimensionality of the material. These compounds do display the quantum anomalous Hall effect, a hallmark of a magnetic TI, where spontaneous magnetization and spin-orbit coupling lead to a topologically non-trivial electronic structure. Magnetic order critical temperatures detected by macroscopic magnetization are T_N=25,13K for n=0,1 and T_C=12K for n=2 with a lower metamagnetic transition at T_M=6K for n=1[1,2,3].

Zero-field µSR (see Fig. 1) shows more than one internal field at the muon site with the majority one decreasing in value when n is increased. The muon spin precessions display very fast relaxations of static inhomogeneous nature, and the longitudinal asymmetry component displays critical slowing down of fluctuations at T_C. Remarkably the high field site disappears above T_M. NMR additionally shows the presence of a small anti-site component (likely Mn in the Bi site) in the n=1 sample. This local information is crucial to correctly interpret macroscopic magnetization data.

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Negative muon spin relaxation in water and ice

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P

MC

Muons are the main component of cosmic ray particles on the earth, and most of the cosmic ray muons are injected into water or ice, which occupy more than 70% of the earth's surface. When negative muons (μ^-) stop in H_2O, they are mainly trapped by oxygen nuclei and form muonic oxygen atoms Oμ^-, and about 15% of Oμ^- atoms finally change to stable nitrogen isotopes ^{14}N or ^{15}N via the neutron emission after the muon capture process. The nitrogen isotopes produced by such a process may be chemically active due to their high recoil energy and may form various nitrogen compounds through reactions with water molecules. In this situation, μ^-SR spectroscopy is suitable for studying the behavior of such active nitrogen in H_2O, since Oμ^- atoms also act chemically as nitrogen. In the present study, we measured μ^-SR spectra in water and ice to approach what kind of nitrogen compounds are formed by cosmic-ray negative muons, and how they affect the surrounding chemical environment.

Experiments were carried out at the D1 beamline in the Materials and Life Science Experimental Facility (MLF) of J-PARC. H_2O and D_2O samples were irradiated with a negative muon beam (47 MeV/c, double pulse), and ZF and LF-μ^-SR spectra were measured. The result shows that the relaxation due to the nuclear dipolar field is observed in solid H_2O and D_2O at 200 K. The field distribution widths were deduced to be Δ_H=0.27 μs^{-1} and Δ_D=0.066 μs^{-1}, for H_2O and D_2O respectively. The relationship between these two values is well explained by the difference in the spins and magnetic moments of proton and deuteron.

In this conference, we will discuss possible chemical states based on the present results.

P

NT

Precise measurement of the hyperfine splitting in muonium with a high intensity pulsed muon beam at J-PARC

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A muonium is a purely leptonic bound system of a positive muon and an electron.

Fundamental properties of such a system can be precisely predicted by the QED, whereas ordinal atoms require to calculate hadronic interactions.

At J-PARC, the MuSEUM (Muonium Spectroscopy Experiment Using Microwave) collaboration aims to precisely measure the ground-state hyperfine splitting of muonium atoms, arising from spins of the muon and electron.

The pulsed muon beam is stopped in a krypton gas cell to form the muonium atoms.

The transitions of spin states are induced with a microwave cavity, which is then measured by positron counters.

In previously performed measurement with a nearly-zero magnetic field [1,2], the resonance of the hyperfine transition was successfully observed with a relative precision of 160 ppb.

As a next step, we plan to perform the measurements with strong magnetic fields, so that the different frequency shifts by Zeeman splitting allow us to more precisely determine the transition rate down to 1.2 ppb.

This unprecedented precision will be achieved by upgrading several components of the experimental setup, including a new high intensity muon beamline which is currently commissioned at J-PARC.

Performing measurements at various magnetic field strengths requires to replace the current cylindrical microwave cavity with a new boxed-shaped cavity.

In this presentation, the general scheme of our experiment and status of the upgrades for the new measurement are reported.

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Evolution of the magnitude of the exchange and Dzyaloshinskii-Moriya interactions under pressure in chiral magnet MnSi

P

SCE

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The intermetallic compound MnSi exhibits a number of properties that have attracted strong interest. In particular it magnetically orders below 29.5 K to an exotic long-pitch helical structure. This type of order is due to the presence of the Dzyaloshinskii-Moriya interaction, authorized by the absence of inversion symmetry in the crystal structure, that coexists with a dominant ferromagnetic exchange interaction.

As often observed in strongly correlated magnets, the properties of MnSi are strongly influenced by the application of a relatively modest pressure. The MnSi ordering temperature decreases with pressure up to 1.5 GPa, above which value its ground state is non-magnetic.

Here we report on recent zero-field μSR measurements aimed at determining the evolution of the magnetic order under pressure. Up to 1.3 GPa, the high statistics asymmetry spectra can be analysed using the model derived a couple of years ago for the interpretation of room pressure measurements [1]. Thanks to a prior determination of the muon site and of the muon coupling parameters, the parameters entering the model are directly those of the magnetic structure.

For each pressure, we find the ordered magnetic moment m to decrease as T^2 from its low temperature value, similar to earlier results obtained at room pressure [2]. This decrease is the signature of the excitations of spin waves (helimagnons) as the temperature is raised. The quadratic temperature dependence reflects the form and anisotropy of the helimagnon dispersion relation. From the slope of $m(T)$ vs T^2 we determine the two parameters of the dispersion relation, from which we quantitatively deduce the magnitude of the exchange and Dzyaloshinskii-Moriya interactions at each pressure. Finally the spectra recorded at 1.44 GPa are discussed.

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P

MC

Near-surface dynamics of 1-ethyl-3-methylimidazolium acetate above and below the glass transition

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Ionic liquids (ILs) are a class of molten salts which are liquid at room temperature. Their properties are determined by strong electrostatic forces and generally include low volatility, negligible vapour pressure, and a low melting point. This makes them attractive candidates for improving battery and capacitor technology. The device effectiveness, however, is often determined by the ion arrangement and dynamics at the interface between the IL electrolyte and the electrode.

A much simpler interface is that of the free surface (vacuum interface). Studies of IL surface chemistry reveal a number of surprising phenomena, such as orientational ordering and regions of surface crystallization. As the ionic constituents may differ greatly in size and shape, many ILs do not crystallize (other than at the surface, perhaps) and will instead vitrify. The unusual behaviour of ILs may help to reveal novel aspects of glassy dynamics.

Having demonstrated that β-NMR was a good probe of IL solvation dynamics and dynamic heterogeneity,[1] we now turn to the question of how the surface modifies these properties, presenting the first depth-resolved β-NMR measurements in 1-ethyl-3-methylimidazolium acetate. The surface clearly has a large dynamical effect in the glassy phase: there is enhancement in the relaxation rate near the surface, resembling a more liquid-like state, yet no significant change in the dynamical heterogeneity. Additionally, the relaxation grows faster as the material is cooled through the glass transition temperature. These two latter aspects are very surprising, and are an extreme departure from the behaviour of other glasses.[2]

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High-pressure phases of Kitaev materials (as seen by muSR)

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P

SL

Bond-dependent interactions between magnetic moments can lead to strong frustration and nontrivial ground states. In particular, the Kitaev-Heisenberg model has a rich phase diagram and can host a spin liquid state or different frozen states depending on the strength of the additional Heisenberg interactions. Experimentally, such phase diagrams can be explored by modifying the relative interaction strengths in materials by applying pressure.

In this presentation, I will describe how the muon spin rotation technique can be used to study such materials under applied pressure and what it can reveal about the transitions between different phases. I will then show examples of our recent high-pressure studies in Kitaev candidate materials. In Na2IrO3 the magnetic order is enhanced by the application of pressure up to at least 4 GPa. Combined with structural studies, we can explain this as a compression of the honeycomb layers [1]. In beta-Li2IrO3, we find that the magnetically ordered state collapses at 1.4 GPa [2], originating from dimerization of the Ir ions. In alpha-RuCl3, a similar phase transition is also observed at about 0.4 GPa [3], which is concomitant with unconventional response in the muon polarization function.

I will summarize the emerging generic picture of Kitaev materials under pressure and will discuss the peculiarities of the muon response in these systems.

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P

SL

Probing Local Magnetic Order in the Frustrated Bow-tie Lattice of Layered Oxide $Ca_2Mn_3O_8$

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Frustrated magnetism continues to be a vibrant area of research in chemistry and condensed matter physics. Geometric frustration arises when the magnetic degrees of freedom are incompatible with the underlying lattice geometry, and contrasts conventional magnetism because the system exhibits numerous degenerate ground states. Hence, rich exotic phenomena are observed as a function of pressure and (or) temperature. A plethora of frustrated layered oxide materials exist, including the delafossite family which is similar to the well-known Kagomé system and is based on a triangular antiferromagnet. One variant of this family with interesting bow-tie connectivity is $Ca_2Mn_3O_8$, which contains two unique manganese sites. It exhibits two magnetic phase transitions, one at T^* = 130 K that is associated with short-range spin correlations and a second at T_N = 58 K that is associated with three-dimensional long-range order. From neutron diffraction studies, the former transition is exclusively linked to the crystallographic*b*-direction but fully ordered one-dimensional chains are not realised. To further investigate this interesting local magnetic behaviour, temperature studies using inelastic neutron scattering, X-ray absorption spectroscopy and muon spin spectroscopy were carried out. Measurements reveal the intriguing correlation between the unique manganese sites such that static-dynamic behaviour between both persists below T^* in an attempt to relieve frustration.

P

NT

Towards a microscopic understanding of charge carrier mobility in dielectrics with muon spectroscopy

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This paper reports the development of a novel technique using spin polarised positive muons to probe local charge redistributions within polymeric dielectrics under externally applied E-fields (EEF's). These materials are used in many high voltage applications, and knowledge of charge dynamics is crucial to their successful use, as it dictates their ultimate ability to function as a dielectric. Conventional bulk characterisation methods are useful tools in this regard, but only give information at a micron level, whereas muons give a molecular view and can therefore bring new insight into how charge transport at this level develops prior to breakdown. Here we report the first investigation of this type, studying muons implanted in a polymer epoxy (DGEBA) subjected to an EEF.

DGEBA consists of long chain molecules, including phenyl groups, where muonium can add to form radical states. We have measured ALC lines in this system and found a broad resonance peak with a coupling consistent to addition to the ring. When exposed to a comparatively large externally applied electric field (EEF), but still well below its intrinsic breakdown voltage (Vbr), a change in the muon asymmetry across the entire resonance peak was observed. The largest change in amplitude was observed at the magnetic field corresponding to the centre of the ALC resonance. Working at this fixed magnetic field, changes in amplitude of the resonance curve were explored as a function of applied EEF. Both negative and positive EEF's were applied along the beam direction.

Measurements show an almost perfect linear dependence of the asymmetry of the ALC line to the applied EEF. However,there is a curious departure in this behaviour when small negative EEF's are applied that merits further investigation. Our contribution discusses early results and considers what they tell us about charge mobility in DGEBA on the microscopic level.

P

SC

The site and high field βNMR properties of ^{8}Li$^+$ implanted into α-Al$_2$O$_3$

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We present high magnetic field βNMR measurements of ^{8}Li$^+$ implanted in single crystals of sapphire, a commonly used backing material for other samples. From the well-resolved quadrupolar splitting, we extract the electric field gradient (EFG) at the implanted ^{8}Li$^+$ site. Comparison with supercell density functional theory calculations of the EFG allows us to identify the octahedral interstitial site as the most likely candidate. In contrast to the zero field βNQR spectra, only a single site is evident at high field. We discuss possible explanations for this discrepancy. The high field spin lattice relaxation is extremely slow ($1/T_1 < 0.02$ s^{-1}) from 4 to 300 K. This regime, where cross relaxation to the ^{27}Al nuclear spins is quenched, extends down to at least 2.2 Tesla.

Time-reversal symmetry breaking in nonsymmorphic type-I superconductor $YbSb_2$

P

SU

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The interplay of superconductivity with nontrivial topological phases exhibit the fascinating topological superconductivity, which has attracted widespan attention from observing quasiparticle like Majorana fermions to its application in fault-tolerant quantum computation [1,2]. It is proposed that the topological superconductivity can be realized in compounds having topological surface states and superconductivity [3]. Only a few superconducting materials with nontrivial topological states have been discovered, and their superconducting ground state/pairing mechanism can not be adequately understood. Therefore, searching and studying the superconducting ground state of materials having nontrivial topological states is vital.

Here, we present the evidence of time-reversal symmetry breaking (TRSB) in the nonsymmorphic type-I superconductor $YbSb_2$, having a distorted Sb square net crystal structure similar to the other topological system ZrSiS [4,5]. The microscopic muon spin relaxation and rotation investigation confirm the fully gapped type-I superconductivity with broken time-reversal symmetry in its superconducting ground state. This indicates that the nonsymmorphic RSb_2 superconductors are an interesting class of materials that exhibit unconventional superconductivity with fascinating properties and warrant great potential for future studies.

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SEMI

Nuclear magnetic resonance of ^{8}Li ions implanted in ZnO

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ZnO is a wide direct bandgap (3.4 eV) semiconductor with promising electronic properties potentially useful in room temperature optoelectronic and spintronic devices. It can be used as a dilute magnetic semiconductor by tuning intrinsic or extrinsic magnetic defects while ZnO also demonstrates many unique surface effects such as a photogenerated metallic state. Imperative to utilizing these unique properties is understanding and controlling point defects in its hexagonal wurtzite structure that may lead to stable hole doping. We implanted a low energy (20-25 keV) beam of hyperpolarized spin-2 ^{8}Li ions and used β-detected nuclear magnetic resonance (β-NMR) to understand the stability, structure, and magnetic state of Li defects in ZnO [Adelman et al., arXiv:2109.08637v1]. Closely related to μSR used to characterize isolated hydrogen impurities in ZnO, β-NMR allows complementary investigations of light isotope dopants in the ultradilute limit.

Using ^{8}Li simultaneously as the defect and probe, distinct Li sites are detected by measuring the coupling of the nuclear electric quadrupole moment to the asymmetric electronic charge distribution surrounding the ^{8}Li nucleus. From 7.6 to 400 K, we find ionized shallow donor interstitial Li is exceptionally stable, verifying its role in self-compensation of the acceptor (Zn) substitutional. Like the interstitial, the substitutional defect shows no resolved hyperfine field above 210 K, indicating it is a shallow acceptor. By pulsing the ^{8}Li beam, the spin-lattice relaxation is measured and indicates above 300 K the onset of correlated local motion of interacting defects. This is supported by resonance spectra collected with a CW frequency comb that enhances the amplitude of well-resolved quadrupolar multiplets and confirms a site change transition from disordered interstitial Li to the substitutional. The quadrupole hyperfine interaction exhibiting a $T^{3/2}$ temperature dependence typical of non-cubic metals is also discussed.

Data analysis for μSR experiments with negative muons.

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Negative muons are often overlooked compared to their positive counterpart, partly due to the loss of around $\frac{5}{6}$ of the μ^- spin polarisation when a μ^- cascades down to the 1s muonic ground state after being captured by a nucleus. One needs to count for around 36 times as long to get statistics comparable to that of a μ^+SR experiment. However, there has been a recent revival of μ^-SR experiments, particularly in the study of hydrogen storage and battery materials [1,2]. When stopped in a material of atomic number Z, μ^- forms a muonic atom and cascades down to its ground state. The muon Bohr radius is 200 times smaller than the electron Bohr radius, and so this probe behaves like an ultra-dilute atom of apparent nuclear charge $Z - 1$. The μ^- will be strongly hyperfine coupled to the nuclear spin of the capture atom, but if that nuclear spin is zero, such as an oxygen in MnO, the only coupling will be to the nuclear dipolar fields in a region very close to that capture nucleus. Because of these difficulties new analysis techniques have been developed in WiMDA [3] for the fitting of μ^-SR data, and we have adapted the DFT+μ^+ technique for the case of a negative muon. Both of these new techniques have been applied to MnO where the dipole field simulations show a large field at the oxygen site, and DFT+μ^- calculations show a Jahn-Teller-like distortion around the negative muon.

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SCE

A wolf in sheep's clothing? Muon-induced magnetism in quantum spin ice

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Compounds of the form $\mathrm{A_2X_2O_7}$ with the pyrochlore structures can exhibit classical or quantum spin ice behaviour if the crystal field environment of the $\mathrm{AO_8}$ arrangement leads to the [111] easy-axis anisotropy. When Pr occupies the A-site, there is a low-lying electronic doublet and $\mathrm{Pr_2X_2O_7}$ compounds are found to be quantum spin ices[1]. $\mathrm{Pr^{3+}}$ is a non-Kramers ion and the presence of the muon can distort nearby $\mathrm{PrO_8}$ units and split the doublet ground states[2], resulting in an enhancement of the Pr nuclear moment due to hyperfine coupling with the electronic moments[3]. We explore this effect using a theoretical model that takes account of the important interactions and compare our simulations with μSR data on samples of $\mathrm{Pr_2X_2O_7}$ (X = Sn, Hf, Zr) and new experimental data on $\mathrm{Pr_2ScTaO_7}$, a candidate system that simultaneously realises spin ice and charge ice structures.

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Phase diagram of the perovskite solid solution $CaCu_3Ti_{(4-x)}Ru_xO_{12}$ elucidated with bulk μ^+SR

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SCE

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The $CaCu_3Ti_{(4-x)}Ru_{(x)}O_{12}$ family, synthesized under high pressure (7.7 GPa) belongs to the perovskite class of materials. The ground state of the extremes of this solid solution are antiferromagnetic insulator for the x = 0 member, and itinerant-electron system, i.e., Pauli-paramagnetic metal, for the x = 4 member respectively**[1,2]**. The suppression of magnetic ordering from the x = 0 to the x = 4 member of the solid solution seems to be accompanied by non-Fermi liquid (NFL) behavior since $CaCu_3Ti_4O_{12}$ manifested indications of such a behavior in heat capacity measurements**[3]**. These features make the solid solution $CaCu_3Ti_{(4-x)}Ru_{(x)}O_{12}$ a promising candidate for possessing a Doniach-type phase diagram**[4]**. In this work we present the results of a bulk muon spin rotation study on the intermediate members of the solid solution, showing the evolution of the magnetic ground state going from antiferromagnetic to paramagnetic. Evidence of highly dynamical ground states are also found among the members of the solid solution and a tentative phase diagram as a function of the Ru content x is proposed.

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NT

Search of ultracold Mu generation material: μSR study in SiC

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Ultracold muonium (UCMu) is an important muonium (Mu) source for the generation of ultraslow muon beam [1-3] for nanotechnological applications and understanding hydrogen dynamics in materials. In order to search a new solid material for the generation of UCMu in vacuum, we have studied n-Si [4], SiC and KCl at low temperatures (5 K – 300 K) using conventional μSR method. The relaxation rates of Mu formed deep inside (full-stop case) and near the rear surface (half-stop case) of the samples at low transverse field (TF 1.2 G) were observed. In n-Si, the difference in relaxation rates below 100K provided the hint for emission of Mu from the surface but the distance dependent study (distance of sample from silver sheet) shows that there is surface effect that causes the change of relaxation rate of Mu in half-stop case. In SiC, we have observed the Mu signal with high relaxation rate and the relaxation rates in full-stop and half-stop cases were found within error-bars. In KCl, we did not observe even a complete spin rotation signal of Mu below 100 K at TF 1.2 G field. In literatures, there is quantum diffusion of Mu in KCl is available [5,6]. In the program, we will present details about our measurement method and result in SiC.

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Probing beneath the surface without a scratch: Developments of elemental analysis using muons at ISIS

P

X

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Using negative muon emission spectroscopy (µXES) can yield unique information by determining the composition beneath the surface whilst being completely non-destructive and has been shown to be a powerful technique for non-destructive analysis of the elemental composition of precious/rare samples. The characteristic muonic X-rays emitted after muon implantation can be used as fingerprints to assign the presence and depth of a given element in a sample. The use of negative muons for elemental analysis has seen a rapid increase in demand, from cultural heritage, advanced manufacturing to energy materials, even though the instrument at ISIS is still under development.

In the past few years there has been some developments in data acquisition electronics, analysis techniques, and future instrument design and in this paper we will review some of the science highlights, and the recent developments, including:

New software has been developed (EVA) to assist in the understanding, this includes easy peak identification, composition analysis and data correction.

Mudirac: A Dirac equation solver for elemental analysis with muonic X-rays is being extended to include the probability of transition, thus potentially making an automatic efficiency and absorption correction.

In addition, a machine learning (mulspec_ml) based technique for analysing and classifying elemental composition from µXES experiments has been developed (see abstract Butler).

Finally, studies for the next generation instrument are in place. The current set-up is composed by four HPGe detectors: the new detector array is expected to increase the solid angle coverage and optimisation which should yield an increase in rate of 10-100x (momentum dependent) and a decrease in measuring time. To evaluate the best geometry, Monte Carlo simulations are performed with the GEANT4 toolkit. Simulations are peformed to evaluate the capabilities of seven hexagonally shaped germanium crystals, placed around the sample stage in a packed geometry.

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SCE

Magnetic Properties of $LiFePO_4$ under Hydrostatic Pressure

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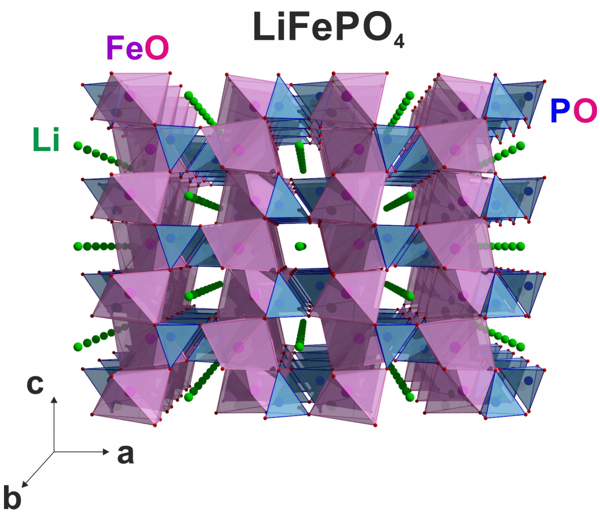

Figure 1

$\mathrm{LiFePO_4}$ (LFPO) is an archetypical and well-known cathode material**[1]** for rechargeable Li-ion batteries. However, its quasi-one-dimensional (Q1D) structure (see Figure) along with the Fe ions, LFPO also displays interesting low-temperature magnetic properties**[2]**. At ambient pressure LFPO display an antiferromagnetic (AFM) spin order below $T_N = 53\ \mathrm{K}$ and neutron scattering**[3-5]** have characterized that LFPO orders in a canted AFM ground state below T_N. Our team has previously utilized muon spin rotation (μ^+SR) to investigate both magnetic order as well as Li-ion diffusion in LFPO**[6]** as well as nano-structured LFPO**[7,8]** and related compounds**[9-11]**. In this initial study we make use of high-pressure μ^+SR to investigate effects on the low-T magnetic order. We find a clear decrease in T_N at $p = 20\ \mathrm{kbar}$ and we can estimate that a complete suppression of magnetic order should appear around $p_c \approx 300\ \mathrm{kbar}$.

