New Applications of μSR

A workshop focussed on
Studies of Soft Matter, Spectroscopy of Excited States and a discussion of Muon Perturbations

3-4 September 2015;
Queen Mary University of London, UK

Science & Technology Facilities Council
ISIS

SEVENTH FRAMEWORK PROGRAMME

Queen Mary University of London

Venue

The meeting is being held on the Mile End Campus of Queen Mary, University of London, in the Mathematical Sciences building (shown on the title page and number '4' on the campus map).

Lectures will be in the Maths Lecture Theatre, and a registration desk will be available in the foyer of the building from about 10:00 on the Thursday.

If you have asked for campus accommodation you should be contacted directly by the University with directions. You should be able to check into rooms from 2pm onwards on the day of arrival. On arrival report to the Residences Reception in France House, this is open 24 hours. Rooms should be vacated by 10am on the day of departure, and you are asked to go to the Reception in France House to check out. Breakfast is served in the Curve which is open 07:00-10:00 hours – you'll receive a breakfast voucher in your key pack.

Travel to the Mile End Campus

Maps to help reach the campus can be found here. Travel around London and from the airports can be planned using the Transport for London website, while the National Rail website is useful for those travelling by train from further away.

For those using the underground, the two closest stations to the campus (within five minutes' walk) are Mile End (Central Line, District Line, Hammersmith & City Line) and Stepney Green (District Line, Hammersmith & City Line).

It's not recommended to drive to the campus as there is no on-campus car park for delegates. If you need a parking space, perhaps because of reduced mobility, please contact Alan Drew to arrange a solution.

Mile End Campus

Educational/Research

ArtsOne	37
ArtsTwo	35
Arts Research Centre	39
The Bancroft Building	31
Bancroft Road Teaching Rooms	10
Computer Science Building	6
Engineering Building	15
Fogg Building	13
G.O. Jones Building	25
Geography	26
Informatics Teaching Laboratories	5
Joseph Priestley Building	41
Library	32
Law	36
Lock-keeper's Graduate Centre	42
Mathematical Sciences	4
Occupational Health and Safety Directorate	12
The People's Palace/Great Hall	16
Queens' Building	19
Temporary Building	61

New Graduate Centre construction site 18

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Albert Stern Cottages	3
Albert Stern House	1
Beaumont Court	53
Chapman House	43
Chesney House	45
Creed Court	57
France House	55
Fellden House	46
Hatton House	40
Ifor Evans Place	2
Lindop House	21
Lodge House	50
Lynden House	59
Maurice Court	58
Maynard House	44
Pooley House	60
Sellincourt House	51
Varey House	49

Facilities

Advice and Counselling Service	27
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Careers Centre	19
Clock Tower	20
CopyShop	56
The Curve	47
Drapers Bar and Kitchen	8
Canalside	63
Ground Café	33
The Hive	24
Infusion	9
IT Services	19
Mucci's	29
Occupational Health Service/ Student Health Service	28
Octagon	19a
Police Box	38
Portering and Postal Services	17
Qmotion Health and Fitness Centre Sports Hall	7
Santander Bank	62
Security/France House Reception	54
St Benet's Chaplaincy	23
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Student Enquiry Centre	19
Village Shop	52
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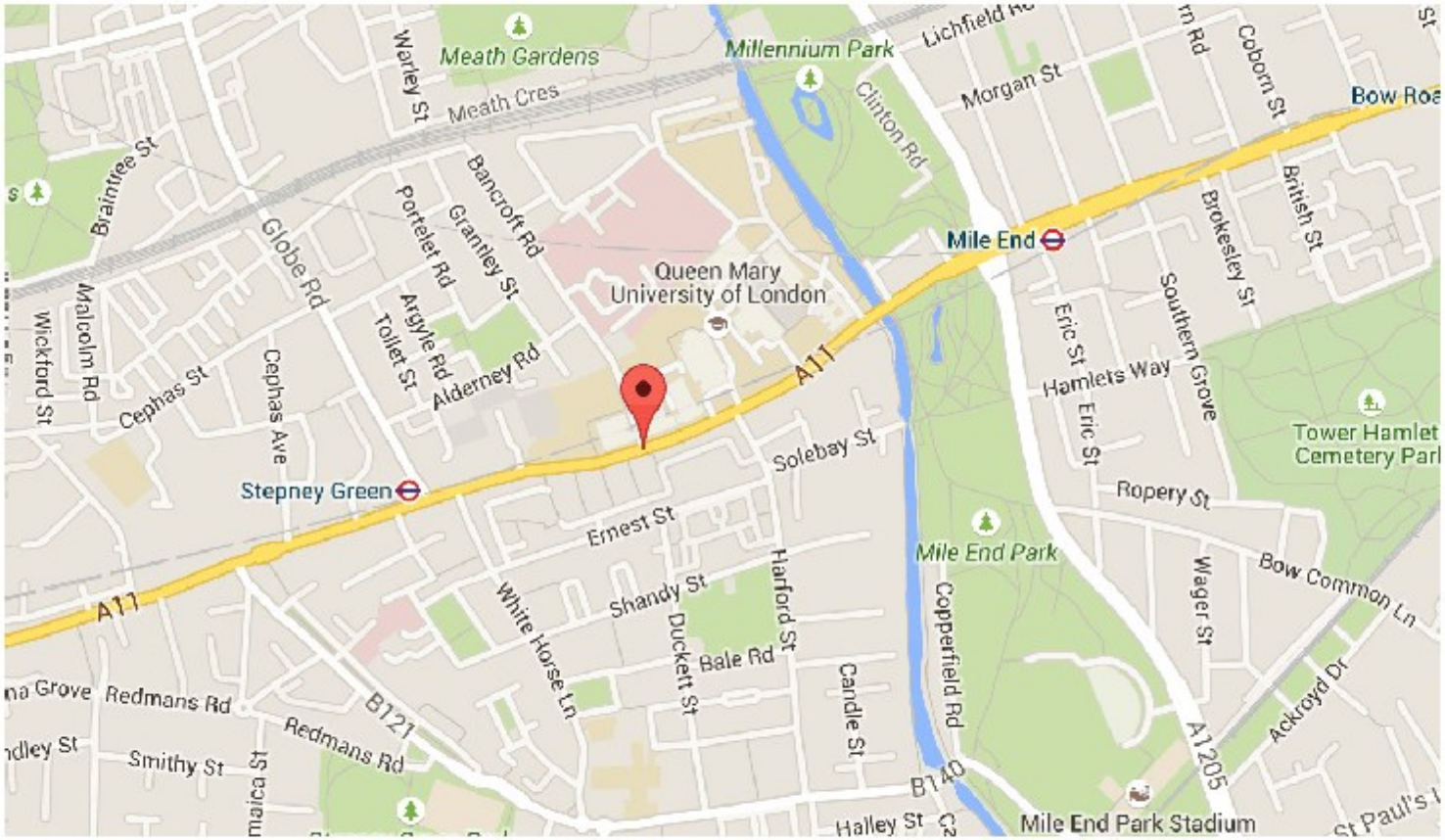

Programme

Thursday, September 3rd

10:00 Refreshments

10:40 Welcome
Alan Drew (Queen Mary, University of London)

Session A: Excitations I *(James Lord)*

10:45 Developing experimental techniques for photo-μSR - Examples in semiconductor physics
Koji Yokoyama (Queen Mary, University of London)

11:15 Foundations of muon-laser spectroscopy
Khashayar Ghandi (Mount Allison University)

11:45 Photo-induced effects in semiconductors probed by Low Energy Muons
Thomas Prokscha (Paul Scherrer Institute)

12:15 Muonium Reactivity and Isotopic Mass Effects from State-Selected Reactants: a case study of the Mu + H_2(v=1) reaction rate
Don Fleming (UBC / TRIUMF)

12:45 Lunch

Session B: Soft Matter I *(Peter Baker)*

13:45 Applications of muon spectroscopy in surfactant based soft matter
Nigel Clayden (University of East Anglia)