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SCE

Anomalous electrical transport in frustrated intermetallic $RCuAs_2$: the role of spin

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The Kondo effect was a longstanding theoretical puzzle, describing the scattering of conduction electrons in a metal due to dilute, localised d- or f -electron magnetic impurities and resulting in a characteristic minimum in electrical resistivity with temperature. Extended to a lattice of magnetic impurities, the Kondo effect likely explains the formation of so called heavy Fermion systems and Kondo insulators in intermetallic compounds, especially those involving rare earth elements like Ce, Pr and Yb. The hybrisation of the 4f electron states with the conduction band and resultant screening of local moments, required for Fermi liquid behavior in the Kondo lattice, competes with interactions between localised moments. The diversity in the low temperature properties of heavy Fermion metals, as well as their highly tunable nature (with magnetic field, pressure, chemical substitution), make these systems invaluable in the investigation of the emergent properties of highly correlated quantum materials.

Counterintuitively, in a class of ternary intermetallic compounds of the type $RCuAs_2$ (R = rare earth) [1], the rare earths like Sm, Gd, Tb, and Dy with strictly localised 4f character, where the Kondo effect is not anticipated, also exhibit a pronounced minimum in resistivity well above their respective magnetic ordering temperatures. Even more surprisingly, no such minimum is observed for Pr, Nd, and even Yb based members of this series. Recent theoretical predictions suggest geometric magnetic frustration plays a role [2]. More generally, frustration is thought to be an important additional tuning parameter in the Kondo lattice model. A muon spin relaxation investigation of these materials is discussed, shedding light on the role of magnetic fluctuations in determining the electronic transport in heavy Fermion materials.

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Possible p-wave parity in Cr-based superconductor $Pr_3Cr_{10-x}N_{11}$

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SU

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Superconductivity with a critical temperature $T_C \sim$ 5.25 K was recently reported in the Cr-based superconductor $Pr_3Cr_{10-x}N_{11}$. The large upper critical field $H_{C2} \sim$ 20 T, and the strong correlation between $3d$ electrons derived from specific heat, suggest the unconventional superconductivity nature of this compound. We performed muon-spin rotation/relaxation (μSR) measurements on a high-quality polycrystalline of $Pr_3Cr_{10-x}N_{11}$ down to 0.027 K, and specific heat measurements under different magnetic fields up to 9 Tesla. Our μSR data indicate that time-reversal symmetry is broken in the superconducting state of $Pr_3Cr_{10-x}N_{11}$, and the superconducting energy gap is consistent with a p-wave model, which is also supported by the specific heat data.

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SEMI

Profiling defect and charge carrier density in the SiO_2/4H-SiC interface with Low-Energy Muons

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Silicon carbide (4H-SiC) is a wide-bandgap semiconductor with promising applications in high-power and high-frequency devices. An advantage of SiC is that it is the only compound semiconductor that has the ability to form native silicon dioxide (SiO_2). The performance of SiC-based devices relies heavily on interface effects. However, characterization of oxidation-induced defects - both in the oxide and the semiconductor - is still challenging.

Low-energy muon spin spectroscopy (LE-μSR) can probe regions very close to the surface and interface up to a depth of 160 nm in SiO_2/SiC structures and is sensitive to charge carrier and defect concentrations.

We have studied SiO_2/SiC interfacial systems with thermally grown and deposited oxides using LE-μSR. The thermal SiO_2 has higher structural order, as indicated by the undisturbed muonium (Mu^0) formation. However, the oxidation process leads to strain in the oxide and to band-bending at the SiC-side of the interface, which affects the SiC faces differently: i) at the (0001) Si-face the results can be explained by the depletion of electrons at the interface and ii) at the $(000\overline{1})$ C-face a carbon-rich n-type region contributes to the increase of the diamagnetic fraction due to Mu^- formation.

Further investigations have been conducted to understand the passivation effects of state-of-the-art post-oxidation annealing (POA) processes on the SiO_2/SiC interface. Particularly, POA in an NO environment leads to an increase in charge carrier concentration near the interface, likely due to N acting as a dopant, which can be quantified based on the measured diamagnetic fraction.

Operando muSR experiment on nano-cystal growing of the Fe-based magnetic material FINEMET(R) under external fields

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In recent years, there have been increasing opportunities to consider about energy issues on a global scale, and the development of energy-saving technologies in various fields is highly desired. It is known that Fe-Cu-Nb-Si-B nanocrystalline alloy, so-called FINEMET(R), have higher magnetic flux density, higher linearity, and higher temperature stability than conventional materials. Nano-crystals of FINEMET is grown by heat treatment of Fe-based amorphous alloys, showing different B—H curves for various conditions of the magnetic field application during the heat treatment. However, the nanocrystallization process during heat treatment under magnetic fields has not been fully understood. To investigate elementary processes such as grain growth of nanocrystals, we have performed operando muon spin rotation experiments. It was reported that a remarkable time variation in crystal growing under several magnetic fields is seen [M. Ohta ¥it et al., JPS Conf. Proc. ¥bf 33, 011053 (2021)]. Recently, more detailed analysis of time spectra with varying temperatures in the magnetic field has revealed the emergence of two distinct phases around the nanocrystal nucleation temperature. It is discussed how these two phases are related to nanocrystal nucleation and grain growth, also using the other technique such as transmission electron microscope (TEM) measurements and theoretical calculations.

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Development of monitoring system for the muon rotating target using an infrared camera

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It is important to measure the temperature of the muon-production rotating target (hereinaf-ter referred to as "rotating target") in order to detect problems of rotating target quickly.

Thermocouples have been installed on the cooling jacket to measure the temperature rise due to thermal radiation from the rotating tar-get. Since the time constant of the thermocou-ples is on the order of minutes, it is not possible to stop the accelerator quickly in case of a sig-nificant temperature rise. In order to construct a rapid temperature detection system for rotating targets, we have installed an infrared camera.

We successfully measured temperature distribution of the rotating target during the 1-MW operation observed by the infrared camera.

Enhancement of strong coupling s-wave superconductivity in the vicinity of a quantum critical point in $(Ca,Sr)_3Rh_4Sn_{13}$

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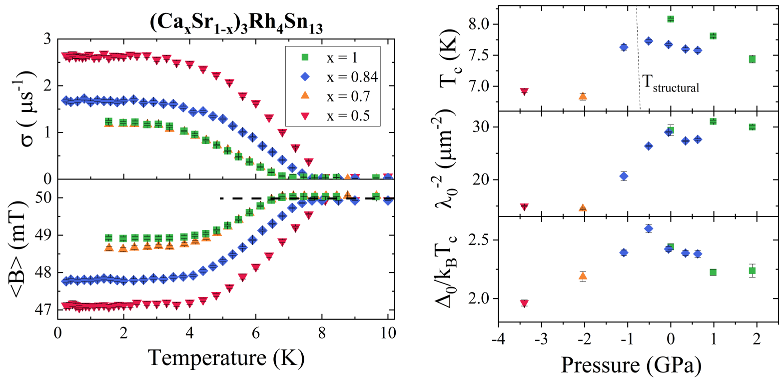

Figure 1: (a) Depolarization rate and center field as a function of temperature at ambient pressure for different chemical compositions. (b) Superconducting state parameters as a function of combined chemical and hydrostatic pressure.

We report muon spin rotation (μSR) studies of the superconducting properties as a function of chemical and hydrostatic pressure on the cubic ternary intermetallic $(Ca_xSr_{1-x})_3Rh_4Sn_{13}$ compounds, which feature strong coupling phonon-mediated BCS superconductivity and a structural phase transition a critical pressure p_c associated with a charge density wave (CDW) formation [1]. A strong enhancement of the superfluid density and a pronounced maximum in the pairing strength provide evidence of a quantum critial point at p_c, which separates a superconducting phase coexisting with CDW from a pure superconducting phase. In both phases superconductivity has a phonon-mediated BCS s-wave character. Together with the related isoelectronic compound $Ca_3Ir_4Sn_{13}$ [2], this system shows that conventional BCS superconductors in the presence of competing orders may display behavior and characteristics of unconventional superconductors.

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P

SCE

Using uniaxial stress to probe the relationship between competing superconducting states in a cuprate with spin-stripe order

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Cuprate high-temperature superconductors have complex phase diagrams with multiple competing ordered phases. Understanding to which degree charge, spin, and superconducting orders compete or coexist is paramount for elucidating the microscopic pairing mechanism in the cuprate HTSs. In this talk, I will report some novel results of muon-spin rotation (μSR) and AC susceptibility experiments on uniaxial stress effect on the static spin-stripe order and superconductivity in the La214 cuprates [1].

We find that in the cuprate system $La_{2-x}Ba_xCuO_4$ with x = 0.115, an extremely low uniaxial stress of 0.05 GPa induces a substantial decrease in the magnetic volume fraction and a dramatic rise in the onset of 3D superconductivity, from 10 to 32 K; however, the onset of at-least-2D superconductivity is much less sensitive to stress [1] (see Figure 1a and b). These results show not only that large-volume-fraction spin-stripe order is anti-correlated with 3D superconducting (SC) coherence, but also that these states are energetically very finely balanced. Moreover, the onset temperatures of 3D superconductivity and spin-stripe order are very similar in the large stress regime. These results strongly suggest a similar pairing mechanism for spin-stripe order, the spatially-modulated 2D and uniform 3D SC orders, imposing an important constraint on theoretical models.

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Tuesday Session

Indico ID	Prog. code	Title	Presenter
105	P-TUE-1	The internal magnetic field in a ferromagnetic compound $Y_2Co_{12}P_7$	Kazuki Ohishi
110	P-TUE-2	Reinventing the Muon Decay Channel	Sydney Kreitzman
133	P-TUE-3	Negative muon spin rotation and relaxation study on Li metal	Jun Sugiyama
135	P-TUE-4	Magnetic dopants and spin-density waves: the $SmFe_{1-x}Mn_xAsO$ case	T. Shiroka
151	P-TUE-5	Development and test of a TDC and amplifier circuit for a multi-channel positron detector (also Student Day presentation)	Marta-Villa de Toro Sanchez
154	P-TUE-6	Tracking Decay Positrons in a Magnetic Field for Muon Microscope Applications	Kenji Kojima
159	P-TUE-7	µSR studies of dynamics in model biomembranes	Iain McKenzie
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247	P-TUE-33	A µSR investigation of the influence of inter-site impurities on quantum spin liquids.	Fabian Hotz
248	P-TUE-34	The new muSR instrument FLAME at PSI	Hubertus Luetkens
249	P-TUE-35	An updated model for muonium in 6H-SiC	Rick (P.W.) Mengyan
250	P-TUE-36	Thin Film and Surface Preparation Chamber for the Low Energy Muons Spectrometer	Zaher Salman
255	P-TUE-37	Superconductivity in $TiSe_2$ Under Hydrostatic Pressure	Frank Elson

Indico ID	Prog. code	Title	Presenter
258	P-TUE-38	Analysis of Positively Charged Muonium and its Diffusion in Cadmium Oxide	Samuel Cathcart
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260	P-TUE-40	The Ultra-Slow Muon beamline at J-PARC: the present status and future prospects	Sohtaro Kanda
302	P-TUE-41	Inducing Quantum Criticality in $CrCl_3$ Under Pressure (also Student Day presentation)	Yuqing Ge
313	P-TUE-42	Progress on the surface muon beamline S-Line at J-PARC MUSE	Akihiro Koda
323	P-TUE-43	Photophysical dynamics in $(CH_3NH_3)PbX_3$ (X=Br, Cl) single crystal perovskites studied by Muon-Spin Spectroscopy	Yasmine Sassa
347	P-TUE-44	Muon Sites in Hexagonal Ice	Amba Datt Pant
307	P-TUE-45	Shallow Muonium radical in κ-Ga_2O_3 thin films	Roberto De Renzi

P

SCE

The internal magnetic field in a ferromagnetic compound $Y_2Co_{12}P_7$

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Various μ^+SR techniques have been widely used for studying internal magnetic fields in assorted materials [1], such as, antiferromagnets, spin-glasses, paramagnets, and superconductors. However, for ferromagnetic (FM) materials, μ^+SR faces a difficulty in determining the correct dipole field at the muon site $(\boldsymbol{H}_{\rm dip})$ because the internal magnetic field at the muon site in ferromagnets is expressed by; $\boldsymbol{H}_\mu = \boldsymbol{H}_{\rm dip} + \boldsymbol{H}_{\rm L} + \boldsymbol{H}_{\rm hf}$, where $\boldsymbol{H}_{\rm L}$ is the Lorentz field and $\boldsymbol{H}_{\rm hf}$ is the hyperfine field at the muon site. Therefore, the muon sites and the magnetic structure need to be apprehended for evaluating $\boldsymbol{H}_{\rm dip}$ but also the saturation magnetization for evaluating $\boldsymbol{H}_{\rm L}$ and the local spin density at the muon site for evaluating $\boldsymbol{H}_{\rm hf}$.

Considering the three contributions to $\boldsymbol{H}_\mu$ in the above equation, a combined work with μ^+SR and DFT calculations are needed to provide a reasonable estimate for the ordered magnetic moment of rare earth (R) ions in $\rm Nd_2Fe_{14}B$ and related magnets [2]. Following upon this work, we attempt to estimate the ordered magnetic moments of R ions in cobalt-based FM materials, $R_2\rm Co_{12}P_7$ with such combined work. As a first step, a powder sample of $R_2\rm Co_{12}P_7$ with $R = \rm Y$ was measured with μ^+SR and three clear muon spin precession signals below its Curie temperature ($T_{\rm C} = 151$ K) were found.

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Reinventing the Muon Decay Channel

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This work describes the new M9H muon decay channel at TRIUMF, which is specifically designed to deliver high quality transversely spin polarized beams. Transverse polarizations in both X and Y of 80% over the momentum range 70-120MeV/c are expected. In contrast to a traditional z-polarized decay beam the key to accomplishing this task lies in the extraction an off-centre momentum-canted distribution of muons exiting the decay solenoid. We describe both the theoretical and practical considerations that have informed the design.

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Negative muon spin rotation and relaxation study on Li metal

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During the μ^-SR measurements on Li-ion battery materials, a part of implanted μ^- is naturally captured by Li nucleus, leading to the formation of muonic-Li species in target materials. The past μ^-SR study on Li metal shows the lack of relaxation in the TF-μ^-SR spectrum at room temperature [1], despite the presence of large nuclear magnetic fields at the muonic-Li position from the surrounding Li nuclei. Such phenomenon was explained by diffusion of a He-like muonic-Li in Li metal. On the other hand, the He diffusion in solids is reported as a thermally activated process based on a thermochronometry gas analysis [2]. Therefore, the TF relaxation rate in Li is expected to increase with decreasing temperature, as the muonic-Li diffusion is suppressed at low temperatures.

Nevertheless, the μ^-SR experiment on both natural Li and ^{6}Li indicates the absence of detectable TF relaxation rates even at the lowest temperature measured. This clearly excludes the scenario that the muonic-Li start to diffuse at a certain temperature below 300 K. Although the mechanism on such a zero TF relaxation rate is not fully understood, we could ignore the contribution from the muonic-Li on the asymmetry μ^-SR spectrum for the Li-ion battery materials.

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Magnetic dopants and spin-density waves: the $SmFe_{1-x}Mn_xAsO$ case

P

SCE

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Electronic correlations play a key role in tuning the properties of parent- and doped (superconducting) iron pnictides, ultimately determining their respective ground states. Parent compounds with magnetic doping are particularly intriguing, since dopant coupling via Ruderman-Kittel-Kasuya-Yosida (RKKY) interactions depends significantly on the strength of electronic correlations, which interact with the underlying SDW phase.

Here, we address the interesting case of Fe-to-Mn substitution in the SmFeAsO parent compound [1] through comparative studies of $SmFe_{1-x}Mn_xAsO$, with x(Mn) = 0.05 and 0.10, via dc-magnetization, Hall-effect, and muon-spin spectroscopy measurements. Our main experimental findings are: (i) the Fe-to-Mn substitution weakens the commensurate spin-density wave (SDW) order of iron, whose transition temperature decreases with increasing Mn content. (ii) At low temperature, well inside the SDW ordered phase, an additional magnetic order sets in at $T^* \sim 10$ K and 20 K, for x = 0.05 and 0.10, respectively. We demonstrate that diluted Mn ions can pin the electronic charges and thus induce a radical reconstruction of the Fermi surface, in turn responsible for a commensurate-to-incommensurate antiferromagnetic (AF) transition at T^*.

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Development and test of a TDC and amplifier circuit for a multi-channel positron detector.

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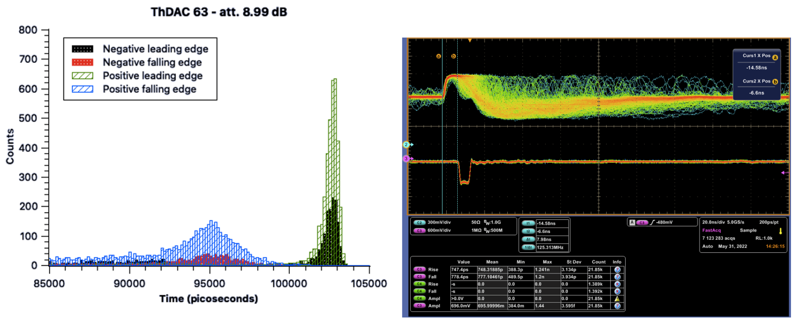

Figure 1

In a continuous beam muon facility positrons are detected by relatively large plastic scintillators without position sensitivity. An idea has been proposed to make these positron detectors multi-channel and able to track the positron trajectories. This will ultimately enable 2-dimensional magnetic imaging of the sample with the µSR technique. To attain this “muon microscope” idea, large numbers of independent photosensors with high-timing resolution will be necessary.

Our group at KEK has developed an amplifier-shaper-discriminator (ASD) circuit named FGATI with 16 channels per chip and a high-resolution time to digital converter, called HR-TDC with a timing resolution on the order of picoseconds. Silicon photomultipliers (SiPMs) from Hamamatsu (MPPC) are employed to give electric pulses for the optical input [1-2]. We have been testing this new set-up at TRIUMF with a pulsed laser to understand the efficiency, transient response, timing resolution, and the data acquisition to a computer. We are now successfully detecting the rising and falling edge timing as well as the time-over-threshold (TOT) of the laser pulses.

The tested circuit will be a basis for the light detection and time recording from scintillation fiber arrays to be used for the multi-channel positron detectors. Multiple layers of such detectors will establish tracking the positron trajectory and aid with the development of the “muon microscope”.

This work is partially supported by a Grant-in-Aid for Scientific Research (No.JP21H04666) from Japan Society for the Promotion of Science (JSPS).

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Tracking Decay Positrons in a Magnetic Field for Muon Microscope Applications

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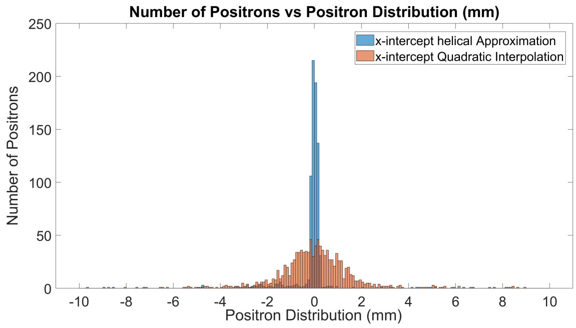

Figure 1: Comparison of the tracked back position for the positron sources at (0,0) in the helical approximation and quadratic approximation

We present a theoretical calculation for feasibility study of the Muon Microscope, which is intended to add positional resolutions within the sample by tracking down the positron trajectories to its source positions. In the presence of a magnetic field, any positrons whose trajectories have components which are perpendicular to the magnetic field will start to move in a helical path due to the Lorentz force. Taking special relativity into account, we have analytically determined the trajectories of the positrons in a uniform magnetic field. This solution serves as a guiding principle before going to a more realistic case, such as the distribution of the magnetic fields and positron scattering from the cryostat walls.

For the first step of the G4beamline simulation, we placed three virtual detectors (meaning they do not interact with the positrons) in the up stream direction at z=100, 150 and 200 mm from the sample respectively. When we apply a uniform magnetic field of 0.3 Tesla in the z-direction, the helical tracking analysis reproduces the source position with the accuracy of 0.3 mm in Full Width Half Maximum (FWHM). It is considerably more accurate than the quadratic interpolation method (FWHM=2.4 mm) as shown in Fig. 1.

Inclusion of the positron scattering from the cryostat wall and the inhomogeneity of the magnetic field will reduce the spatial resolution, and we will discuss them quantitatively from our G4simulation results from the realistic settings.

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MC

μSR studies of dynamics in model biomembranes

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Avoided level crossing muon spin resonance (ALC-μSR) has been used to study the dynamics of the alkyl chains and cholesterol within model biomembranes composed of phospholipids (DPPC and POPC) and cholesterol. ALC-μSR is sensitive to motions on timescales between that measurable by NMR and neutron scattering. Muonium adds to the unsaturated C=C bonds of POPC and cholesterol to give in situ spin probes. The muon and methylene proton hyperfine coupling constants (hfccs) were determined from the Δ_1 and Δ_0 resonance fields in the ALC-μSR spectra. The dipolar muon hfccs ($D_\mu^\parallel$) and the electron spin flip rates were determined by modelling the Δ_1 and Δ_0 resonance lineshapes using Monte Carlo simulations. These parameters provide information about the motion of the spin probes in the alkyl chains. In all cases, the spin probes are undergoing restricted reorientational motion, but the addition of cholesterol leads to more restricted motion of the alkyl chains, evident from the larger $D_\mu^\parallel$, and tighter packing of the chains, which is deduced from the magnitude of the muon hfccs. The goal of this project is to determine how the dynamics at different positions within the biomembrane depend on the composition.