14:15 Muons for Energy and Environmental Science
Martin Månsson (KTH)

14:45 Antioxidant Capacity
Upali Jayasooriya (University of East Anglia)

15:15 Spintronic properties of organic spin valve devices measured with muon spin rotation
Leander Schulz (Sichuan University)

15:45 The magnetic field dependent crossover between hyperfine and spin-orbit interactions in organic semiconductors
Ke Wang (Queen Mary University of London)

16:00 Refreshments

Session C: Muon Perturbations I *(Francis Pratt)*

16:30 Muon sites and spin dynamics in the one-dimensional molecular spin chain $Cu(pyz)(NO_3)_2$
Tom Lancaster (Durham University)

17:00 A DFT+μ study of Pr-based pyrochlores: the effect of muon-induced distortions in quantum spin ice
Franz Lang (Oxford University)

17:30 The Non-Centrosymmetric Helical Magnet MnSi: a μSR Study
Alex Amato (Paul Scherrer Institute)

18:30 Posters and pre-dinner drinks

19:30 Dinner

Friday, September 4th

Session D: Excitations II *(Fiona Coomer)*

09:00 Applications of photomusr – a local probe investigation of excitons
Alan Drew (Queen Mary, University of London)

09:30 Muon probing of spin-polarized conduction electrons in semiconductors
Harry Tom (University of California, Riverside)

10:00 Microwave assisted chemical reactions – applications of a muon-microwave interface
Khashayar Ghandi (Mount Allison University)

10:30 Refreshments

11:00 New Science with Radio Frequency Techniques
Stephen Cottrell (STFC)

11:30 Bulk non-destructive elemental analysis using muons
Adrian Hillier (STFC)

Session E: Muon Perturbations II *(Francis Pratt)*

12:00 Wien Effect for Magnetic Monopoles in Spin Ice
Steve Bramwell (University College London)

12:30 What do muons do inside spin ice?
Steve Blundell (University of Oxford)

13:00 Lunch

Session F: Soft Matter II *(Adrian Hillier)*

14:00 Muon studies of polymers
Nicola Morley (University of Sheffield)

14:30 Probing artificial [Fe,Fe] Hydrogenase systems
Joseph Wright (University of East Anglia)

15:00 First Evidence for the Interaction of a Free Radical, the MuC_6H_6 Radical, with a Au NP Surface in a Mesoporous Silica Enviroment
Don Fleming (UBC / TRIUMF)

15:30 Close of meeting

Participants

Alex Amato	Paul Scherrer Institute
Peter Baker	STFC
Adam Berlie	STFC
Pabitra Kumar Biswas	STFC
Stephen Blundell	Oxford University
Steve Bramwell	UCL Physics
Dominic Carter	Queen Mary University of London
Shuqun Chen	Queen Mary University of London
Nigel Clayden	University of East Anglia
Fiona Coomer	STFC
Steve Cottrell	STFC
Steve Cox	STFC
Alan Drew	Queen Mary University of London
David Dunstan	Queen Mary University of London
Donald Fleming	UBC/TRIUMF
Khashayar Ghandi	Mount Allison University
Adrian Hillier	STFC
Upali Jayasooriya	University of East Anglia
Tom Lancaster	Durham University
Franz Lang	University of Oxford
Tom Loe	STFC
James Lord	STFC
Martin Mansson	KTH Royal Institute of Technology
Jingliang Miao	Queen Mary University of London
Nicola Morley	University of Sheffield
Prashantha Murahari	Queen Mary University of London
Anthony Phillips	Queen Mary University of London
Francis Pratt	STFC
Thomas Prokscha	Paul Scherrer Institute
Leander Schulz	Sichuan University
Christopher Scott	University of Southampton
Paul Shaver	Mount Allison University
Mingyign Song	Queen Mary University of London

Pardis Tabaee	Queen Mary University of London
Harry Tom	University of California, Riverside
Ke Wang	Queen Mary University of London
Tom Wood	STFC
Joseph Wright	University of East Anglia
Koji Yokoyama	Queen Mary University of London
Sijie Zhang	Oxford University