Calculating muon sites and couplings from a high-throughput modelling perspective

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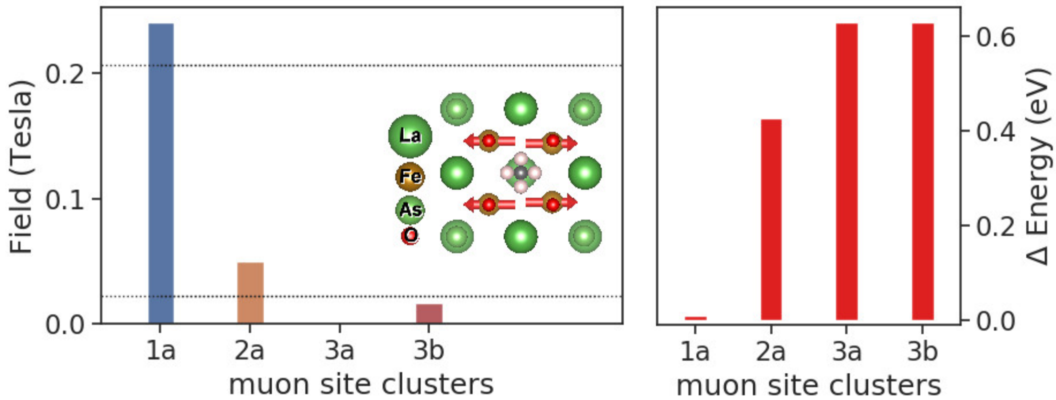

Figure 1: Typical workflow results: In this case for LaFeAsO [2]

In muon spin spectroscopy, the knowledge of muon implantation sites and hyperfine couplings is of importance to the analysis of the experimental data. Over the past decade there has been significant progress in calculating muon sites using first-principles methods such as density functional theory (DFT) [1,2]. However, the protocols required for muon calculations are both resource and task intensive. They are performed sequentially in steps with strenuous human intervention required to track, coordinate and analyse these calculations. The recent advent of the DFT-based high-throughput (HT) approach and the development of dedicated frameworks has opened the possibility of performing this type of sequential large-scale calculations in an efficient way. Here, we present our efforts towards the design and implementation of workflows within the AiiDA integrated platform for high-throughput DFT-based muon calculations aimed at i) the design of a user-friendly approach available to every muon user; ii) benchmarking the scope of sustainable DFT calculations. We started from identifying material selection criteria to exclude the well-known harder cases. We have benchmarked the workflow at its current stage over 16 magnetic compounds. Our preliminary benchmark results demonstrated the feasibility of this plan and have further allowed us to understand the workflow capabilities, its limitations and the likely improvements to be considered for more accurate results of the calculated muon properties. These improvements include; taking into account the muon charge states and spotting the right compromise between sustainable and accurate treatment of electronic correlation effects.

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Metal State with Spontaneously Broken Time-Reversal Symmetry above the Superconducting Phase Transition

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Fundamentally, what distinguishes a superconducting state from a normal state is a spontaneously broken symmetry corresponding to the long-range coherence of Cooper pairs, leading to zero resistivity and diamagnetism.

Here we report a set of thermodynamic, transport and muon spectroscopy observations on a series of hole-doped $Ba_{1-x}K_xFe_2As_2$. Our specific-heat measurements indicate the formation of fermionic bound states when the temperature is lowered from the normal state. However, at the doping level $x \approx 0.8$, instead of the characteristic onset of diamagnetic screening and zero resistance expected below a superconducting phase transition (T_c), we observe the opposite effect: the generation of self-induced magnetic fields in the resistive state, measured by spontaneous Nernst effect [1] and muon spin rotation experiments [2,3] (see Fig.1). This combined evidence indicates the existence of a bosonic metal state in the temperature range $T_c \leq T \leq T_{Z2}$ in which Cooper pairs of electrons lack coherence, but the system spontaneously breaks time-reversal symmetry (Z2). The observations are consistent with the theory of a state with fermionic quadrupling, in which long-range order exists not between Cooper pairs but only between*pairs of pairs*.

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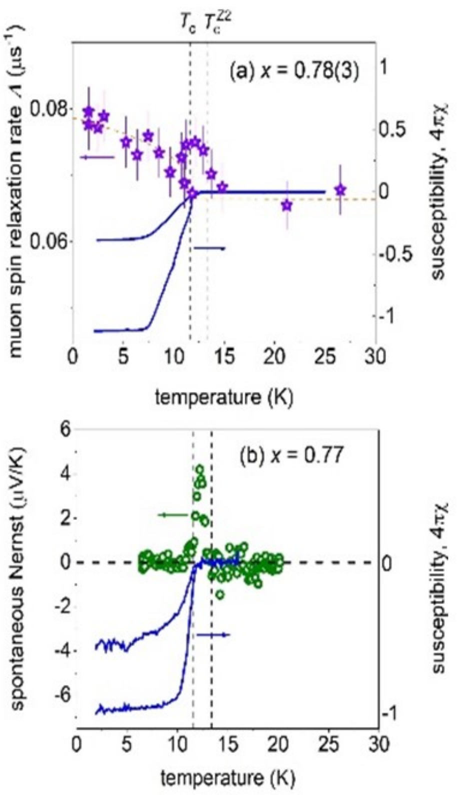

Figure 1: (Top panel) Temperature dependence of the zero-field muon spin relaxation rate (left) and the magnetic susceptibility measured in $B \parallel ab = 0.5$ mT (right) for the stack of single crystals with x = 0.78(3) [3]. (Bottom panel) Temperature dependence of the spontaneous Nernst effect (left) and the magnetic susceptibility measured in $B \parallel ab = 0.5$ mT (right) for a sample with $x = 0.77$. The comparison suggests that the origin of the spontaneous Nernst effect at T_{Z2} is the appearance of spontaneous magnetic fields.

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Inverse Laplace Transform Approaches to βNMR Relaxation

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Spin lattice relaxation is the simplest type of βNMR measurement. The usual approach is to implant a pulse of hyperpolarized nuclei and monitor the time-resolved β-decay asymmetry, yielding the ensemble average spin-lattice relaxation. In the simplest case, the asymmetry decays exponentially with a characteristic time constant T_1, but this ideal is rarely obtained in practice. In most data, the relaxation is more complicated. This can be the result of multiple crystallographic sites for the implanted probe each having a distinct T_1. The sample may also be inhomogeneous due to: impurities or defects (including interfaces important for thin films); intrinsic phase separation; or, if it is a glass. There may also be a background signal from probe ions that stop outside the sample. The general approach to this problem has been the*ad hoc* development of an appropriate relaxation model that avoids overparametrization.

Given the prevalence of more complicated relaxation, it is crucial to develop a*systematic* approach to relaxation modelling. The decomposition of a relaxing signal into exponentials is, however, a mathematically ill-posed problem[1]. This feature is intrinsic and unavoidable, but there are a number of methods to accommodate it for noisy real-world data, including nuclear spin relaxation [2].

Here we demonstrate regularization methods for the inverse Laplace transform adapted to the particularities of βNMR relaxation data, most importantly the strong time dependence of the statistical uncertainty stemming from the radioactive lifetime of the probe.

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Intense Lyman-alpha light source for ultra-slow muon generation

P

NT

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Reduction of the momentum width in the muon beam is required in particle physics and material science. A small-momentum-width muon beam so called ultra-slow muon beam can be realized by laser ionization of muonium which can be produced by stopping of surface muons in a solid target and thermally diffusing them. Such an ultra-slow muon generation technique reduces the momentum width to about 100 meV. The application of this ultra-slow muon beam to μSR measurement will enable to measuring of the physical properties from the surface to the interface of materials more clearly with extremely high depth resolution. In order to efficiently generate ultra-slow muons, two coherent lights are required: the so called Lyman-alpha light, which resonantly excites muonium from the ground state to 2p, and the 355 nm light, which ionizes excited muonium to the unbound state. In particular, the generation of intense Lyman-alpha coherent light for resonant excitation is a challenging task in laser technology because the wavelength of the Lyman-alpha light is in vacuum ultraviolet. At J-PARC MLF the Ultra-Slow Muon beamline, we have successfully generated muonium resonant Lyman-alpha coherent light exceeding 10 μJ using an all-solid-state laser and high-efficiency vacuum ultraviolet light generation technologies, and we have applied the Lyman-alpha light to the generation of ultra-slow muons. In this presentation, we will describe the current status of our intense Lyman-alpha light source, and future upgrade of the light source will be presented.

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SU

LE-muSR Study of the Meissner state. New Results on an Old Problem.

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The Meissner state (MS) is the state with the most pronounced superconducting properties. Therefore, knowledge and understanding properties of the MS is a necessary condition to understand and predict properties of all other states of all superconductors. The standard interpretation of the MS is based on the theory of F. and H. London, with minor modifications adopted in the Ginzburg-Landau and Bardeen-Cooper-Schrieffer theories. Londons' theory rests on three postulates: (i) the magnetic permeability μ and dielectric permittivity ε are equal to unity; (ii) the induction B and, consequently, the intensity $H(= B/\mu)$ of the magnetic field is zero; and (iii) the penetration depth λ is independent of the applied field H_0. Quite long-ago, using thermodynamic considerations, H. London showed that λ must depend on H_0. The first application of Pippard's microwave resonator technique was to verify this statement. Pippard found a weak increase of λ vs H_0 nonmonotonically changing with temperature, and concluded that λ can be viewed as independent of H_0. This result was (and still is) regarded as a confirmation of the London theory (F. London, 1950). However, the standard diagram of the Abrikosov vortices suggests that λ strongly decreases with the field. Soon after Pippard's experiment, Shoenberg noted that Londons' theory conflicts with the law of energy conservation. Besides, Londons' postulate $\mu = \varepsilon = 1$ implies that the electromagnetic properties of superconductors are identical to those of vacuum. To sort out with these and other fundamental issues in the MS interpretation, we launched the LE-μSR project aimed at measuring the field dependence of the induction profile near the surface of high-quality type-I and type-II superconductors in the MS. The entire profile (from $B = H_0$ to zero) was measured for the first time. The results obtained to date and the challenges we are encountering in this investigation will be reported.

^{8}Li Spin Relaxation as a Probe of the Modification of Molecular Dynamics by Inelastic Deformation of Glassy Polystyrene

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MC

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Glasses occupy more volume than required for molecular close packing. The distribution of this “free volume” is related to other key properties such as dynamic heterogeneity (stretched exponential relaxation). As a glass ages, it equilibrates by thermally activated structural relaxation producing permanent densification with slowed relaxation times. Mechanical deformation can significantly alter glassy structure and relaxation, leading to apparent over-aging or rejuvenation via irreversible plastic shear flow that explores microscopic configurations that are otherwise inaccessible[1].

Nanoimprint[2] is a technique that deforms thin polymer films by indentation of a patterned die for lithographic patterning and measuring mechanical properties. Few techniques are capable of studying local properties of polymer films, however the spin-lattice relaxation of implanted ^{8}Li^{+} is sensitive to the molecular dynamics in the glassy state, including modification by processing parameters[3]

We report initial results on a 300 nm thick atactic polystyrene film plastically modified by nanoimprint stamping[4] using a 1 mm ultra-smooth spherical die. While the beam can easily be stopped in the film, the beamspot is ~ 2 mm in diameter, so a large array of imprints was produced over an area ~ 3 mm^2, leaving an inelastic strain of a few tenths of a percent over an areal fraction ~ 20

To ensure the beam overlapped the imprinted area, a new method was developed. Using scintillation from an Al_2O_3 crystal, the beamspot image was fit with a Gaussian profile. Partially automation allowed the overlap to be maximized in real time. We find a small but significant change in the bulk of the film (away from the surface), compared to an unimprinted control, the relaxation is slower and more inhomogeneous (lower stretching exponent).

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Small Sample Measurements at the Low Energy Muon Facility of PSI

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with
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The low energy μSR (LE-μSR) spectroscopy is primarily used to study thin films, surfaces, and interfaces of materials. However, because of the large beam spot and low implanted muons rate, LE-μSR measurements on small samples are difficult, requiring an optimal sample area of 25×25 mm^2. Recently, we have boosted our ability to measure small samples, down to 5×5 mm^2 area by beam collimation and tuning. This advance is crucial for measurements of many magnetic and superconducting samples. Furthermore, we have devised a method that allows us to measure five small area samples mounted together on the same sample plate. We expect this method to further improve the efficient use of beam at LEM.

A muon-spin relaxation study of type-I rhenium investigating time-reversal symmetry breaking in the superconducting state

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SU

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with
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Time-reversal symmetry breaking is a signature of unconventional superconductivity and can be observed from zero-field muon spin relaxation measurements as an increase of the muon relaxation rate through the superconducting transition temperature. Time-reversal symmetry breaking, although rare, has been observed in several noncentrosymmetric rhenium-based intermetallic superconductors [1].

Recent results indicate that elemental rhenium powder, exhibiting type-II superconductivity with a transition temperature of 2.7 K, also breaks time-reversal symmetry [2]. This suggests that the local electronic structure of rhenium may be intrinsically linked to the unconventional superconductivity in the rhenium-based materials. However, removing internal strain from the rhenium by melting or annealing reduces the transition temperature to 1.7 K and leads to type-I superconductivity.

In the present study, we have investigated the superconductivity in type-I rhenium using zero-field muon-spin relaxation measurements [3]. No unconventional behaviour is observed, and time-reversal symmetry is preserved in the superconducting state. Instead of the muons remaining stationary over their lifetime, we observe muon diffusion across the full temperature range studied, with muons quantum-mechanically hopping between interstitial sites. The hopping rate exhibits metallic behaviour in the normal state. In the superconducting state, the behaviour can be described qualitatively by including the presence of the superconducting energy gap and energy asymmetries between muon sites from crystallographic defects.

These results call into question the role the electronic structure of rhenium plays in the breaking of time-reversal symmetry in rhenium-based intermetallic superconductors and demonstrates that the behaviour of muon spectroscopy data can be governed by muon diffusion effects.

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The Muon Spectroscopy Computational Project

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This poster presents an overview of the software tools and techniques that have been developed as part of the Muon Spectroscopy Computational Project (MSCP). The MSCP is an initiative that currently includes: (a) the Muon Group at ISIS; (b) the Scientific Computing Department; (c) the UK Software Sustainably Institute and (d) Members of the [Galaxy][1] platform. The main objective of the MSCP is to support users of muon sources via the development of a sustainable and user-friendly set of software tools and a software platform that can be used for interpreting muon experiments.

Currently, the MSCP has developed and is maintaining the following software tools:

- **pymuon-suite**: a Python library that can be used to estimate potential stopping sites for the mu+ and the muonium.
- **pm-nq**: can be used to estimate the quantum effects on the muon in accordance with the harmonic approximation.
- **muspinsim**: used for studying the spin dynamics of a system of a muon and other spins. You can simulate LF, ZF, TF and ALC experiments. One of the important features of this tool is that it can be run in parallel and it can also be used for fitting experimental results.
- **Mudirac**: can be used for the prediction of frequencies and probabilities of transition between energy levels of muonic atoms.

These tools can be easily downloaded and installed and, as they have been designed in modular way, they can be combined to tackle different problems related to muon science.

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Development of non-destructive and depth-selective quantification method of sub-percent carbon contents in steel by negative muon lifetime measurement

CT

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When a negatively charged muon stops in a material, the muon makes muon atomic orbitals around an atomic nucleus in the material. The muon orbiting its 1s orbital is absorbed into the nucleus with a mean lifetime depending on the atomic number of the nucleus (Z). This no-electron-emission process competes with the natural decay of the muon into an electron with a lifetime of 2.2 µs. The nuclear absorption rate becomes faster as Z increases. The apparent lifetime of the muons gets shorter with Z; e. g. 2.0 µs in carbon and 0.20 µs in iron. It is possible to identify the element that captured a muon by measuring the lifetime. A compound's elemental composition can be non-destructively determined by measuring the electron lifetime spectrum. We have conducted a feasibility study on the non-destructive identification of carbon contents in steel (iron-containing carbon).

The muon experiment was conducted at the D1 area of the Muon Science Establishment in the Japan Proton Accelerator Research Complex (J-PARC MUSE). The decay electrons were measured by the large-solid angle plastic scintillation counter system Kalliope for µSR. Standard steel samples with known carbon content were used for obtaining a calibration curve. A stacked steel sample consisting of three steel plates with carbon contents of 0.51%, 0.20% and 1.03% of 0.5 mm in thickness was irradiated by three different muon beam momenta to stop muons in the middle of each layer.

The lifetime spectrum was fitted by four components; iron, carbon, air (N, O and Ar) and a long-lifetime background. The carbon contents in the stacked sample determined by the lifetime spectra agreed well with the known carbon contents in each steel layer. In summary, we successfully demonstrated the non-destructive and depth-selective determination of sub-percent carbon contents in steel by muon lifetime measurement.

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SEMI

Investigation of doping and dopant dependence of n-type 4H-SiC with low-energy muon spin spectroscopy

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with
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Silicon carbide (4H-SiC) is a wide-bandgap semiconductor with applications in high power devices. Epitaxial growth of SiC is crucial to produce structures with controlled thickness and doping concentration. Ion implantation with nitrogen (N) and phosphorus (P), on the other hand, is used to create spatially defined n-type regions in SiC. Implantation is usually followed by a post-implantation annealing step, to ensure lattice recovery and electrical activation of the donors. However, mitigating implantation-induced defects remains a challenge.

The narrow defective regions (200-300 nm) are not accessible by conventional techniques, but can be studied with low-energy muon-spin spectroscopy (LE-μSR). The LE-μSR experiments were performed at the low-energy muon facility at the SμS (PSI, Switzerland). The 4H-SiC samples were either doped with N during epitaxial growth ($N_D = 4\times10^{15}$ and 1×10^{17} cm^{-3}) or using ion-implantation of N and P ($N_D = 1\times10^{17}$ and 1×10^{18} cm^{-3}). The goal was to compare the different doping processes and to establish a μSR baseline for different doping concentrations in n-type SiC.

We find that an effective electron concentration (n) of 4×10^{15} cm^{-3} in SiC is below the sensitivity limit of LE-μSR. For $N_D >1\times10^{17}$ cm^{-3}, there is an intermediate space charge region where muonium (Mu^0) formation dominates and the diamagnetic fraction (F_D) decreases. In the deeper probed region, F_D increases with doping concentration due to Mu^- formation. F_D also increases between 10 and 0.5 mT indicating delayed Mu^- formation, having a Mu^0 precursor state. For the implanted samples, 10 K measurements indicate higher defect density for 1×10^{18} cm^{-3}, which can be related to the higher implantation dose.

Furthermore, Monte Carlo simulations were used to generate muon decay histograms for different electron capture rates, to determine F_D and the phase of the diamagnetic signal as function of*n*, which agree with the experimental results. This means, that*n* can be determined for a SiC sample with unknown carrier concentration by comparing the experimental results of F_D and the phase with the results of the simulation.

Local electronic structure of dilute hydrogen in gallium oxide

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SEMI

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Gallium oxide β-Ga_2O_3 is currently drawing much attention as a material for high-voltage power devices because of its large band gap (E_g ∼4.9 eV). We investigated the electronic structures of muon as a pseudo-hydrogen in β-Ga_2O_3 in which the dilute hydrogen is under the central focus as a crucial factor for the bulk conducting properties. We demonstrate by μSR study combined with the first principles calculations that muons in β-Ga_2O_3 have two electronic structures: a state corresponding to hydrogen that acts as an electron donor (Mu_1), bounded to three-coordinated oxygen, and a hydride-like state in rapid motion (Mu_2). Furthermore, we imply from the Hall effect measurements that the fractional yield of Mu_2 exhibits a close link with the mobility and density of the carriers (electrons).

In the presentation, we will compare our results with those of previous study and discuss the electronic structures of Mu_1 and Mu_2 in terms of our recently proposed ambipolar model of muon in oxides.

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X

Negative muons for the characterization of thin layers in Cultural Heritage artefacts

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Muonic X-ray Emission Spectroscopy (µXES) is a novel technique based on the detection of high-energy X-rays emitted after the interaction of a negative muon beam with matter. Thanks to the multi-elemental range, a negligible self-absorption effect of the x-rays and very low residual activity left in the sample after irradiation, the technique has been applied to a wide range of studies, with special attention to cultural heritage artefacts. In addition, the technique offers the possibility to perform depth profile studies. By tuning the energy of the incident muon beam, indeed, it is possible to investigate the different layers that constitute a sample. Here we report preliminary results of the analysis on two fire-gilded surfaces, in which the gold layer was supposed to be around 10 microns. In particular, in this work, the technique is coupled with a Monte Carlo based simulation software. Simulations are a powerful tool for improving the data analysis and the interpretation: for µXES especially, by exploiting a simulation software like SRIM or GEANT4, it is possible to assess the thickness of a given layer. To perform a depth profile characterization, the samples were analysed at different beam energies (or momentum). Each of the resulting x-ray spectra was then analysed and gaussian fitted with a data analysis software. Then, the normalised area values were plotted against the momentum to obtain a profile of the variation of the elements as the penetration depth of the beam increased. The output of the simulations was compared with the experimental data and a remarkably good agreement was reached. The results of the work are promising and with this approach, it will be possible to enhance the capability offered by the technique both in terms of data analysis and data interpretation.

Breaking the barriers in understanding your data: Unbiased model selection for muon spin relaxation spectroscopy

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The analysis of muon spin relaxation experiments typically relies on model fitting under conditions that are ill-posed. Typically models are selected to fit the data based on the inductive bias (physical intuition) of the experimentalist. Although recent studies have demonstrated the application of unsupervised machine learning to automatically detect model changes [https://doi.org/10.1088/1361-648x/abe39e], the use of physical models remains essential for gaining insights into the physics and chemistry of the systems under study. This invites the question - can we use a principled approach, in concert with the inductive bias of experienced researchers to select the best models for fitting a given data set? In this contribution we demonstrate how Bayesian model selection can be applied to select the optimal model from a finite set, for fitting data from a given experiment, avoiding both over- and under-fitting. We use a series of simulated experimental data sets, with different underlying models and levels of noise. We show how comparison of Bayes factors, obtained by integration of Markov Chain Monte Carlo (MCMC) sampling of the parameter space, provides robust and principled comparison of possible models for fitting the data, and also provides parameter estimation with associated uncertainties. The latter can be used to determine the point at which sufficient experimental data have been collected to satisfactorily assign parameters to the underlying model. Finally, we also explore the application of nested sampling [https://doi.org/10.1063/1.1835238], a method of efficiently sampling posterior distributions, which could allow the extension of this scheme of model selection to higher-dimensional models (D>5) while remaining computationally tractable.

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SL

The interaction between positive muons and multiple quadrupolar nuclei

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A positively charged muon implanted in copper sits at an octahedral interstitial site and experiences a magnetic dipolar coupling with six nearest-neighbour quadrupolar $I = 3/2$ copper nuclei [1]. The resulting avoided level crossing resonance observed as a function of magnetic field [2] provides a means of studying these interactions and understanding the effect of the electric-field gradient due to the muon experienced by the quadrupolar nuclei. The effect is usually modelled by considering the interaction between the positive muon and a single copper nucleus, but the other five copper nuclei are equally important. By solving the problem in the full $2(2I+1)^6 = 8192$-dimensional Hilbert space, we demonstrate the effect of these additional interactions.

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Negative muon spin rotation and relaxation study on antiferromagnetic order of Na clusters in sodalite

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P

NT

μ^+SR is used in various research fields as a sensitive local magnetic probe. Although the implanted μ^+ stop at interstitial sites in the crystal, it is often difficult to determine the sites precisely. On the other hand, the implanted μ^- are captured by nuclei and have different lifetimes for each nuclide. Thus, the μ^- position is unambiguously determined by measuring the lifetime. However, the spin polarization of μ^- is reduced down to about 1/6 during the capture process, requiring much higher statistics than μ^+SR. Recent improvements in the beam intensity and detection efficiency of pulsed-muon facilities have made μ^-SR experiments feasible, and such an advanced μ^-SR is used to study ion dynamics in solids.[1] We here report an attempt to investigate magnetic materials with the advanced μ^-SR.

Na_4^{3+} clusters can be arranged in a bcc structure in sodalite crystal. Antiferromagnetic ordering occurs below $T_N = 50$ K due to the exchange interaction between the s-electrons in the arrayed clusters. In ZF-μ^+SR, a homogeneous local field of 92 Oe is observed at low temperatures.[2] Our recent study shows it's due to the Fermi contact at the cage center. In the present μ^-SR, the lifetime analysis shows the signal at the oxygen site is dominant. The initial asymmetry of the time spectra dropped sharply below T_N, but muon spin precession due to a homogeneous local field couldn't be observed. The decoupling by longitudinal field shows the local field of about 0.4 kOe. This value can be explained as the local field of oxygen sites when the spatial distribution of s-electron wave function is approximately incorporated. These results demonstrate the importance to study the magnetic nature of materials with $\mu^{\pm}$SR.

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The mechanism of superconductivity in the controversial spinel oxide $LiTi_2O_4$ clarified with LEμ^+SR

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The very first low-energy muon spin rotation (LE-μ^+SR) study performed on $LiTi_2O_4$ films in the Meissner state is presented. $LiTi_2O_4$ is a unique spinel type superconductor in which the mechanism underlying superconductivity is highly debated**[1]**. LE-μ^+SR is a direct probe for the characterization of depth dependent properties in thin films, which allowed us to extract the London penetration depth ($\lambda_L = 241 \pm 15$ nm) and the temperature dependence of the superconducting order parameter for $LiTi_2O_4$, among other relevant quantities. The order parameter was found to not follow any of the standard models within the realm of the mean field theory. In particular, the value of the critical exponent, close to 1, suggests that the superconductivity in $LiTi_2O_4$ is of unconventional nature. Indeed, by plotting the correlation between the critical temperature Tc and the London penetration depth for $LiTi_2O_4$ in Uemura's scaling relation for doped cuprates, we see that its behavior is close to the one of electron doped cuprates. We concluded that the observed behavior is compatible with a superconductivity of BCS type, with disturbance by Ti3+ spin fluctuations, which introduce a time reversal symmetry breaking perturbation in the system. This measurement gives a robust indication that LTO is a nonconventional SC and sets an important step forward in understanding the controversial nature of superconductivity in this material.

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A simulation study of muon transport in the Ultra-Slow Muon beamline at J-PARC

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The Super-Omega beamline at J-PARC Materials and Life Science Experimental Facility provides an intense pulsed surface muon beam. Combined with a muonium production target and a laser for muonium ionization, the pulsed ultra-slow muon facility has been developed. At the facility, a spectrometer for the muon spin rotation measurements using the ultra-slow muons is under commissioning. In this poster presentation, we will report on the beam optics optimization of surface muon transport and ultra-slow muon extraction to improve the intensity and quality of the ultra-slow muon beam.

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Super-MuSR scientific design: Progress towards a step-change in muon capabilities at ISIS

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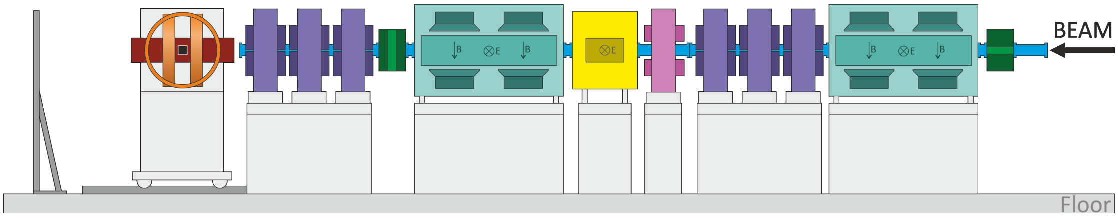

Figure 1: Planned layout of the Super-MuSR beamline and spectrometer

Super-MuSR is a major project to upgrade the MuSR instrument at ISIS that aims to provide an order of magnitude increase in resolution and counting rate in separate modes of operation. This now forms an early part of the ISIS-wide Endeavour programme, an estimated £90m investment in new and upgraded instruments, which we are aiming to start in the 23/24 financial year.

Experiments using the current MuSR instrument generally focus on magnetism and superconductivity, particularly those situations where weak relaxation rates are observed. To extend these capabilities a new detector array will increase the data collection rate by more than fifteen times. This will also enable detailed studies of quantum coherent muon states and in-operando diffusion measurements of battery cells. The present instrument is limited in the frequency range it can study by the intrinsic muon pulse width at ISIS. This issue will be overcome using a pulse slicer to remove both ends of the incoming pulse and increase the time resolution approximately ten-fold, albeit reducing the muon flux. Complementing this will be spin rotators to allow transverse field measurements over 0.1T. These will increase the range of magnetic and superconducting samples that can be studied. A new cruciform will permit either fly-past measurements for smaller samples with lower backgrounds or quick changes between cold dilution fridges for high experiment throughput for larger samples as now.

We have now completed the scientific design of the instrument and are now prototyping individual beamline and spectrometer components. Here we report the progress made with the scientific design of the beamline and instrument to realise our scientific goals, with likely performance evidenced through simulations.

Status of negative muon at D-Line

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The D-line of the J-PARC MLF MUSE has a pion decay section, which makes it possible to use decay muons. The superconducting solenoid magnet used in the pion decay section has a large bore and thus produce the world's highest positive and negative muon intensities. Since the D-line is currently the only beamline at MUSE where practical negative muon intensity is available, various user experiments are being conducted using negative muons, especially in nondestructive elemental analysis, negative muon spin relaxation, soft errors in semiconductors, and so on. In addition, the beamline has been commissioned in various ways including beam tuning to meet the requirements of these experiments. In this talk, we will report on the recent progress of upgrading at D-line.

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Low temperature spin dynamics in the $S = 2$ kagome magnet $Fe_4Si_2Sn_7O_{16}$: An AC susceptibility, NMR and µSR study

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Fe4Si2Sn7O16 displays an undistorted kagome lattice of Fe2+ (3d6, S = 2) ions. We present results of DC-pulse-field magnetisation up to 50 T, Nuclear Magnetic Resonance (NMR), AC-susceptibility and muon-spin-resonance (µSR) measurements down to 19 mK on powder sample of Fe4Si2Sn7O16. The magnetization measurement at 2 K excludes the presence of strong Ising anisotropies. In the temperature range of 3 K to 8 K, the maximum in the real part of AC-susceptibility shows frequency-dependent shift and indicates the presence of spin-glass-like behavior. An additional frequency-independent magnetic regime is observed below T = 0.7 K. The transverse-field and zero-field µSR results show the onset of static magnetic correlations below 30 K. Further, below T = 1 K, ZF-relaxation rate remains relatively constant which indicates the presence of persistence spin dynamics down to 19 mK. Based on the longitudinal field decoupling µSR studies, we discuss the coexistence of static and dynamic magnetic correlations below 250 mK. From our combined AC-susceptibility and µSR results, we demonstrate that in Fe4Si2Sn7O16 the dynamic magnetic correlations increase below 250 mK and a possible gapless-spin-liquid behavior is achieved.

Studies of μ^+ Diffusion and Trapping in dilute Fe Alloys by Longitudinal μ^+ Spin Relaxation Technique

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MC

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In the late 1970s and 1980s μ^+spin rotation experiments were performed elaborately to study μ^+ diffusion and trapping in Fe and Fe alloys. In Fe alloys not many experiments were performed, probably because the unavoidable inhomogeneity of the magnetization in ferromagnetic Fe alloys bring about the fast dephasing of spin rotation and may obscure the diffusion and trapping effects. Recently at J-PARC MUSE we have found that the measurement of the longitudinal μ^+spin relaxation time T_L in ferromagnetic Fe alloys is the effective new microscopic technique to study the μ^+ diffusion and trapping in Fe dilute alloys and to investigate how the hydrogen interacts with the principal alloying elements in an attractive or repulsive manner and how the local lattice strain induced by them affect the hydrogen diffusion. We revisit the μ^+SR studies of diffusion and trapping in Fe alloys. We have measured the temperature dependence of the T_L in several dilute Fe alloys containing principal alloying elements such as Ni, Mn, Cr, Ti, Al, Si and interstitial impurities C and O. In some alloys the temperature dependence of $1/T_L$ exhibits the peaks and in some other alloys a hump in a broad temperature region. We have developed the 'two-state' model of ferromagnetic dilute Fe alloys: the trapped state by impurity atom and the freely diffusing state of μ^+. The μ^+SR results are well explained by this model. The peaks are due to the motional narrowing effect where the μ^+-impurity interaction is repulsive and the μ^+ diffuse in the crystal apart from the impurity atoms. The broad hump is due to the trapping and de-trapping of μ^+ by impurities. The 1st principle calculations of hydrogen-impurity interactions, the magnetic moment of the impurity and the local strain induced by the impurity in dilute Fe alloys are compared with the μ^+SR results.

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Present status of J-PARC MUSE

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J-PARC MUSE is responsible for the inter-university user program and the operation, maintenance, and construction of the muon beamlines, namely D-line, S-line, U-line, and H-line, along with the muon source at MLF.

At D-line, which provides the world's most intense pulsed negative and positive muon beams, various scientific studies, including those on industrial applications, archeology, and fundamental physics, have been performed. In FY2021, non-destructive analysis was carried out on samples brought back by Hayabusa2 from the asteroid Ryugu, which are thought to preserve the elemental composition of the solar system in its primordial state.

Stable operations have been achieved in S1 area of S-line for µSR. In addition, a group at Okayama University constructed a new experimental area, S2, in FY2020 for muonium 1s-2s measurement.

U-line, uses electrostatic lenses to focus low-energy muons obtained by laser ionization of thermal muonium to produce energy-variable and high time-resolution ultra-slow pulsed muon beams for various experiments. A muon spin spectrometer for materials science research using the µSR method has been installed in the U1A area, and is being upgraded and upgraded for the start of the inter-university user program. The spectrometer is located on a high-voltage stage and the depth of penetration into the sample can be controlled in the range from sub-keV to 30 keV.

The H line is a high-intensity muon beamline where experiments such as high-statistics fundamental physics experiments and transmission muon microscopy are planned. The first beam observed in the H1 experimental area, the first branch, in January 2022.

At present, the beam commissioning is being carried out in collaboration with several research groups that plan to conduct experiments at the H-line.

Monopole-limited nucleation of magnetism in $Eu_2Ir_2O_7$

P

SCE

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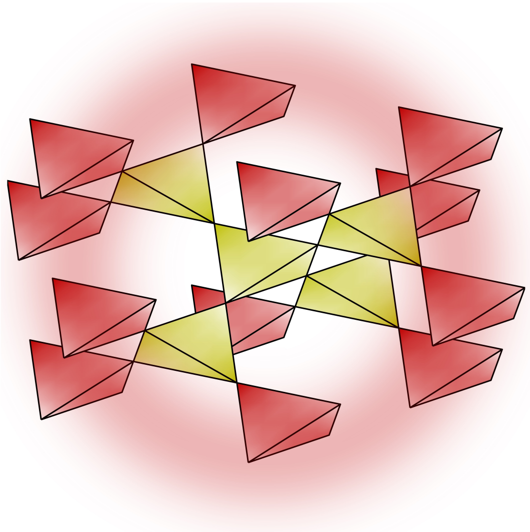

Figure 1: Nucleation of magnetism radiating from topologically non-trivial ordered tetrahedra (yellow) immersed in topologically trivial paramagnetic tetrahedra (red).

The arrangement of magnetic moments at the vertices of a pyrochlore lattice - composed of corner-sharing tetrahedra - leads to a great variety of electronic ground states for $R_2M_2O_7$ materials. Here, we present an in-depth analysis of muon-spin spectroscopy measurements of $Eu_2Ir_2O_7$ under the effect of the $Eu_{1-x}Bi_x$ isovalent and diamagnetic substitution [1] as well as of external pressure [2]. Below T_N, $Eu_2Ir_2O_7$ shows a topologically non-trivial 4-in/4-out order where the Ir^{4+} magnetic moments all point inwards or outwards the tetrahedron they are located at (magnetic hedgehog monopole). Our results evidence an anomalous correlation between the magnetic volume fraction and the order parameter only for stoichiometric $Eu_2Ir_2O_7$, pointing towards highly unconventional properties of the magnetic phase developing therein [3]. We argue that magnetism in $Eu_2Ir_2O_7$ develops based on the nucleation of magnetic droplets at T_N, whose successive growth is limited by the need of a continuous generation of magnetic hedgehog monopoles [3].

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P

EM

Na^{+} self-diffusion in Co-substituted $Na_2Ni_{2-x}Co_xTeO_6$ Na-ion battery cathode material

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with
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$Na_2Ni_2TeO_6$ honeycomb layered oxide has suitable properties for use as a Na-ion battery cathode material. The substitution of Ni with Co has been shown to have a detrimental effect on the energy density of $Na_2Ni_{2-x}Co_xTeO_6$, whereas the plateau potential vs Na^{+}/Na increases. Thus, to ascertain the cause of the electrochemical properties change upon substituting Ni with Co Na-ion self-diffusion properties are investigated with the use of zero field and longitudinal field $^{+}$SR methods in $Na_2Ni_{2-x}Co_xTeO_6$ with x of 0.0, 1.0 and, 1.5. Na-ion site occupancies and crystal structure was determined from neutron powder diffraction measurements and used for the determination of Na-ion jump paths. All measurements were performed in a temperature range from 50 K to 550 K. Three distinct Na-ion sites are determined from the neutron powder diffraction measurements. In addition, two distinct temperature regions for Na-ion self-diffusion, with different Na-ion diffusion pathways, are determined and analysed. The Na-ion diffusional pathway dependence on the substitution of Ni with Co is shown and discussed. Based on the obtained results we propose a cause for the decrease in the capacity, with the simultaneous increase in plateau potential vs Na^{+}/Na, with the increased substitution of Ni with Co. Based on the results, a roadmap on how to further improve $Na_2Ni_{2-x}Co_xTeO_6$-based Na-ion battery cathode materials is given.

A μSR investigation of the influence of inter-site impurities on quantum spin liquids.

P

SL

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with
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Quantum spin liquids (QSLs) represent a state of matter governed by long-range quantum entanglement. These states are stabilized by geometric frustration and remain magnetically disordered even at zero temperature. Of particular interest, are the new exotic fractional excitations with S = ½, so-called spinons. Kagome antiferromagnets are known as one of the most promising systems for the realization of QSLs, and the dynamical spin fluctuations are preserved down to the lowest temperatures. On the other hand, kagome antiferromagnets such as Zn-Brochantite or Zn-Barlowite are polluted by intersite disorder between the copper atoms, with effective spin ½, and the nonmagnetic zinc atoms. Therefore, true observation of QSLs is a formidable task. Nevertheless, sophisticated techniques such as μSR can unambiguously distinguish the slow fluctuations of QSLs from magnetic order or fast paramagnetic fluctuations and thus identify possible QSL candidates. More detailed information is also obtained from muon Knight shift measurements, which directly probe the local magnetic susceptibility, providing information on the gapped nature of the QSL ground states. Moreover, the spinon Kondo effect has been observed in a gapless QSL, in which the magnetic impurities seen by the muons are screened by the surrounding spinons.

P

NT

The new muSR instrument FLAME at PSI

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A. Raselli, A. Stoykov, Paul Scherrer Institut, Switzerland

Here, we report on the status of the setup, commissioning and first performance tests of the newest muSR instrument FLAME (FLexible and Advanced MuSR Environment) at PSI. Commissioning started in spring 2022 after the delivery of the superconducting experimental magnet.

FLAME is designed to allow ZF, LF and TF muSR measurements over a broad temperature range from 25mK to 300K with magnetic fields from true zero field up to 3.5T with high spatial homogeneity and temporal stability.

Due to its forward and backward veto system, it should be possible to study small samples with practically no background.

We anticipate a time resolution of approximately 150ps due to a compact detector design allowing for high TF measurements with good spectroscopic accuracy and large observable signal amplitude.

FLAME will have the possibility to mount up to 2 samples (later up to 3 samples) on a ladder holder on the dilution fridge which can successively be brought into the beam at low temperatures. This feature is thought to reduce the ratio between “down” and “up” periods of the instrument, which is a key factor on a heavily oversubscribed facility as SmuS.

The magnet and muSR spectrometer are designed to be compatible with other cryogenic environments already used at the µSR facility making FLAME a very versatile instrument and ready for future upgrades.

In addition, it is foreseen to use FLAME for in-situ modification of samples by external stimuli like uniaxial pressure, electric fields or electric currents.

By the time of the muSR conference, we will hopefully be able to present the user community positive results of the commissioning of the instrument and of the first performance tests.

An updated model for muonium in 6H-SiC

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with
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We present an updated model for muonium properties and behavior in silicon carbide (polytype 6H; SiC) based on new (unpublished) and published results from our group's TF-, LF-, RF- and photoexcited MuSR measurements.

SiC is known and widely used for structural ceramics due to its physical properties (e.g. high thermal conductivity; hardness; strength; resistance to corrosion and abrasion) all being stable to near 1920 K. The electrical and optical properties (E_G 3.0 eV, for 6H-SiC) of SiC are of great interest to the device community as, for example, its electrical resistivity can be tuned from high resistivity (intrinsic) to a more conductive variety via p- or n- type doping. Isolated hydrogen impurities in semiconductors is an unavoidable, abundant and electrically active impurity in many materials. Direct study of isolated hydrogen impurities in semiconductors is not generally possible due to hydrogen's high reactivity or solubility limitations within the host; however, muonium is an experimentally accessible analogue allowing for an investigation into the stability and dynamics of these impurity centers.

One of the most popular polytypes of SiC is a 6 layer, hexagonal (Wurtzite; 6H-SiC). In this polytype, T-sites with Si neighbors at the end of a short-c axis have estimated hyperfine constants of 3009.5 MHz (Mu1) and 3026 MHz (Mu1b). A Si antibonding site has an estimated hyperfine constant of 2768 MHz (Mu2). A carbon antibonding site is identified with an estimated hyperfine constant of 2801 MHz (Mu3). Donor and acceptor levels were initially estimated based on thermal ionization; later, laser-based measurements identified possible ionization energies with some of these states. LF- and RF- MuSR has been completed to develop the most complete available characterization of muonium states in 6H-SiC.

P

MC

Thin Film and Surface Preparation Chamber for the Low Energy Muons Spectrometer

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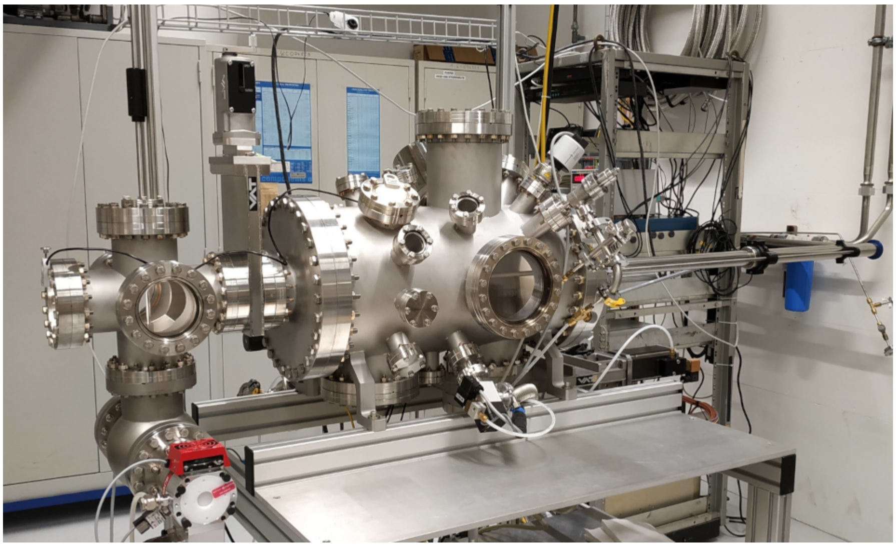

Figure 1: The LEM preparation chamber

We have designed and constructed a thin film preparation chamber with base pressure of $< 2 \times 10^{-9}$ mbar. Currently, the chamber (see figure) is equipped with two large area evaporators (a molecular evaporator and an e-beam evaporator), an ion sputtering gun, a thickness monitor and a substrate heater. It is designed such that it can handle large area thin film samples with a future possibility to transfer them in vacuum directly to the LEM spectrometer or to other advanced characterization facilities in the Quantum Matter and Materials Center (QMMC) which will be constructed in 2024. Initial commissioning of the chamber resulted in high quality, large area and uniform molecular films of CuPc and $TbPc_2$ on various substrate materials. We present first results from a low energy μSR measurements on these films.

Superconductivity in $TiSe_2$ Under Hydrostatic Pressure

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J. Philippe, M. Janoschek, R. Khasanov, G. Simutis, Paul Scherrer Institute, Switzerland
M. Abdel-Hafiez, Uppsala University, Sweden

P

SU

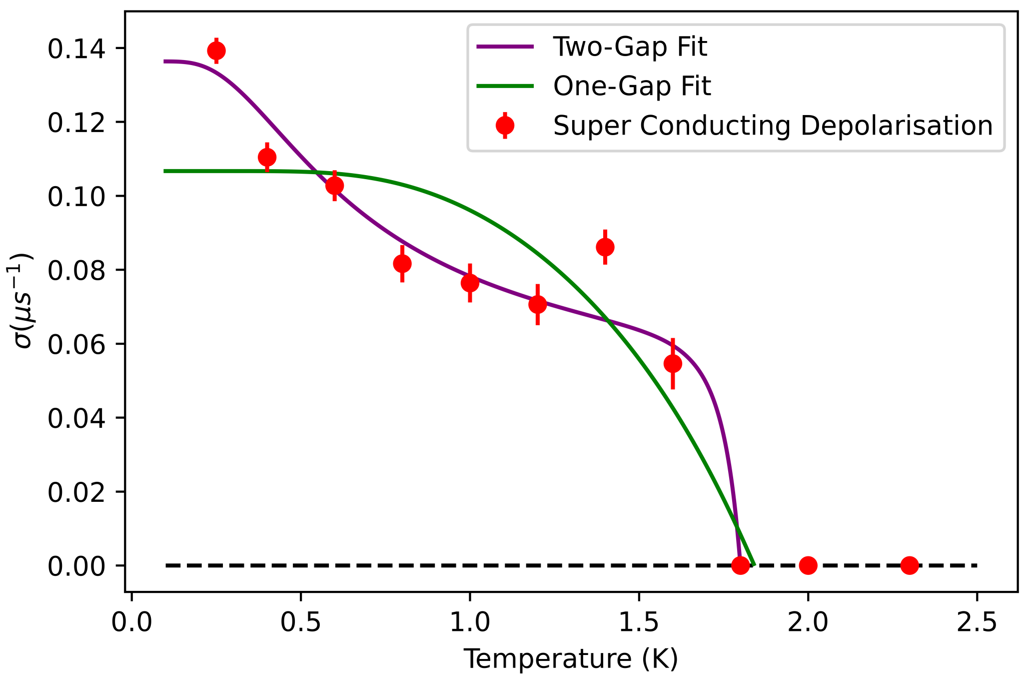

Figure 1: Temperature dependence of the relaxation rate from $TiSe_2$ under pressure.

One of the key challenges in the condensed matter research field is understanding the pairing mechanisms that give rise to unconventional superconductivity. Transition metal dichalcogenides MX_2 (M = Nb, Ti, Ta, Mo and X = S, Se) are a class of materials that have been shown to exhibit competition between a charge density wave (CDW) and superconducting state [1]. In ambient conditions, $TiSe_2$ displays a CDW state in ambient conditions and has also been shown to undergo a superconducting transition when intercalated with Cu [2] and when hydrostatic pressure is applied [3]. Here, we have conducted a muon spin resonance (µ+SR) experiment on a powder sample of $TiSe_2$ under hydrostatic pressure. The measurements were conducted at the GPD beamline, Paul Scherrer Institute. Measurements were taken at high pressure (22.9 kbar) and at zero pressure in order to compare, and at two muon momentums of 100 MeV/c and 95 MeV/c. All these measurements were taken in field cooled conditions under 100 Gauss. We can say that the response from the lower momentum muons is mainly from the pressure cell, and the larger momentum muons respond more to the sample. We see a possible two s-wave gap behaviour for the high-pressure results, fixing T_C = 1.8K, Δ_1 = 1.03meV and Δ_2 = 0.096 meV where Δ is the maximum value of the gap for each contribution. Results from other µ+SR studies using copper doped $TiSe_2$ show a similar behaviour [4], suggesting these mechanisms are similar. Further analysis on these results shall allow us to put this material on an Uemura plot.

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Analysis of Positively Charged Muonium and its Diffusion in Cadmium Oxide

P

SEMI

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with
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Cadmium oxide is a transparent conducting oxide (TCO) that has many applications in optoelectronic devices, such as solar cells, photo transistors and diodes. CdO is a naturally n-type TCO with hydrogen acting as a shallow donor. MuSR zero field measurements were collected, from 20 K to 800 K, to investigate the diffusion properties of positive Mu defects in a CdO powder sample. The neutral Mu shallow donor signal is seen up to 200 K. At this temperature the neutral Mu ionizes. The calculated ionization energy is 119 meV +/- 20 meV. This result in agreement with Cox, et. al. [*J. Phys.: Condens. Matter* **18**, 1061 (2006)]. Two positive Mu sites are seen below 425 K. Above 425 K, one of the positive Mu sites becomes mobile and transitions to the second positive Mu site. By 550 K, all positive Mu have transitioned to the second site. Details relating to the transition between sites, barrier energies, and diffusion processes will be discussed in the presentation.

P

SEMI

Analysis of Positively Charged Muonium in Tin Oxide

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with
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Tin oxide is a transparent conducting oxide (TCO) that has many applications in optoelectronic devices, such as solar cells and LED's. Tin oxide is naturally n-type with hydrogen acting as a shallow donor. MuSR zero-field measurements were taken on a single crystal sample from 2 K to 710 K in a closed cycle refrigerator and from 300 K to 1080 K in an optical furnace. The zero-field measurements allow for analysis of positively charged muonium defects in samples. The analysis of the results shows two positive muonium states with hints of an additional state at temperatures below 300 K. The current model shows a high occupancy positive muonium state and a low occupancy positive muonium state with a slow migration of muonium from the high occupancy state to the low occupancy state above 300 K. We will present details of an updated model and the muonium sites, energies barriers, and diffusion processes of the positively charged muonium determined from the model.

The Ultra-Slow Muon beamline at J-PARC: the present status and future prospects

P

NT

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At J-PARC MLF, MUSE provides the world-highest flux of pulsed muon beams. U-Line, one of the four beamlines in the facility, features an intense surface muon beam from Super-Omega and Ultra-Slow Muon (USM) generated by laser ionization of thermal muonium in a vacuum. The beamline has two branches: U1A for muon spin spectroscopy using USMs and U1B for transmission muon microscope. The unique feature of the USM is variable low-energies from sub-keV to tens of keV, compared to the energy of 4 MeV of a surface muon beam. This feature makes it possible to use muons not only as a probe for the bulk but also as a depth-resolved probe for surfaces and interfaces. Commissioning of the beamline and instruments is underway in preparation for the start of user programs. This contribution will present an overview of the facility, its current status, and its prospects.

P

SL

Inducing Quantum Criticality in $CrCl_3$ Under Pressure

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Accelerated by the discovery of graphene, research on two-dimensional (2D) materials have attracted tremendous attention both from fundamental and applied sciences. Among the large number of 2D materials, chromium trihalides CrX3 (X = Cl, Br, I) van der Waals (vdW) magnets have also raised a large interest due to the existence of many magnetic subtleties that cannot be explained by their magnetic and/or structural transitions.

Numerous studies were performed on CrI3, but only a few have been reported so far on its analogue CrCl3. The 2D vdW CrCl3 compound is stabilized under a rhombohedral symmetry, consisting of 2D Cr layers arranged in a honeycomb web fashion and surrounded by octahedrally coordinated Cl, with weak vdW inter-layers coupling. The layer structure and inter-layer coupling make CrCl3 an ideal system to study under external stimuli such as pressure or magnetic field, where new intriguing states of matter can be unveiled. With such expectations, studies of CrCl3 under room temperature, high pressure have been reported[1]. However, its spin dynamics at low-temperature and high-pressure regime remain unexplored.

In this study, we present the results of our recent muon spin rotation (MuSR) investigations performed on hydrostatically pressured CrCl3. Our previous MuSR results at ambient pressure revealed successive transitions from paramagnetic to short-ranged-order-ferromagnetic then to antiferromagnetic states with strong spin dynamics as the temperature decreases[2]. When applying pressure, we observed that the magnetic ground state is gradually suppressed. A linear extrapolation points toward the suppression of magnetism at about p_c= 30 kbar indicating the possible existence of a quantum critical point at p_c.[3]

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Progress on the surface muon beamline S-Line at J-PARC MUSE

P

NT

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The surface muon beamline (S-Line) in the experimental hall No.1 of the Materials and Life science experimental Facility (MLF), J-PARC is designed to provide low-energy muon beam, which is mainly utilized by materials and life science experiments. The final goal of S-Line is a beamline with four experimental areas from S1 to S4, of which the first experimental area S1 started in 2017 for user experiment programs. In 2022, beam tests in the second experimental area S2 finally started, where a group led by Prof. Uetake at Okayama University has set up an apparatus for laser spectroscopy of muonium. Using the electric beam kicker in the S line, a double-pulse muon beam can be used as a single-pulse muon beam in the S1 and S2 areas simultaneously. Beam commissioning started in January 2022 confirmed that 3×10^6 /s of positive muons are extracted to the S2 area when the proton beam of 700 kW is operated. Besides, we have had several beam kicker problems due to failures in the Marx high voltage circuits using semiconductor devices. It is the beamline component that requires improvement for stable operation at the highest priority.

P
EM

Photophysical dynamics in $(CH_3NH_3)PbX_3$ (X=Br, Cl) single crystal perovskites studied by Muon-Spin Spectroscopy

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In our efforts to help the earth recover from ecological burnout we have been trying to bridle the sun's energy since 1954, when the first practical silicon solar cell was introduced. Today we are researching for ever higher efficiencies, while we try to make use of earth-abundant materials. Perovskite solar cells are promising candidates for next generation photovoltaic technology due to their energy gap tunability and significantly long carrier lifetime which leads to a high diffusion length.

This study focuses on ion diffusion in (CH3NH3)PbX3 (X=Br, Cl) hybrid perovskites, structures that contain moving organic cations confined in a cage structure of PbX6 octahedra. Diffusing ions can affect the local magnetic field distribution. We employ muon spin spectroscopy (μ+SR) to exploit this effect by studying the relaxation of muon spin in local electronic and nuclear fields. Single crystals were studied in a 30-340 K temperature range with and without illumination. We investigate the thermally activated regions, compare the extracted diffusion rate coefficients and activation energies. However, the dynamical structure and structural transitions of hybrid perovskites make theoretical interpretations challenging. With μ+SR we are able to detect these structural changes and study their effect on the diffusive properties of the crystals.

Muon Sites in Hexagonal Ice

P
SC

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Theoretical study using density functional theory (DFT) calculations supports to estimate the stopping site of muon in materials and understand the muon spin rotation and relaxation (μSR) measurements. To understand the temperature dependent zero-field (ZF) μSR measurement in water, we have performed DFT calculations and quantum simulation to estimate the muon sites in hexagonal (Ih) ice. Taking initial lattice parameters from the high-resolution neutron powder diffraction study [1], the muon stopping site was calculated in the Ih supercell containing 2×2×1 conventional cells using Quantum ESPRESSO [2]. The supercell contains 12 water molecules and a muon. The added muon in Ih ice behaves as a defect in a solid which leads to the relaxation of immediate surrounding structure. The water molecules nearby the muon site found reoriented. The stopping site of muon is found at around 2 A distance from three protons (one proton of a water molecule and two of another, total four spin-half (4S) system). It seems like H_2O-Mu-H_2O^+ but the muon site is found neither L-defect nor D-defect but like interstitial. Based on this result and quantum simulation [4], only the slow-oscillating term of ZF spectra at 270 K can reproduce. To satisfy the fast-oscillating term of the ZF spectra, quantum simulation indicates that the muon should be at least 0.99 A distance from one of the protons in the 4S system (indicating two sites of muon). In the program, we will present DFT calculations and quantum simulations to interpret the oscillating ZF spectra at 270 K.

References

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P

SEMI

Shallow Muonium radical in κ-Ga2O3 thin films.

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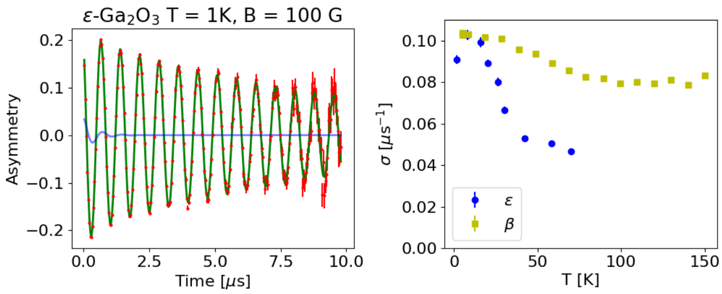

Figure 1: Left: ϵ-Ga_2O_3 time-dependent asymmetry; right: relaxation rate vs. temperature.

Ga_2O_3 is an emerging wide-gap semiconductor with a broad variety of applications, from transparent conduction to high voltage applications, therefore considered as a possible replacement for SiC. Its alpha polymorph, which can be grown in bulk crystalline form, is intensely investigated. An important technological development relies on the growth of thin film of the epsilon polymorph, since the small amount of required material allows for considerable cost reductions.

The role of hydrogen (H) in doping and passivation of vacancies, or dangling bonds, is very prominent in semiconductors, whereas spectroscopic technique capable of detecting H are not abundant. Muon spin spectroscopy is unique in its ability to provide insight on the behaviour of muons as light H isotopes in the extreme dilution case, which is impossible to access with 1H.

A Muonium (Mu) shallow donor center is reported [1, 2] in the β polymorph, with a tiny hyperfine coupling of Bhf 100 G and an activation energy for conversion to other muon species $E_a = 20(4)$ meV.

Here we present the result of a surface muon investigation of κ-Ga_2O_3 30 micron-thick film grown on sapphire. The experiment required a special kapton degrader, obtained after careful tuning of its thickness, assisted by SRIM simulations. The measurements reveal a shallow Mu center with a similar tiny hyperfine coupling, but a significantly different activation energy (see figure)

References

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Thursday Session

Indico ID	Prog. code	Title	Presenter
119	P-THU-1	Hydrogen diffusion observed in photoinduced YO_1H_2 thin films	Yuya Komatsu
131	P-THU-2	Sodium Diffusion in Hard Carbon Studied by Small-Angle Neutron Scattering and Muon Spin Relaxation	Kazuki Ohishi
136	P-THU-3	Development of a stable measurement system for Radio-Frequency studies of muonium reactivity with metal nanoparticles and surface-adsorbed molecules in mesoporous hosts	Stephen Cottrell
348	P-THU-4	In-flight muon spin resonance and muonium interferometer	Sohtaro Kanda
152	P-THU-5	BEAMS: A New User-Friendly Program for Analyzing µSR Data	Alec Petersen
174	P-THU-6	Development of Transient µSR at J-PARC	Shoichiro Nishimura
180	P-THU-7	Broadband Adiabatic Inversion Cross Polarization (BRAIN-CP) for beta-NMR	Sydney Kreitzman
196	P-THU-8	LE-muSR Study of the Field Distribution and the Domain Shape near the Surface of Superconductors in the Intermediate State*	Vladimir Kozhevnikov
201	P-THU-9	Muon-spin relaxation investigation of magnetic bistability in a molecule-based material	Alberto Hernandez-Melian
208	P-THU-10	Low Energy Measurements in Low-Energy μSR	Thomas Prokscha, Zaher Salman
215	P-THU-11	Magnetic ground state of rutile-type oxide RuO_2 inferred from muon	Masatoshi Hiraishi
220	P-THU-12	Development of magnetic resonance imaging (MRI) system using beta-NMR technique (also Student Day presentation)	Takato Sugisaki
229	P-THU-13	Magnetic nature of wolframite $MnReO_4$	Elisabetta Nocerino
233	P-THU-14	Online learning to train users of muons and neutrons at ISIS	Peter Baker
251	P-THU-15	In situ, operando investigation of thin film devices using LE-µSR	Zaher Salman
257	P-THU-16	A MaxEnt-µSR study: Precursor effects of the Fe3O4 Verwey transition	Carolus Boekema

Indico ID	Prog. code	Title	Presenter
261	P-THU-17	Mott-insulating state of alkali-metal clusters in sodalite studied by μSR	Takehito Nakano
262	P-THU-18	TrimSP Simulations for Pressure Cell Stopping Fraction	Frank Elson
265	P-THU-19	Quadrupolar split resonance of ^{8}Li in $LaAlO_3$	Victoria Karner
266	P-THU-20	Structure of muoniated trimethylsilylvinyl radicals	Iain McKenzie
271	P-THU-21	Elemental Depth Profiling using Negative Muon Implantation and X-ray Tomography of a Copper based Bust representing: the Head of Crying Child.	Adrian Hillier
276	P-THU-22	CHNET-TANDEM experiment: Muonic Atoms X-Rays Spectroscopy for elemental characterization of ancient metal artifacts	Massimiliano Clemenza
278	P-THU-23	Ion Diffusion in Na Super Ionic Conductors (NaSICON)	Rasmus Palm
279	P-THU-24	Development of a highly pixelated detector array and a novel digitising DAE for the next generation ISIS instrument, Super-MuSR	Sam Franklin
280	P-THU-25	Magnetic surface state on pure and iron-doped palladium thin films	Gesa Welker, Thomas Prokscha
284	P-THU-26	Anisotropic hyperfine coupling of muonium in CeO_2 studied by muon spin relaxation	Akihiro Koda
291	P-THU-27	*Withdrawn*	
292	P-THU-28	^{8}Li βNMR studies of Epitaxial Thin Films of the 3D topological Dirac semimetal Sr_3SnO	W. Andrew MacFarlane
294	P-THU-29	Development of ultra-slow negative muon production	Hiroaki Natori
297	P-THU-30	Magnetic ground state of $YbCo_2Zn_{20}$ probed by muon spin relaxation	Wataru Higemoto
298	P-THU-31	Depth profiling of LE-μSR parameters with musrfit	Maria Mendes Martins
299	P-THU-32	Thermal desorption spectrometry system for complementary hydrogen measurements of μSR experiments	Ryosuke Kadono
301	P-THU-33	Simulating muon spin depolarisation in a nanostructured magnetic material	Rhea Stewart

Indico ID	Prog. code	Title	Presenter
303	P-THU-34	Investigating magnetic skyrmion in Pt/CoFeB/Ru multilayers with low-energy MuSR	Yasmine Sassa
304	P-THU-35	Anomalous behaviour of the mixed phase of superconducting $LaFeAsO_{1-x}F_x$	Giacomo Prando
306	P-THU-36	Confirming the phase diagram of the Shastry-Sutherland model with μ^+SR	Yuqing Ge
308	P-THU-37	Development of a drift tube for study of a quantum mechanical scattering of muons in helum gas	Shiro Matoba
310	P-THU-38	Phase diagram and charge-dynamics of electron-doped osmium based $Ba_2Na_{1-x}Ca_xOsO_6$ spin-orbit-coupled Mott insulator	Samuele Sanna
312	P-THU-39	Thermal integrity test to muon production target by the induction heating system	Wonjun Lee
315	P-THU-40	Magnetic structure refinement in the Mott insulator NiS_2	Jonas A. Krieger
318	P-THU-41	Piezoelectric-driven uniaxial pressure cell for muon spin relaxation experiments	Hans-Henning Klauss
319	P-THU-42	Negative muon spin rotation and relaxation on superconducting MgB_2	Jun Sugiyama
321	P-THU-43	Muonium 1S-2S spectroscopy with improved statistics	Shinsuke Yamamoto
328	P-THU-44	Using the TCDFT method to determine muon quantum effects	Yue Yuan
210	P-THU-45	$KAgF_3$: Using F–μ–F states to measure magnetic materials	John Wilkinson

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SEMI

Hydrogen diffusion observed in photoinduced YO_1H_2 thin films

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Materials showing high photoresponsive electrical resistance have attracted considerable attention due to their photoelectronic applications.[1] Recently, we have reported that yttrium oxyhydride (YO_xH_y) epitaxial thin films exhibit a repeatable photo-induced insulator-to-metal transition by UV laser illumination and thermal relaxation.[2] The photo-induced metallization likely originates from the carrier generation reaction: $H^- + h\nu \rightarrow H^+$ + $2e^-$, which generates excess electrons and protons.[2,3] This suggests that a local environmental change around hydrogen in the epitaxial YO_xH_y thin film plays an important role in the photo-induced metallization process. To further understand the hydrogen dynamics in the YO_xH_y epitaxial thin film, here, we used ^{8}Li β-NMR for pristine and UV-illuminated thin films. For the as-fabricated sample, the spin-lattice relaxation rate ($1/T_1$) is constant as 0.2 s^{-1} in the temperature range between 100 to 300 K. For the UV-illuminated sample, the temperature-independent 1/T1 of 0.3 s^{-1} is also observed at temperatures below 200 K, indicating an increase in $1/T_1$ by UV illumination. There are two possible origins for the increase in $1/T_1$: one is the generation of color centers and the other is the enhancement of the interaction between dilute paramagnetic moments and photocarriers. Furthermore, we found that $1/T_1$ increases with increasing temperature only for the UV-illuminated sample at temperatures above 200 K; this implies a change in the nuclear magnetic field due to hydrogen dynamics. These results suggest that the hydrogen dynamics are thermally activated and a change of the local environment around hydrogen under UV illumination.

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Sodium Diffusion in Hard Carbon Studied by Small-Angle Neutron Scattering and Muon Spin Relaxation

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EM

The recent surge of Li-ion batteries has triggered an increased interest to investigate Na-ion battery materials [1,2], because Na is more abundant than Li, resulting in lower material costs. Although many Na transition metal oxides are available as a cathode material for the Na-ion battery, there is, at present, no suitable anode material [1]. The most common anode materials for the Li-ion battery are not compatible for the Na-ion battery, because graphite is electrochemically inactive in an intercalation and deintercalation reaction of Na^+ ions.

Since non-graphitizable carbon (hard carbon) is electrochemically active as a Na insertion host, hard carbon is heavily investigated as an anode material for the Na-ion battery. However, the relationship between the structure of hard carbon and dynamics of Na insertion is still not fully clarified despite huge efforts in the past decade [2]. We have therefore attempted to study the microscopic structural nature of sodium intercalated hard carbon (NaC_x) with small-angle neutron scattering (SANS) and the dynamics of Na diffusion in NaC_x with muon spin rotation and relaxation (μ^+SR).

The transverse field μ^+SR measurements on NaC_x clearly showed a motional narrowing behavior above around 150 K, which indicates that Na+ starts to diffuse above 150 K. The zero field and longitudinal field measurements clarified the presence of the two muon sites (μ1 and μ2). Since the Na concentration around the μ1 site is higher than that around the μ2 site, the μ1 site locates in the graphene layer and the μ2 site in the amorphous region [3]. At the presentation, we will also discuss the results of SANS on NaC_x.

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Development of a stable measurement system for Radio-Frequency studies of muonium reactivity with metal nanoparticles and surface-adsorbed molecules in mesoporous hosts

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with
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We have recently begun an investigation of paramagnetic (free-radical) final states formed on metal nanoparticles by muonium reactivity with surface-adsorbed molecules. The nanoparticles are incorporated into mesoporous silica, facilitating specific reaction steps in the silica host that involve H-atom transfer reactions important to studies in heterogeneous catalysis. Radio-frequency (RF) methods are an essential tool for characterising final state species in these systems, and a non-metallic sample cell is essential for running these measurements to ensure the RF field penetrates the sample. Initial measurements were carried out using an existing cell with a body made from PEEK polymer, using a 1/16" capillary to enable vapour to be introduced into the cell in-situ. Unfortunately, several significant problems were encountered during initial experiments, the most serious being a temporal instability in the signals measured for both pure silica and for systems loaded with small pressures of benzene. This paper reports in detail on the problems encountered using the PEEK cell, and then discusses the development of a more reliable experimental setup giving better reproducibility for these measurements. The new sample cell has been fabricated from Shapal, a ceramic material with good thermal properties. Previous experience of using Shapal components in gas RF cells has suggested this is a 'clean' material that gives none of the outgassing issues previously associated with PEEK. While rebuilding the cell, the opportunity was also taken to improve the conductance of the vapour transfer tube. The success of the new cell is demonstrated both through off-line tests and by muon measurements, including a series of TF 2G muonium spin precession measurements designed to verify the temporal stability of the experimental setup. Finally, an RF cavity was fashioned, and RF measurements made for muons stopped in bare silica, with signals from both diamagnetic and paramagnetic muon states clearly seen.

In-flight muon spin resonance and muonium interferometer

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The muon and muonium play a unique role in materials science as a tiny magnetometer and an emulator of hydrogen in matter. However, there are few examples of their application as matter waves. This is because the surface muon and its simple slowing-down in a degrader cannot keep sufficient coherence. Low-energy muons from laser ionization of muonium can be used to obtain slow muonium with small temporal and spatial spread. Like an ordinary atomic interferometer, a muonium interferometer has a variety of potential applications. For example, muonium spectroscopy using interference effects, studies of quantum interference effects such as a measurement of Berry phase, and precise measurements of fundamental constants will be possible using muonium interferometry. In this contribution, we discuss the in-flight spectroscopy of muonium and the potential of muonium interferometry.

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BEAMS: A New User-Friendly Program for Analyzing μSR Data

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with
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To support the continued growth of μSR, it is important to encourage prospective new users by minimizing any barriers to entry to the μSR community. As with any other scientific approach, one such barrier to entry can be the software tools necessary to extract useful information from the data. Although excellent software options for μSR currently exist, in our experience, students and other new μSR practitioners often struggle to learn how to use these tools. For this reason, we have developed BEAMS, a comprehensive, user-friendly computer program for μSR data analysis designed to complement existing μSR programs as an accessible entry point into μSR data analysis. BEAMS is an open-source, python-based graphical program that enables interactive inspection of μSR data and flexible fitting of mathematical functions to asymmetry spectra through non-linear least-squares optimization. The program currently accepts data from TRIUMF, PSI, and ISIS. The software is available for Windows, Mac, and Linux operating systems through a simple installation procedure. The source code, helpful tutorial videos, and detailed documentation are available at https://github.com/FrandsenGroup/beams to help new users take advantage of BEAMS as an easy-to-use tool for analyzing μSR data.

Development of Transient μSR at J-PARC

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To obtain one time-differential μSR spectrum using a conventional technique, we must wait around 10^2 minutes. In the majority of μSR experiments, the μSR spectrum is recorded as a function of temperature. Thus, such a long recording time (t_{record}) has not been a serious problem, because the lead time (t_{read}) for stabilizing temperature requires typically 10-20 min, which is shorter than the recording time ($t_{lead} < t_{record}$). However, due to the developments of the high-intensity pulsed muon beam with a repetition of 25 Hz in J-PARC MUSE and the multi-detector counting system, the recent data recording time is very short compared with the time to stabilize the measurement condition ($t_{record} < t_{lead}$), which makes t_{lead} a significant bottleneck for the advanced μSR measurements. In order to solve this problem, we are developing a novel data record and analysis technique to use a high-intensity muon beam more efficiently. In the novel technique named transient μSR, the sample environment, such as temperature and magnetic field, is continuously changing during the μSR measurements. Positron events in each muon pulse are recorded as multidimensional data, i.e., along with the number of pulses and the changing parameter. The whole data is then resorted as a function of the parameter. This transient μSR technique also enables us to study a transient phenomenon that is now unavailable with the standard μSR technique. It should be emphasized that the feasibility of this technique crucially depends on the intensity of the pulsed muon beam. We have also developed a new software based on ROOT to analyze the huge number of the μSR spectrum within a reasonable amount of time. We will introduce the analysis software how to analyze the transient μSR data and report the results obtained under dynamic sample environments.

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Broadband Adiabatic Inversion Cross Polarization (BRAIN-CP) for beta-NMR

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Cross-polarization techniques provide a rich playground which allows NMR practitioners a large variety of tools to extract detailed spin-hamiltonian parameters of inhomogeneous systems. Beta-detected NMR is almost an ideal arena, i.e. one spin-polarized 8Li residing in a local structure, for which to apply such multi-resonant pulse sequences.

As such, an adaptation of NMR's BRAIN-CP RF pulse sequence is described which can in principle extract the dipolar and/or quadrupolar spin parameters of the 8Li near neighbours. The polarization transfer is achieved in a specifically tuned "double" rotating frame during an adiabatic inversion of the 8Li spin, and is detected as loss or fine structure in the monitored 8Li z-polarization.

LE-muSR Study of the Field Distribution and the Domain Shape near the Surface of Superconductors in the Intermediate State*

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SU

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As known (Landau, 1937), the equilibrium domain structure of the magnetic flux in type-I superconductors in the intermediate state is formed due to the competition between the energy contributions to the sample free energy arising from the superconducting/normal interfaces, on one side, and the contributions due to an inhomogeneous field distribution and the domains shape (FDDS) near the sample surface, on the other. Landau suggested two scenarios for FDDS, other scenarios were proposed by Tinkham, Marchenko and Abrikosov. However, none of these scenarios meets the fundamentals of the Laplace-based magnetostatics being simultaneously consistent with observed flux structure. We will report on for the first time performed direct measurements of the FDDS near the surface of planar samples in the intermedium state, i.e., on high purity indium films in a normally applied field. The measurements were carried out using LE-μSR. The range of the probed distances from the surface extends from 0.1 μm inside to 1 μm outside the sample. It was found that, contrarily to what follows from the Laplace equation, the current-free space outside the samples contains voids extending over a large-scale distance, which can exceed the thickness of the samples. More specifically, at low fields the measured FDDS is close to that suggested by Tinkham. However, at high fields the real FDDS differs from all predictions: the width of the superconducting domains widens instead of expected narrowing and outside the samples the field passes through a maximum, in apparent violation of Earnshaw's theorem. It will be shown that the observed FDDS is thermodynamically the most favorable for the superconducting sample, which leads to inapplicability of the Laplace equation and, consequently, the Earnshaw theorem in a wide vicinity of the sample in the intermediate state.

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SCE

Muon-spin relaxation investigation of magnetic bistability in a molecule-based material

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We present the results of a muon-spin relaxation (μ^+SR) investigation of the crystalline organic radical compound 4-(2-benzimidazolyl)-1,2,3,5-dithiadiazolyl (HbimDTDA), in which we demonstrate the hysteretic magnetic switching of the system that takes place at $T = (249 \pm 13)\,\mathrm{K}$ caused by a structural phase transition. Muon-site analysis using electronic structure calculations suggests a range of candidate muon stopping sites. The sites are numerous and similar in energy, but, significantly, differ between the two structural phases of the material. Despite the difference in the sites, the muon remains a faithful probe of the transition, revealing a dynamically-fluctuating magnetically disordered state in the low-temperature structural phase, which was previously believed to be diamagnetic. This is evidenced by relaxation following the Redfield formula in longitudinal field (LF) measurements, which is observed only in the low temperature phase. In contrast, in the high temperature phase the relaxation is caused by static nuclear moments, with rapid electronic dynamics being motionally narrowed from the muon spectra.

Low Energy Measurements in Low-Energy μSR

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In the context of μSR studies on magnetic materials in the ordered state, often a strong initial depolarization is found in the zero field spectra. For transverse field measurements this is often referred to as a loss in asymmetry. In case of the low-energy muSR (LE-μSR) setup this needs a more detailed discussion since effects such as time-of-flight distribution decay, back scattering, and muon reflection will change the spectra at early times and low implantation energies ($E < 3$keV). These effects are well understood and reproducible allowing to correct for in any given experiment. We will discuss them and show how to correct for in experiments at low implantation energies.

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SCE

Magnetic ground state of rutile-type oxide RuO_2 inferred from muon

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Ruthenium dioxide RuO_2 is a well-known catalyst applied in various fields due to its high electrical conductivity and chemical stability. Although rutile RuO_2 has long been regarded as a Pauli paramagnetic metal, recent neutron diffraction experiments and resonant X-ray scattering have suggested the presence of an antiferromagnetic order ($T_{\mathrm{N}} > 300$ K: Ru moment size ∼0.05 μ_{B}) associated with the lattice distortion. This has triggered a growing interest regarding the details of the electronic state. We were thus motivated to investigate the magnetic ground state of high-quality single crystal RuO_2 (residual resistivity ratio RRR>1,000) by muon spin rotation/relaxation experiment. We found no clear evidence from μSR measurements to suggest the development of a quasi-static antiferromagnetic order from 400 K to 4 K. The remaining possibility is that the muons happen to reside at a site where the internal magnetic field is canceling. In the presentation, we will also report the evaluation of muon site in the rutile structure deduced by first principles calculations to examine this possibility.

Development of magnetic resonance imaging (MRI) system using beta-NMR technique

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NT

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Today, the technology of magnetic resonance imaging (MRI) has been established and it is essential in the medical field. MRI is the method of making an in-situ image by utilizing nuclear magnetic resonance (NMR). However, the MRI technique has rarely been put to practical use for elements other than hydrogen because of the sensitivity issue. On the other hand, the technique of beta-ray-detecting NMR (beta-NMR) makes it possible to observe NMR for various elements with extremely high sensitivity by measuring the asymmetry of the beta-ray emission from polarized radioisotopes (RIs). By utilizing beta-NMR, we aim to create a 3-dimensional (3D) MRI system. We have developed a detector set with plastic scintillation fibers, which enables us to track back the trajectory of beta-rays. Moreover, by seeking the beta-ray asymmetry at each position in the sample, we can create a magnetic resonance image. We conducted experiments using a spin-polarized $^{12}\mathrm{B}(I = 1, T_{1/2} = 20\ \mathrm{ms})$ beam at HIMAC heavy-ion synchrotron facility of the National Institutes for Quantum Science and Technology. We obtained the data from various samples of mixtures as well as simple substances. We have successfully obtained a 1D image of the beta-ray asymmetry for $^{12}\mathrm{B}$ in Si. The data analysis for 3D imaging are now in progress.

It is expected that this new technique will be applied to non-destructive and non-contact testing related to various fields such as medical and materials science.

In this conference, we will present our new results of the analyses. We will also show some idea that a combination of beta-NMR and mu-SR will expand this technique.

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Magnetic nature of wolframite $MnReO_4$

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Rhenium oxide compounds of the type $AReO_4$ where A is a first-row transition metal cation, exhibit interesting electronic properties. Among this family of compounds, $MnReO_4$ was the first of this kind, synthesized with a high-pressure technique at 25 kbar in 1970**[1]**. It has a wolframite structure where both cations have partially filled d shells, and an anisotropic electrical resistivity that makes it suitable for potential applications in the development of electrical devices**[2]**. Although this material was already known for several years, the magnetic properties of $MnReO_4$ have never been studied in detail. In this work we present the very first investigation of the magnetic nature of the wolframite insulator $MnReO_4$ carried out by muon spin rotation. The aim of the experiment was to clarify the occurrence a static antiferromagnetic order, and the possibility for the formation of magnetic multipole order at low temperatures, which is expected due to the lack of an inversion symmetry at the Re6+ site and a strong spin-orbital coupling of its 5d1 electron. The occurrence of the static antiferromagnetic ordering was clearly observed in $MnReO_4$ and the order parameter of the transition was determined.

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Online learning to train users of muons and neutrons at ISIS

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Online learning is being adopted across a wide range of disciplines as remote access to resources, widening participation in training, and an appreciation of the diverse approaches of learners have come to prominence. Online resources can also be used to augment more traditional in-person training by bringing a cohort of learners up to a common minimum level beforehand, distributing materials during the course, and reinforcing learning after the event.

Over the last six years ISIS has developed online learning materials about muon and neutron science that sit alongside other neutron science materials produced as part of the SINE 2020 project. The materials include lecture videos, quizzes, and introductions to science areas, experimental techniques, and computational methods. These have been used by hundreds of students, those participating in training schools, those preparing for experiments or data analysis, and those with another interest in these subjects. Users have provided consistently positive feedback on the available content. Following the conclusion of the SINE2020 project, the materials are now hosted by the PaNOSC and ExPaNDS projects at: [https://e-learning.pan-training.eu/][1].

We will describe the materials now available, the opportunities and challenges of online training for facility users, and the developments planned for coming years.

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In situ, operando investigation of thin film devices using LE-μSR

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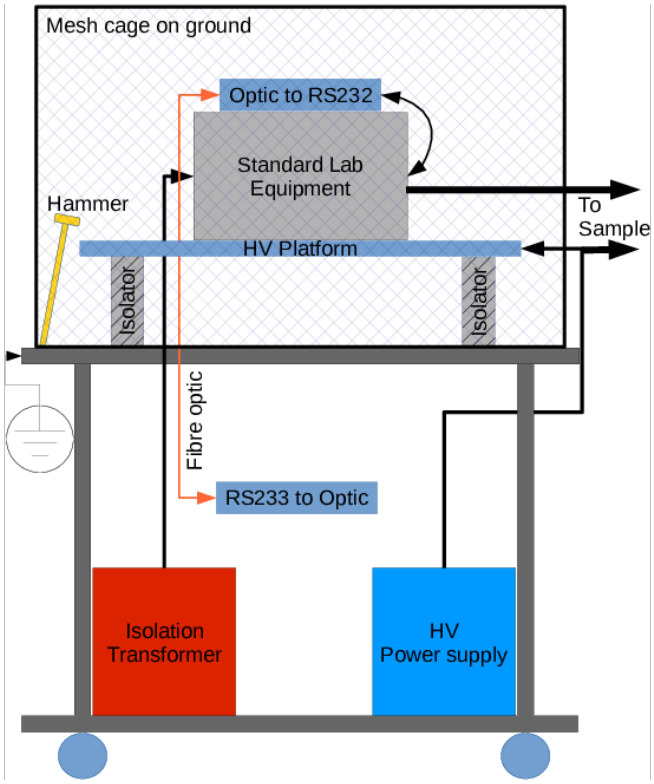

Figure 1: Schematic of the LEM high voltage table

Tuning the energy of incoming muons in the low energy muons (LEM) spectrometer is done primarily by applying a high voltage (HV) on the sample plate to accelerate or decelerate the implanted muons. Therefore, any manipulation on the sample that requires the use of direct contacts to it becomes complicated. For example, in order to run a current through the sample or apply an electric field on the sample, the power supply and contacts have to be on the same HV as the sample. A simple way to achieve this is to place the power supply (or any other standard lab equipment or device) on an insulated platform outside the cryostat and bias both the sample and the device by the same HV. Although the idea is simple, its application requires serious safety and reliability considerations. Here we present the design of this HV table (see figure) and discuss some applications in various thin film devices.

A MaxEnt-µSR study: Precursor effects of the Fe3O4 Verwey transition

P

SCE

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Using muon-spin rotation (µSR) [1] the magnetic fields of Fe3O4 have been previously investigated. The Verwey transition at Tv (123 K) and a transition at Tw (247 K) are observed. Using Maximum-Entropy (MaxEnt) µSR data of single-crystal Fe3O4 are analyzed with much improved precision. [2,3] We review earlier results [3] and report on our analysis of the temperature dependence of fields with B (720 Oe) // <110>. Below the demagnetization field, extra µSR signals are found at Bext // <110> indicating two frequencies at room temperature (RT) and two at 205 K. [3] At RT, the upper frequency follows the zero-field trend seen in the Tv-Tw region of the zero-field (ZF) phase diagram. At 205 K, the lower frequency follows the extension of the ZF trend above Tw. These two ZF trends indicate plausible short-range ordering related to the “extra” 3d-electron conduction behavior. This should further be interpreted as precursor effects to the Tv transition. [1] Our MaxEnt-µSR finding is consistent with diffuse [4] & x-ray [5] scattering results above Tv providing a clear picture of the magnetic environments in Fe3O4. This new interpretation indicates two T-dependent magnetizations, reflecting different short-range orders [3-5] in the ZF phase diagram of this Mott-Wigner glass.[6]

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SCE

Mott-insulating state of alkali-metal clusters in sodalite studied by μSR

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In Mott insulators, band electrons are localized due to strong electron-electron interactions. Although the s-electrons of alkali metals are very delocalized, by confining them in the periodic nanospace of zeolite crystals and making them moderately localized, such a strongly correlated electron system can be created.[1] In sodalite, β-cages with an inner diameter of 0.7 nm are arranged in a bcc structure. By loading alkali atoms, an A_4^{3+} cluster (A: alkali atom) is formed in the cage. The cluster has one unpaired s-electron. Antiferromagnetic order of Mott insulating state has been identified in $A =$ Na, K, and K-Rb alloy clusters.[2] T_N systematically increases from 50 K (Na) to 90 K (K-Rb alloy). In ZF-μ^+SR, a uniform local field is observed below T_N, and its value is higher for clusters with heavier chemical compositions.[2]

To clarify the mechanism of the systematic change in the local field and its relation with the Mott-insulating state of this system, we investigate the muon Knight shift by high TF-μ^+SR using NuTime at TRIUMF. We successfully obtained the hyperfine coupling constants between μ^+ and the s-electron above T_N from the $K-\chi$ plot. By combining the ZF-μ^+SR local field,[2] we determined the size of the ordered moments, which systematically decreases from $\simeq$ 0.5 μ_B (Na) to $\simeq$ 0.3 μ_B (K-Rb alloy). It correlates perfectly with the increase in T_N, namely, the decrease in the electron correlation U/t in the Mott-Hubbard model. From DFT calculations, we found that μ^+ is in a hydride (Mu-) state at the cage center. This also explains that the systematic increase in the local field corresponds to the decrease in U/t due to the shallower potential of the heavier alkali atoms.

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TrimSP Simulations for Pressure Cell Stopping Fraction

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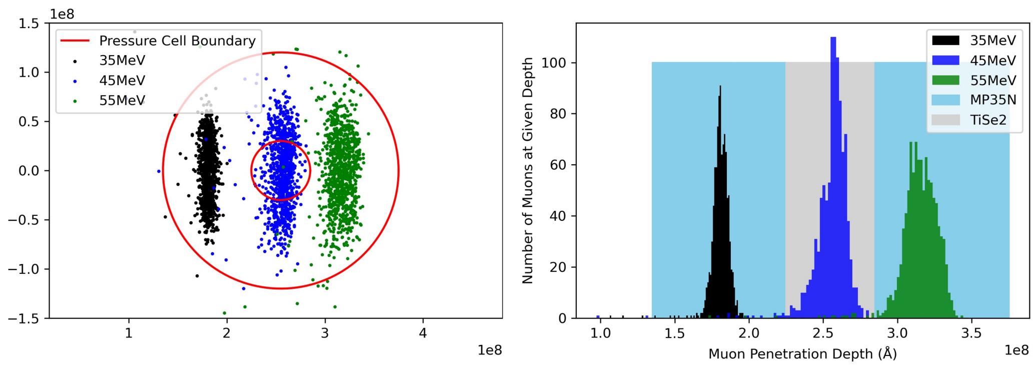

Figure 1: Example of simulation results

For quantum systems/materials, a standard procedure for probing this behaviour is to try to tune these properties using external parameters to put the different phases of the material onto a phase diagram. Pressure application is a widely used tool to tune these properties, using a given pressure cell device. This can be a problem when using Muon Spin Rotation/Relaxation (μ+SR) as a large proportion of the muons will be implanted in the pressure cell rather than in the sample. This is a problem as in most cases the pressure cells give their own temperature responses. This issue gets amplified when the temperature dependant response from the sample is much smaller than that of the pressure cell, where the sample response can be lost in the background and cause alignment issues. As pressure dependant μ+SR studies increase in popularity, the need to tackle this issue becomes greater. We have used pySRIM [1] to make a tool that helps alleviate some of these problems, specifically for the pressure cell setup at the GPD beamline at the Paul Scherrer Institute, with the use of TRIMSP simulations. The goal is to make it easy to estimate how many muons will be stopping in the sample and how many in the pressure cell at a given muon momentum. This will allow the user to know before their experiment what they expect in terms of alignment and also what kind of fractions to be inputting into their fit procedures to extract the background accurately. The aim is to make this tool into an available GUI so users can easily use this before their experiment or append the simulation results to their proposals for the GPD beamline (and maybe also other beamlines in the future).

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SEMI

Quadrupolar split resonance of ^{8}Li in $LaAlO_3$

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$LaAlO_3$ is a wide bandgap, transparent oxide commonly used as a substrate for epitaxial film growth and as a vacuum-like electrically insulating layer in heterostructures. Below a soft-mode structural phase transition at about 800 K, it is rhombohedrally distorted from the ideal cubic perovskite structure as the AlO_6 octahedra rotate about the cubic $\langle 111 \rangle$ directions[1]. It is a popular substrate, in part, because Al does not support multiple oxidation states like Ni or Ti and because it is well matched to materials such as $LaNiO_3$ due to the similarity of their lattice constants. Here, we establish the behaviour of ^{8}Li in the bulk as a prerequisite to probing the surface effects of the rhombohedral distortion[2].

We report β-detected NMR of $^{8}Li^{+}$ implanted into a single crystal of rhombohedral $LaAlO_3$. Like other insulating perovskites[3], the resonance is quadrupole split, since even in the cubic phase, its interstitial site (the P-site, Wyckoff $3d$ in the cubic phase) is noncubic. In fact, the splitting in the perovskites[4] is the largest observed for ^{8}Li. The splitting is comparably large in $LaAlO_3$ ($\nu_q \approx$ 191.3 kHz), but there is additional splitting due to the rhombohedral distortion.

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Structure of muoniated trimethylsilylvinyl radicals

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MC

Muoniated vinyl radicals can be produced by Mu addition to triple bonds. Rhodes et al. observed a muoniated radical formed by Mu addition to trimethylsilylacetylene but were unable to determine the structure.¹ We have performed additional transverse field muon spin rotation measurements on trimethylsilylacetylene at 298 K and observed that two muoniated radicals were formed; a major product with muon hyperfine coupling constant (A_μ) of 587.3(1) MHz and a minor product with A_μ of 570.9(5) MHz. DFT calculations show that Mu addition is preferred to the unsaturated carbon bonded to H and that the resulting radical has a non-linear radical centre. Calculated muon hyperfine coupling constants were used to assign the observed radicals, which are the cis and trans isotopomers with respect to the trimethylsilyl substituent, respectively.

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Elemental Depth Profiling using Negative Muon Implantation and X-ray Tomography of a Copper based Bust representing: the Head of Crying Child.

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Copper based busts in the shape of heads or shoulder high length, are known from the Renaissance, e. g. the small statuettes of the Virgin and Christ, with heights under 15cm by François Duquesnoy [1] to busts of heights over half a meter [2]. The bust presented in this paper has no comparison to Renaissance statuettes. The contorted face of the Bust, height about 22cm, reminds one of the Character Heads of Franz Xavier Messerschmidt (1736–1783) [3]. The bust of a crying child has been investigated using negative muons. Negative muons are implanted at a known depth and during the capturing process X-rays are emitted, characteristic of the capturing atom. This statuette comprises of CuZn24. At higher momentum implantation the composition of the inner core of the statuette comprises of calcium sulphate. The material depth profile as obtained from negative muon experiment has been compared with the X-ray tomography on the bust of the crying child.

Since the bust is open on the bottom, we were able to check the core body and confirm calcium sulphate as core material and confirms our results. One also observes a small iron object in the middle of the core material which was identified by X-ray tomography as a nail.

The zinc content of the studied bust, 24%, is much higher than one normally finds in Renaissance bronzes and brasses and indicates a later manufacture date. The results show that the method can be used for 'closed' statuettes: providing information on the core material and alloy composition in a non-destructive way.

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CHNET-TANDEM experiment: Muonic Atoms X-Rays Spectroscopy for elemental characterization of ancient metal artifacts

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X

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In the past years, in the framework of a successful collaboration between RIKEN-RAL and INFN, (CHNET-TANDEM collaboration) a series of experiments were carried out to optimize Muonic Atoms X-rays Spectroscopy as a non-invasive and non-destructive probe for quantitative elemental characterization of ancient metal artefacts of particular interest. We present the results on late Bronze-age artefacts found in Tuscany and a silver Portuguese ancient coin. A series of measurements on 2 bronze oil lamps, with the shape of small ships, found in Vetulonia in the Tomb of the "Tre Navicelle", part of the collection of the National Archaeological Museum of Florence (n. inv. 6779; 6780) and on a Portuguese coin of the eighteenth century utilized for an IAEA inter comparison round robin were analysed. The goal was to determine the chemical composition of the samples with the possibility of carrying out both "superficial" and "bulk" measurements by elemental profiles from the sample surface to a depth of several millimetres.

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EM

Ion Diffusion in Na Super Ionic Conductors (NaSICON)

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Lithium-ion (Li-ion) batteries are commonly used as energy storage device for both mobile and stationary applications. Even though the Li-ion technology is clearly a huge success story for modern electrochemistry, lately, there has been serious concerns regarding several aspects, e.g., availability and price of lithium raw material**[1]**. Consequently, the industry is currently and actively looking for alternatives to the Li-ion technology. Here one option might be to simply replace lithium with its neighbour in the periodic table i.e. sodium (Na)**[2]**, which is a more abundant, accessible and less expensive element. A famous group of such compounds is the so-called Na Super Ionic Conductors (NaSICON). One of the materials within the NaSICON family that is known to have highly mobile sodium ions is $Na_{1+x}Ti_{2-x}Fe_x(PO_4)_3$**[3]**. Electrochemical measurements have suggested that substitution of Fe for Ti results in higher capacity and better retention. Finally, our own studies**[4,5]** have revealed enhancements of the battery performance by introducing a nano-scale coating of carbon onto the submicron-sized NaSICON particles. However, the underlying mechanism for such effect is still partly unknown. In this study we have investigated the microscopic Na-ion self-diffusion in $Na_{1+x}Ti_{2-x}Fe_x(PO_4)_3$ using the muon spin rotation (μ^+SR) technique**[6,7]**. We present values of both activation energy of the diffusion process as well as temperature dependent Na-ion self-diffusion coefficients (D_{Na}).

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Development of a highly pixelated detector array and a novel digitising DAE for the next generation ISIS instrument, Super-MuSR

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The development of the next generation 'Super-MuSR' instrument at ISIS will provide a transformational improvement in counting rate (to 1000M ev/hr) and timing resolution (to better than 2ns) for pulsed beam measurements. Key to delivering this capability is the highly pixelated cylindrical detector array, built as 64 long 'barrel staves'. This totals 704 pixels providing 75% solid angle coverage. The detector array is combined with novel readout, where the analogue waveforms are fully digitised and processed using digital signal processing (DSP) methods at either software or firmware level.

Each detector pixel will use a Hamamatsu S10362 series SiPM, optically coupled to a BC408 scintillator using wavelength shifting fibre. The fibre is embedded into a scintillator tile, with the ends protruding to ensure good optical coupling. The tile and fibre are surrounded by a reflective inner (PTFE) and light tight outer (Aluminium) wrapping. This design was chosen to maximise the light collection and homogeneity for each of the 8 different pixel sizes used to preserve solid angle across the stave length.

The data pipeline will combine a series of 'firsts' for ISIS. Digitisation will be achieved using the Xilinx Zynq UltraScale series of 'system on a chip' operating with ADCs running at 1G Sample/s, data handling using Kafka event streaming technology, and full digital signal processing to provide advanced data correction techniques.

We will present our design considerations, first results from our 12-pixel prototype stave and discuss the benefits of implementing a DSP 'data pipeline'.

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EM

Magnetic surface state on pure and iron-doped palladium thin films

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Elemental palladium (Pd) is a well-known paramagnetic transition metal. Doping with iron impurities leads to giant magnetic moment formation and spin glass behavior. Pd surfaces often show different behavior than bulk Pd [1,2], which is particularly relevant in research fields working with Pd nanomaterial, such as for example catalysis and spintronics.

We present depth-dependent transversal field µSR measurements with low-energy muons (1 keV-25 keV) on 100 nm Pd thin films at temperatures of 3.7-200 K and external magnetic fields of 10-330 mT. These measurements reveal a magnetic surface state both on pure elemental Pd and on iron-doped (170 ppm) Pd samples. The surface state is characterized by an increased muon field and increased muon depolarization rate at the sample surface and at the interface with the silicon substrate. The interior of all thin films shows bulk-like Pd properties, in accordance with earlier bulk-µSR measurements [3]. The surface is different from the bulk for all samples, in one case, we even found a strong indication for a paramagnetic to ferromagnetic phase transition at the surface. We argue that orbital moments induced at the surface / interface by localized spins and charges are the most likely origin of the observed surface state [4].

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Anisotropic hyperfine coupling of muonium in CeO_2 studied by muon spin relaxation

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SEMI

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CeO2 is a material that has been widely used in industrial fields such as catalysts and sensors. It is believed that oxygen deficiencies and hydrogen at the deficient positions play an important role in these functions, but the details, including the electronic state, have not been clarified. It has been reported that muons implanted in CeO2 are bound to electrons and form muonium [S.F.J.Cox*et al.*, J. Phys.: Condens. Matter**18**, 1079-1119 (2006)]. However, the sample used in the experiment was a powder, and the information about the oxygen deficiency in the measured sample is unknown. Therefore, we perform the muon experiment using a single crystal sample. By using a single crystal, we can deduce the oxygen deficiency from other measurement technique, and by combining this information with our result of muon experiments, we can clarify the details of the electronic state of hydrogen in CeO2.

It was seen in our muon experiments that muon spin relaxation suggesting the existence of muonium in single crystals of CeO2 appears at temperatures below 60 K under zero external field. The temperature dependence is qualitatively in good agreement with that reported by Cox*et al.* As the longitudinal magnetic field along the [100] crystalline axis being increased, the spin polarization at $t = 0$ recovered. It is noted, however, that the obtained magnetic field dependence of the spin polarization at $T = 9$ K is different from the behavior expected for muonium with isotropic hyperfine coupling, strongly suggesting the anisotropy of the hyperfine coupling constant at the muon stopping site. Furthermore, we observed how the anisotropic behavior seen in longitudinal magnetic fields changes with changing the crystal orientation, taking advantage of the single crystal sample. From these results, we discuss the position of muonium in the crystal lattice and its electronic state.

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SEMI

^{8}Li βNMR studies of Epitaxial Thin Films of the 3D topological Dirac semimetal Sr_3SnO

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The inverse perovskite Sr_3SnO is a 3D cubic Dirac semimetal with a very small energy gap, a so-called topological crystalline insulator [1]. The unusual electronic structure confers a variety of novel properties, such as chiral topological surface states, and very strong itinerant electron orbital magnetism. Remarkably, when doped it also becomes superconducting [2]. In the most insulating samples, the Fermi level lies close to the Dirac points, and orbital magnetism is maximal. We report the results of ion-implanted $^{8}Li^{+}$ βNMR in Au capped epitaxial thin films of Sr_3SnO as a function of carrier content which can be finely tuned by the growth conditions. In addition, we stop the ^{8}Li in the Au overlayer to seek proximal evidence of the chiral surface state.

In high magnetic field (6.55 T), we find remarkably little contrast in spin-lattice relaxation between low carrier density Sr_3SnO and the Au overlayer. In the insulator, $1/T_1 \sim 0.14$ s^{-1} is slightly faster than Au at 300 K, while, in the overlayer, there is a small but systematic enhancement in $1/T_1$. The resonance in the insulator is broad with a long tail towards negative shift without resolved quadrupolar splitting.

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Development of ultra-slow negative muon production

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Ultra-slow negative muon production is under development in J-PARC.

It may explore new fields in material science, such as surface science, precise depth analysis of sample materials after re-acceleration, and 2 or 3 dimensional scanning of samples after re-acceleration and focusing. It may also contribute to explore new fields in Particle physics. Production of both the negative and positive ultra-slow muons will make it possible to generate undiscovered true-muoniums and re-acceleration and focusing them may introduce muon collider.

Though the ultra-slow positive muon beams are already offered or under development, the study of ultra-slow negative muon production is not intensively done because capture by nuclear makes it difficult.

We will present about our ultra-slow negative muon production and the current status of the development.

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SCE

Magnetic ground state of $YbCo_2Zn_{20}$ probed by muon spin relaxation

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In intermetallic Ce- and Yb-compounds, the hybridization between the $4f$ and itinerant conduction electrons induces the magnetic instability and charge configurations, and the ground state properties of heavy fermion located in the vicinity of a magnetic quantum critical point (QCP) is one of important issue for strongly correlated electron systems. The cubic compound $YbCo_2Zn_{20}$ has huge electronic specific heat coefficient γ=7900mJ/molK^2 [2] and its ground state could be located in the vicinity of the QCP or a long-range ordered phase. Indeed, a magnetic long-range order was observed under pressure above 1-2 GPa[2].

To investigate magnetic ground state, we have carried out muon spin relaxation measurements and confirm non-magnetic ground state with fluctuating tiny magnetic moment. Detail of the magnetic state will be reported in the presentation.

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Depth profiling of LE-μSR parameters with musrfit

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The study of thin-film and multi-layered structures with nanometer resolution is possible with low energy μSR (LE-μSR). The average stopping depth of the positive muons with implanted energies between 1 and 25 keV extends over a few nanometers and depends on the density of the probed material.

Modeling of the measured μSR parameters such as diamagnetic asymmetry and relaxation rate as a function of sample depth can be obtained from a series of experimental implantation energy measurements and its correlation with the simulated stopping profiles. The fitting approach assumes a sharp transition between regions with distinct properties, such as layers with different materials, defects, and intermixing near the interface, or, depletion regions where the charge carriers concentrations may change. The fitting method, previously developed in matlab, is being implemented in musrfit, a free μSR data analysis framework written in C++. The main goal is to make this fitting method widely available for energy dependent measurements and increase the modeling possibilities within musrfit.

We will present the added functionality, its implementation, and different examples where the systems measured with LE-μSR could be better understood by quantifying the width of physically relevant regions.

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Thermal desorption spectrometry system for complementary hydrogen measurements of μSR experiments

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Figure 1: Snapshot of commissioning status of TDS system

Muon probing hydrogen study is based on the fact that the target material contains at least a small amount of hydrogen. Therefore, a high-sensitivity measurement of hydrogen abundance would be useful as a complementary measurement of μSR experiments. We are developing a high-sensitivity thermal desorption spectrometry (TDS) system to perform such complementary measurements.

TDS is known as a method to evaluate the hydrogen abundance in a material[1]. The principle is that a sample is heated in an ultra-high vacuum, the partial pressure of the released gas is measured with a quadrupole mass spectrometer, and the gas abundance is quantitatively evaluated by integrating the spectrum. Recently, the development of a TDS system that detects hydrogen with a high sensitivity of 10^{16} atoms cm^{-3}, the highly hydrogen sensitive TDS (HHS-TDS) system, was reported[2,3]. Our system is a modified version of this HHS-TDS system suitable for complementary measurements of μSR experiments.

While a conventional TDS system consists of a stainless steel UHV chamber, the HHS-TDS system consists of a chamber made of Be-Cu alloy. This alloy, which has a precise composition of $Be_{0.2}Ni_2Ag_{0.1}Zr_{0.2}Cu_{97.5}$, is suitable as a chamber material because of its good thermal conductivity, low hydrogen solubility, and hardness to form a vacuum flange[4]. In our system, the sample geometry was designed to allow measurement of thin-film substrates mounted on a flag-style sample holder, which is to make the measurement compatible with experiments using ultra-slow muons. We will report on the commissioning of the vacuum chamber and the infrared laser of the TDS system.

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Simulating muon spin depolarisation in a nanostructured magnetic material

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Artificial spin ices, which are composed of dipolar coupled arrays of elongated nanomagnets, host a broad range of physical phenomena usually the preserve of bulk condensed matter[1]. In particular, collective phase transitions between ordered and disordered states have been well documented in these nanomagnetic systems[2]. The complex phases observed in artificial spin ices occur as a consequence of dipolar interactions between neighbouring magnetic moments. In order to better control the collective behaviour of the spins one must tune the interactions between nanomagnets. Traditionally this has been achieved by either varying the lengthscales within the lattice or by altering the dimensions of the individual nanomagnets themselves. However, when one pushes to smaller dimensions direct imaging techniques can no longer be used to characterise the phase transitions due to limitations in resolution.

In recent years, low energy muon spin relaxation has been used to great effect in order to study the behaviour of artificial spin systems[3]. Here we present our recent work on modelling the muon spin depolarisation in nanostructured magnetic materials. We use Monte Carlo simulations to compute the static nanomagnet moment configurations, and from these configurations calculate the net stray field distribution at the muon site. Muons are then implanted and their spin evolution determined *via* solution of the Landau-Lifshitz precession equations. By performing a full spatial integration over the plane of the sample and the muon stopping profile, we are able to simulate experiment[4].

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Investigating magnetic skyrmion in Pt/CoFeB/Ru multilayers with low-energy MuSR

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SCE

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After the first observation of magnetic skyrmion in 2009, the so-called skyrmionics research field is still rapidly evolving. To this day, intense research effort is still carrying on in understanding their intrinsic properties for the potential realization of future energy efficient nanodevices. Magnetic skyrmion in thin multilayer films are appealing because their emergence, stability, and physical properties can be engineered by controlling dipolar, perpendicular anisotropy and Dzyaloshinskii-Moriya (DM) interactions at interfaces through the choice of materials, layer thickness, and film stacks. Among numerous multilayers systems, Pt/CoFeB/Ru is an excellent platform to study the skyrmion phase, but also other magnetic fluctuations that may arise from competing orders. In addition to the DMI at the Pt/CoFeB interface, in thick multilayers, dipolar interactions favorize the formation of the Néel-type chiral domain walls close to the edges of the multilayer, and results in the creation of skyrmions with hybrid chirality.

Here, we present a low-energy muon spin rotation study on Pt/CoFeB/Ru multilayers as function of temperature and magnetic field. From both transverse field (TF) and longitudinal fields (LF) measurements, a clear magnetic transition between T= 475-500 K is observed, with fluctuations appearing at $T \leq$ 550 K. Interestingly, the relaxing components for the LF measurements show a change of fractions and depolarization rates as function of temperature, but not as a function of magnetic field. Our results suggest the presence of domain wall dynamics in these systems, which are independent of the skyrmion phase.

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SU

Anomalous behaviour of the mixed phase of superconducting LaFeAsO$_{1-x}$F$_x$

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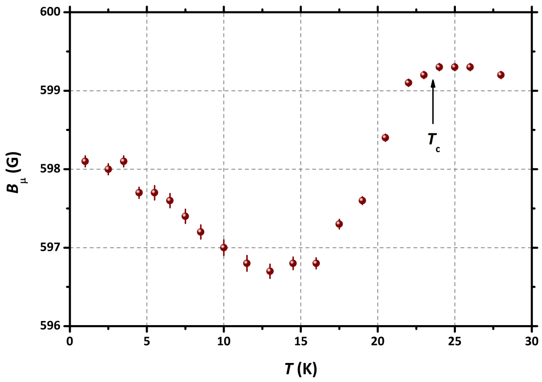

Figure 1: Temperature dependence of the internal magnetic field at the muon site for LaFeAsO$_{1-x}$F$_x$ ($x = 0.1$) field cooled in a transverse external field $B_{ext} \simeq 600$ G. An anomalous enhancement is observed in the low temperature regime.

The Fe-based superconductors have been extensively investigated in view of the intimate interplay of the magnetic and superconducting phases developing therein. Here, we show an anomalous behaviour of the mixed phase in the family of superconducting compounds LaFeAsO$_{1-x}$F$_x$ as detected by transverse-field muon spin rotation. This technique is the best tool to probe both the flux line lattice distribution and any additional source of magnetism through both the muon depolarization rate and the local magnetic field at the muon site B_μ. Although the typical shielding behaviour is expected to saturate to a constant value well below the superconducting transition T_c, our results for LaFeAsO$_{1-x}$F$_x$ show that B_μ is enhanced in the low-temperature regime (see figure). We discuss an extensive investigation of this phenomenon as a function of F doping, external magnetic field and temperature alongside different interpretations for the observed phenomenology, including a spontaneous magnetic re-entrance and a possible change of the flux line lattice distribution [1].

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Confirming the phase diagram of the Shastry-Sutherland model with μ^+SR

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SL

One famous model for a two-dimensional magnetic system is the Shastry-Sutherland (SS) model, which considers an orthogonal dimer network of spin S = 1/2 [1]. The model predicts a dimer ground state for J/J' < 0.5, and a 2D antiferromagnetic (AFM) phase with significant quantum fluctuations is expected for J/J' > 1 [2]. However, the ground state of the intermediate region (0.5 < J/J' < 1) has been debated and various grounds states have been suggested: AFM order [3], helical order [1] or even columnar dimer [4]. The only known realisation of SS model is SrCu2(BO3)2 (SCBO). In order to confirm and determine the intermediate state of the SS model, series of hydrostatic pressure studies were initiated [5,6] and an intermediate frustrated plaquette phase above 21.5 kbar was determined by inelastic neutron scattering. [5]

We have initiated a ^+SR study to investigate the temperature/pressure dependency of the magnetic properties of SCBO [7]. Measurements in zero field and transverse field confirms the absence of long rang magnetic order at high pressures and low temperatures. These measurements suggest changes in the Cu spin fluctuation characteristics above 20 kbar, consistent with the formation of a plaquette phase. Therefore, the ground state of the SS model for the intermediate region is confirmed to be a plaquette state.

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MC

Development of a drift tube for study of a quantum mechanical scattering of muons in helum gas

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The first principle calculation involving muon needs to consider the effect of quantum fluctuations as well and it is still in a state of development. In order to verify the first principle calculation, the basic data for the collision cross section at low energy region corresponding to the binding energy of the muon and the target molecule is necessary. Especially the elastic scattering cross sections and the potential energy surfaces in the thermal energy region are extremely important for studying the muon behavior in the envi-ronment. However, since the collision experiment in this energy region is technically difficult, the report of experimental results for the interaction between two bodies in an isolated system, especially for the elastic scattering, is sparse. By applying the drift tube technique to the muon collision experiment, we consider that information of interactions between a muon and a molecule in gas can be obtained for less than 1 eV region.

The positive muons (2.7 MeV) generated are passed through an thin aluminum plate and to decelerate it to 100 keV. The decelerated muons enter the drift tube and travel a few centimeters by repeatedly colliding with buffer gas (100 kPa) and then thermalizes. The thermalized muon travels with certain mobility toward the back due to the uniform electric field (100 V/cm) applied to the inside of the drift tube. After the muons travel a few centimeters from the point where it thermalized, they decay to positrons. The positrons pass through the double scintillation fiber installed on the outside of the drift tube.By installing the fibers in double, the flight direction of the positron can be determined and the projection diagram to the central axis of the drift tube at the decay point can be obtained.

We have successfully measured the muon stop position at the S-line.

Phase diagram and charge-dynamics of electron-doped osmium based $Ba_2Na_{1-x}Ca_xOsO_6$ spin-orbit-coupled Mott insulator

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P

SCE

In recent years, 5d transition metal oxides have been the focus of increasing research interest, owing to their rich physics emerging from the interplay between electron correlations and strong spin-orbit coupling (SOC). Such SOC-induced insulating phases are frequently accompanied by the transition of the 5d ion to a magnetic state triggered by local structural distortions, in competition with ground states with exotic multipolar ordering [1].

Osmium based double perovskites $Ba_2Na_{1-x}Ca_xOsO_6$ (BNCOO), constitute a remarkable example of SOC-driven physics. In this system, electron doping of Os 7+ by etherovalent substitution of Na by Ca provides a further degree of freedom which strongly affects its magnetic ground state and raises TN from a few kelvin (x = 0) up to $\approx$ 40 K (x = 1). 23Na NMR provides evidence that the onset of magnetic order is anticipated by local static distortions of the cubic perovskite cell, breaking the local point symmetry [1].

Here we report on a combined muSR and NMR experiment which allows us to draw the full phase diagram whith both the local magnetic and structural symmetry breaking and ordering phases. In addition unambiguous evidence for the slow diffusion of dynamic lattice distortions in Ca-substituted BNCOO at temperatures well above their magnetic transitions is reported. Their occurrence in conjunction with electron doping support their identification with small polarons [2], as predicted by recent theoretical studies. We argue that such polarons may play a role as the dynamic precursors of the low-temperature static symmetry-breaking distortions which, in turn, seemingly trigger the magnetism in the system.

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NT

Thermal integrity test to muon production target by the induction heating system

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We report progress of which examines the thermal stability of the muon production target up to high temperature regime. We employed the high-frequency induction heating system as an indirect heater to target material, graphite, used with various purposes such as kitchenware, small blacksmiths. Prior to applying muon production target, we tested simple disc graphite with small chamber and RF feedthrough made by stainless steel, heat was delivered well to graphite, but metal RF feedthrough is bad for high temperature due to heating-up. We designed the flange for RF coil and supporters made by acetal (polyoxymethylene, POM). Tested with small chamber again, it worked under high vacuum condition (10^{-7} torr) and high temperature with full power loaded, but still plastic components are damaged by high temperature due to close to heating source. The thermal test is undertaken systematically at muon production chamber, combined with the engineering simulations, Ansys Mechanical/Maxwell simultaneously. This may be significant method to test various target as a thermal aspect without beam irradiation.

Magnetic structure refinement in the Mott insulator NiS_2

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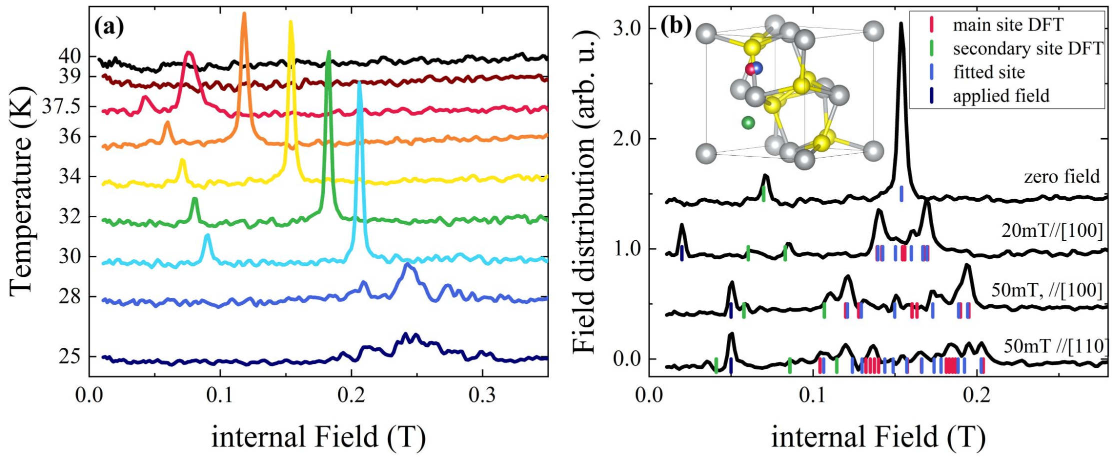

Figure 1: Local field distribution in (a) zero field and (b) transverse field. The curves are offset for clarity. The inset shows the candidate muon stopping sites.

We present muon spin spectroscopy (μSR) measurements on the antiferromagnetic Mott insulator NiS_2. This compound features two subsequent magnetic phase transitions around 38.9K and 29K associated with the opening of a Mott gap. From the the rotation dependence of transverse field μSR measurements (Fig. 1b) we confirm the magnetic space group 205.33 in the 38.9K to 29K phase, refined from neutron diffraction [1]. Using dipolar field calculations, we identify a candidate muon stopping site on a 24d Wyckoff position (blue site in Fig. 1b inset). We then calculate the muon stopping sites by using ab-initio density functional theory (DFT) and relaxing a supercell containing a single muon (i.e. hydrogen) impurity. Indeed the lowest energy muon site is found within 0.2 Angstrom of the experimentally determined one (red site in Fig. 1b inset). In addition, DFT predicts a second stopping site at an 8c Wyckoff position (green site in Fig. 1b inset), that can fully explain a small satellite frequency that we observe in the spectra. We then use the number of observed frequencies in the low temperature phase as a constraint to exclude magnetic order parameters inconsistent with our results.

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Piezoelectric-driven uniaxial pressure cell for muon spin relaxation experiments

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We present a piezoelectric-driven uniaxial pressure cell operable at cryogenic temperatures and optimized for muon spin relaxation and neutron scattering experiments. These methods often require larger sample sizes, and so the cell is designed to generate a force of up to 1000 N. It incorporates calibrated displacement and force sensors, the combined knowledge of which can determine quickly whether the sample and its mounts remain within their elastic limits. An earlier version of this cell was presented in [1] and cells of the current design [2] have accumulated use in multiple beamtimes [3-5], demonstrating its practicality. We anticipate this cell will be useful for a range of other materials, in which the Fermi surface or magnetic interaction strengths can be tuned leading to strong modifications of the electronic state.

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Negative muon spin rotation and relaxation on superconducting MgB_2

P

SU

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Although μ^+SR is widely used as a tool for studying a microscopic internal magnetic field in condensed matters over 40 years, the counterpart technique, i.e., μ^-SR is less common for such purpose mainly due to a low counting rate for reaching reliable statistics. However, the recent progress in the beam power and counting system overcame such problem. We therefore started a new μ^-SR project to measure a nuclear magnetic field in hydrogen storage materials and battery materials since 2018 [1].

In order to expand the μ^-SR work, we have attempted to measure the μ^-SR spectra on superconducting MgB_2 in ISIS to join the time reversal symmetry breaking business. This is because the past μ^+SR work on MgB_2 [2] reported the dynamic change in a nuclear magnetic field even below $T_c = 39$ K due to muon diffusion, resulting in difficulty to know the variation of the nuclear magnetic field below T_c. From a μ^-SR viewpoint, Mg almost lacks nuclear magnetic moments (since the natural abundance of ^{25}Mg with $I = 5/2$ is 10%), and as a result, the μ^-s captured by Mg feel a nuclear magnetic field formed by surrounding B and could detect the change in it accompanied with the superconducting transition. Note that the natural abundance of ^{10}B with $I = 3$ is 19.9% and that of ^{11}B with $I = 3/2$ is 80.1%. Thus, the μ^- captured by B should exhibits a fast decay due to its own nuclear magnetic moment, and the corresponding asymmetry will disappear.

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NT

Muonium 1S-2S spectroscopy with improved statistics

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Our purpose is precision measurement of the 1S-2S energy interval in Muonium, which is an exotic hydrogen-like atom consists of a positive muon and an electron. This purely leptonic system enables a precise calculation of the energy interval with the Standard Model without any concerns of the uncertainty from the charge radius of the nucleus, unlike the hydrogenatom. This advantage motivates us to measure the precise 1S-2S energy interval in Muonium with technology of laser spectroscopy and to determine the muon mass with the highest accuracy of 10 ppb. The improvement of muon mass accuracy has an impact on verification of the Standard Model, muon g-2/EDM experiment, for example. In addition, our technique of Muonium laser ionization is related to muon accelerator or muon microscope.

The energy interval accuracy has been statistically limited since 1999[1]. However, more powerful muon beam is available now at J-PARC in Japan and we are developing new UV laser system.

We will report a recent result of Muonium 1S-2S energy interval measurement at J-PARC. The event rate in our experiment is 50 times higher than the previous experiment. This dramatic improvement gives promising prospect for higher accuracy of 1S-2S energy interval and the muon mass accuracy in the future. **References**

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Using the TCDFT method to determine muon quantum effects

P

SC

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In calculations supporting μSR, it is important to deal with muon quantum effects. In previous studies, people have gone beyond the point-like muon approximation by using methods such as vibrational analysis of the zero point motion and path-integral molecular dynamics.[1-3] We now use a new method called Two-component DFT (TCDFT), which treats the muon as a fully quantized particle with its own wave-function.[4]

By modifying the Quantum Espresso DFT code[5], we have included the potential generated by a muon trial wave-function into the DFT calculation of electronic structure and optimum geometry. Once we have the crystal and electron structures, the new muon wave-function can be calculated by solving its Schrödinger equation via a finite difference method. Repeating iteratively the two-component calculation, we could get a self-consistent result for both the electron and muon wave-functions.

Due to many-body quantum effects, we need to use the Quantum Monte Carlo method to simulate the correlation energy and pair-correlation function. The former is used for the TCDFT calculation and the latter is used for coupling the individual wave-functions of the muon and electrons when calculating a specified physical quantity. In this work, we have already applied the new method to some ferromagnetic systems (Fe, Co, Ni) and the calculations are now being extended to some examples of semiconductors (Diamond, Si, Ge) and single molecules (TCNQ and acetone). From the results obtained so far, we have calculated muon hyperfine contact fields, which agree well with experiments and show good potential for further application of the method to other materials.

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SCE

$KAgF_3$: Using F–μ–F states to measure magnetic materials

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$KAgF_3$ is an antiferromagnet, consisting of Ag ions in the rare 2+ oxidation state which magnetically order at low temperature [1, 2]. Here we present a detailed μSR study of the compound, showing how measuring high statistics data in the high temperature, non-magnetic phase can be used to obtain information about the muon site. Knowledge of the muon site then guides the analysis of the high time resolution low-temperature data to reveal details of the magnetic ordering, the magnetic structure and the size of the magnetic moments. We also show, for the first time, how the Larmor precession of the perturbed nearest-neighbour fluorine nucleus can be observed with μSR, as this leads to a splitting of the muon precession frequencies allowing one to follow the magnetic order parameter in detail.

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Virtual Session

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NT

Studies and R&D efforts of the EMuS muon facility at CSNS

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CSNS (China Spallation Neutron Source) is a large scientific facility which was completed and entered in operation in March 2018. It is based on a high-power proton accelerator complex and is mainly for multidisciplinary research based on neutron scattering techniques. Other applications including muSR techniques have been considered from the beginning. The design study for an experimental muon source (the so-called EMuS) was started in 2007. Now a simplified scheme of EMuS is included in the CSNS-II project which has been approved and will start the construction soon. A study collaboration team from different institutions in China has devoted to the scheme design, physics design and R&D studies including prototyping of key devices. The user league for research at the future EMuS was also formed. EMuS will employ a proton beam of 1.6 GeV in beam energy, 25 kW in beam power and 2.5 Hz in repetition rate, which shares about 5% of the total beam power of 500 kW provided by the accelerator. Two design schemes on the target station and muon beamlines have been studied. The Baseline Scheme uses a conical graphite target that is placed in a superconducting solenoid of 5 T in magnetic field, and the muon beam transport line is also mainly based on superconducting solenoids. Up to eight endstations for different research fields using different kinds of muon beams can be arranged. The Simplified Scheme uses a free and stab-like graphite target of long interaction length, and four muSR spectrometers are foreseen. The two schemes share the same general layout, thus the simplified Scheme can be upgraded to the Baseline Scheme easily. This presentation will introduce the design aspects and R&D efforts of EMuS.

Physical design of the EMuS muon beamlines

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NT

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with
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The accelerator complex of China Spallation Neutron Source (CSNS) is delivering a proton beam of 100 kW in beam power, 1.6 GeV in kinetic energy and 25 Hz in repetition rate, which will be upgraded to 500 kW in the CSNS-II project. A muon facility, the so-called Experimental Muon Source (EMuS), will be added to CSNS in the upgrading project. As a standalone facility located in a new experimental hall, EMuS will employ 25 kW or 5% of the total beam power. EMuS is planned to provide multiple muon beams for different applications. This presentation will introduce the physics design of the muon beamlines in the baseline scheme. With a conical graphite target located in a high-field superconducting solenoid, EMuS can provide muon beams of different characteristics to meet the requirements of different applications. For example, surface muon beams and a decay muon beam are for μSR applications, a negative muon beam for Muonic X-ray analysis, a high-momentum muon beam for muon imaging, etc. The trunk muon beamline that covers a large momentum range from 28 MeV/c to 450 MeV/c is based on superconducting solenoids. The branch beamlines to different endstations are based on either room-temperature magnets or solenoids. A one-to-three spatial beam splitting method with the surface muon beam is applied to serve three μSR spectrometers simultaneously. Sophisticated beam collimation systems are designed to provide muon beams with higher polarization and smaller beam spots at the μSR spectrometers.

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SU

Superconducting Gap Structure in La$_2$(Cu$_{1-x}$Ni$_x$)$_5$As$_3$O$_2$: A μSR Study

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The relationship between magnetism and superconductivity has been one of the most discussed topics in condensed matter physics. Within the BCS framework, magnetic impurities can act as pairing breaking agents rapidly suppressing superconductivity. However in unconventional superconductors, such as cuprates and iron-based superconductors, magnetic impurities may enhance superconductivity. In the newly discovered layered superconductor La$_2$(Cu$_{1-x}$Ni$_x$)$_5$As$_3$O$_2$ (x = 0.37, 0.45), when Cu^{2+} is replaced by Ni^{2+}, the superconducting transition temperature T_c exhibits a dome structure as the substitution ratio increases and the superconductivity can be preserved until the substitution ratio exceeds 60%.

Here, we report muon spin rotation and relaxation (μSR) measurements on the newly discovered superconducting material La$_2$(Cu$_{1-x}$Ni$_x$)$_5$As$_3$O$_2$ (x = 0.37, 0.45), which help to further study the superconducting gap symmetry of this Ni-doped compound in both underdoped and overdoped regions.

Transverse-field μSR experiments of both samples show that the superfluid density tends to saturate at low temperatures, indicating a nodeless superconducting gap. The single-gap s-wave BCS model best fits the temperature dependence of superfluid density in the overdoped areas and the $s + d$-wave model for the underdoped areas, repectively. The absolute values of zero-temperature magnetic penetration depth $\lambda_{ab}(0)$ were found to be 421 nm and 422 nm for x = 0.37 and 0.45, respectively.

Zero-field μSR rate of $x = 0.45$ does not show an obvious increase with the temperature cooling down, revealing no spontaneous magnetic moments below the superconducting transition temperature T_c, indicating that time-reversal symmetry (TRS) is preserved in the superconducting state of the overdoped region.

Fluctuating magnetic droplets immersed in a sea of quantum spin liquid

P

SL

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The search of quantum spin liquid (QSL), an exotic magnetic state with strongly-fluctuating and highly-entangled spins down to zero temperature, is a main theme in current condensed matter physics. However, there is no smoking-gun evidence for deconfined spinons in any QSL candidate so far. The disorders and competing exchange interactions may prevent the formation of an ideal QSL state on frustrated spin lattices. Here we report comprehensive and systematic measurements of the magnetic susceptibility, ultralow-temperature specific heat, muon spin relaxation (µSR), nuclear magnetic resonance (NMR), and thermal conductivity for NaYbSe2 single crystals, in which Yb3+ ions with effective spin-1/2 form a perfect triangular lattice. All these complementary techniques find no evidence of long-range magnetic order down to their respective base temperatures. Instead, specific heat, µSR and NMR measurements suggest the coexistence of quasi-static and dynamic spins in NaYbSe2. The scattering from these quasi-static spins may cause the absence of magnetic thermal conductivity. Thus, we propose a scenario of fluctuating ferrimagnetic droplets immersed in a sea of QSL. This may be quite common on the way pursuing an ideal QSL, and provides a brand-new platform to study how a QSL state survives impurities and coexists with other magnetically ordered states.

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Design of the First μSR Spectrometer at China Spallation Neutron Source

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The Phase II upgrade project of the China Spallation Neutron Source includes the construction of a surface μ beam line and a μSR spectrometer, which will be the first μSR spectrometer built in China. Here we report the conceptual design of the spectrometer including the sample environment. Based on the design parameters of the muon beam, we design the spectrometer with a large number of detector units to maximize the counting rate. We designed the sample chamber with a fly-past structure to reduce the background. In this report we describe the conceptual design and simulation of the spectrometer.

Intrinsic new properties of a quantum spin liquid

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SL

Quantum fluctuations are expected to lead to highly entangled spin-liquid states in certain two-dimensional spin-1/2 compounds. We have synthesized and measured thermodynamic properties and muon spin relaxation rates in the copper-based two-dimensional triangular-lattice spin liquids $Lu_3Cu_2Sb_3O_{14}$ and $Lu_3CuZnSb_3O_{14}$. The former is the least disordered of this kind discovered to date. Magnetic entropy generation at high temperatures has been ruled out after carefully correcting for the lattice specific heat. Surprisingly, roughly half of the magnetic entropy is missing down to temperatures of$O(10^{-3})$ the exchange energy, independent of magnetic field up to $g\mu_B H > k_B \Theta_W$, where Θ_W is the Weiss temperature. The magnetic specific heat divided by temperature $C_M(T)/T$ and muon spin relaxation rate $\lambda(T)$ are both temperature-independent at low temperatures, followed by logarithmic decreases with increasing temperature. This behavior can be simply characterized by scale-invariant time-dependent fluctuations with a single parameter. Since no cooperative effects due to impurities are observed, the measured properties are intrinsic. They are evidence that in $Lu_3Cu_2Sb_3O_{14}$ massive quantum fluctuations lead to either a gigantic specific heat peak from singlet excitations at very low temperatures or, perhaps less likely, an extensively degenerate possibly topological singlet ground state.

P

NT

Intensity measurement of the surface muon beam of MELODY

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with
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A Muon station for sciEnce, technoLOgy and inDustrY (MELODY) project will be constructed at China Spallation Neutron Source. The Phase I project will provide a surface muon beam with a pulse width of 100 ns at a rate over 10^{5+}/pulse. Accurate monitoring of the muon beam intensity is essential for the calibration of the µSR spectrometer. The key of the beam intensity measurement is to distinguish positrons, the major contamination of the muon source. A double-stacked scintillator detector scheme has been proposed, which can use pulse shape discrimination method to determine the intensity of positrons and muons. Detailed description of the detector principle and simulated result will be presented.

Design and optimization of the surface muon beamline of MELODY

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We report the surface muon beamline design of the Muon station for sciEnce, technoLOgy and inDustrY (MELODY) project based on China Spallation Neutron Source (CSNS). Based on the 1.6GeV proton beam, a surface muon beam line has been designed to deliver a muon flux of 10^5+/s to the μSR experiment area. In order to transport the large emittance muon beam, a series of solenoids for focusing combined with large-aperture dipoles are used. Moreover, we use genetic algorithm to optimize the muon beam line to maximize the beam intensity in a small beam spot.

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Target design of MELODY

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The Muon station for sciEnce, technoLOgy and inDustrY (MELODY) is foreseen to be the first muon source in China and to be located at the China Spallation Neutron Source in Dongguan. The stand-alone target station has been studied for the surface muons and the pions production. In this report, we aim to describe the design of the target station, including the mechanical design, the radiation shielding and optimization of the target in order to provide the highest rates of surface muons and pions to the capture solenoids under certain emmittance selections.

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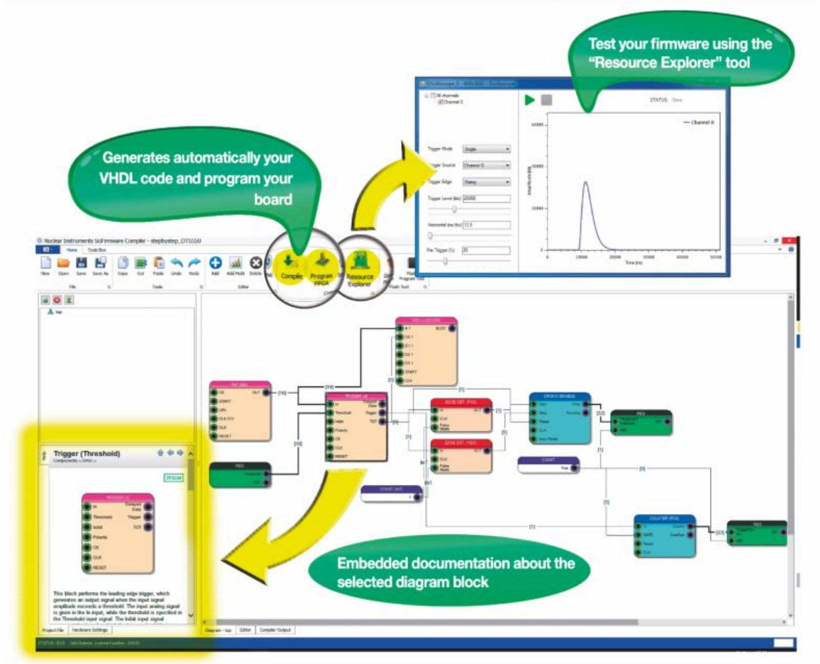
SCI-Compiler and open FPGA platforms

HIGHLIGHTS

- **Block-diagram-based** firmware generator and compiler for CAEN programmable boards
- **Automatic VHDL generation** starting from a block diagram
- **Blocks** implementing high-level functions: oscilloscope, charge integration, TDC, logic gates, digital signal processing, ….
- Suited even for **non-expert** firmware programmer
- **SCI-Compiler SMART kit** for evaluation and learning with basic hardware
- Automatic generation of drivers, libraries and demo software
- **Remote customization service** to generate firmware with no need of any FPGA compiler installed locally



We introduce an innovative method to **simplify the firmware development** on **CAEN Open FPGA boards**. This method is based on a **block-diagram-based** software, called **SCI-Compiler**, that uses a set of high-level functionalities (blocks) to mask the real firmware coding. In this way, it is possible to obtain a **fpga firmware** and **readout libraries for Windows and Linux** starting from a rather simple block diagram structure

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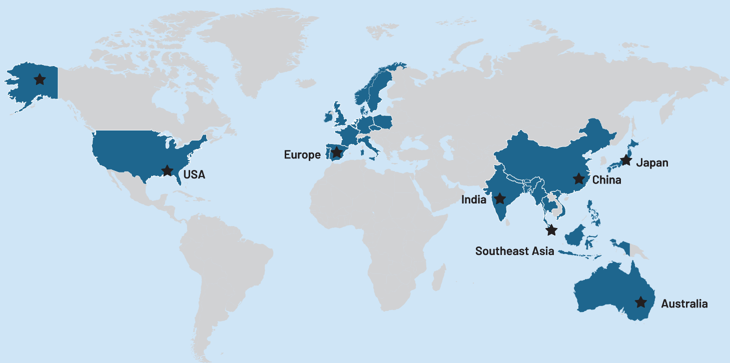

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