Abstracts

Talks

Koji Yokoyama (Queen Mary University of London)

Developing experimental techniques for photo-μSR - Examples in semiconductor physics

Koji Yokoyama

The ERC funded project, Muon Spectroscopy of Excited States (MuSES), has started in 2013 and installed a high-power laser system in the HiFi spectrometer. After successful commissioning and a few in-house experiments the system is now open for users. In this talk we introduce the laser system: the overall design, specification of the laser system, and a few experimental techniques. Then we show our recent measurement on photo-carrier lifetime in silicon as an example of photo-μSR experiment in HiFi.

Khashayar Ghandi (Mount Allison University)

Foundations of muon-laser spectroscopy

Khashayar Ghandi

In this presentation I will describe our original works on laser muonium chemistry at ISIS. This will be more of a presentation on a historical journey, describing the original ideas from a few successful proposals that I have submitted to ISIS as well as published data from some of those and some unpublished data that is in the preparation for publication. The presentation will discuss the science and technical challenges that we had so far as well as new works that could be done via collaborations using the new laser system at ISIS.

Microwave assisted chemical reactions – applications of a muon-microwave interface

Khashayar Ghandi

Microwave (MW) assisted chemical reactions are of interest as a green, energy efficient alternative to conventional thermal heating for chemical processes. MW irradiation interacts with the chemical reactants in two broad ways. The first is through thermal heating, whereby MW energy is absorbed and converted to thermal energy. The second is through non-thermal microwave effects (NTME), whereby the observed changes in chemical reactions cannot be rationalized by the thermal heating. Despite the use of MW in industry and in the lab scale for synthesis and other applications very little in situ data exist to understand the effects of microwave in material science and chemical applications at the microscopic and in the range of ns to microseconds time scales. In this presentation I will discuss some of the applications of a muon-MW interface for such studies as well as discuss the challenges for such studies

Thomas Prokscha (Paul Scherrer Institute)

Photo-induced effects in semiconductors probed by Low-energy Muons

Thomas Prokscha, PSI

The controlled manipulation of the charge carrier concentration in nanometer thin layers is the basis of current semiconductor technology. Besides applying electric fields to control charge carrier concentrations, photo-generated charge carriers provide another fascinating possibility to tune the charge carrier concentration at semiconductor surfaces or interfaces. Low-energy μSR is ideally suited to study photo-induced charge carrier concentration profiles at the surface of semiconductors due to the tunable muon range between a few nm and about 200 nm, providing a perfect overlap of muon stopping distributions and the region of highest photon absorption close to the surface. The change in carrier concentration is detected by a change of the μSR relaxation rates or/and a change of diamagnetic and paramagnetic fractions. We present a description of the current experimental setup and the results of recent experiments on Ge – where we discovered a persistent, photo-induced inversion of the Ge surface layer [1], and observed the depletion of holes at the surface of p-type Ge – and ongoing work on GaAs.

[1] T. Prokscha et al., Scientific Reports **3**, 2569; DOI:10.1038/srep02569 (2013).

Don Fleming (UBC/TRIUMF)

Muonium Reactivity and Isotopic Mass Effects from State-Selected Reactants: a case study of the Mu + H_2(v=1) reaction rate.

Abstract:

The use of isotopes in the sciences and particularly in the study of mass effects on reaction rates dates from the discovery of deuterium in 1932. However, with only a factor of two difference in mass between H and D atoms their comparison of reaction rates as a "test" of rate theory has a limited impact. A far greater impact is provided by muon science and in particular from long-standing studies of muonium (Mu) reactivity, the lightest isotope of hydrogen, and more recently of the reaction rates of its heaviest isotope, the muonic He atom (^{4}Heμ). Examples will be presented.

The use of lasers in the broadly based field of reaction kinetics studies, from both state-selected reactants as well as probing rovibrational final states, has a long history, hugely facilitated by the use of stable mass probes. It is *much more difficult* to embrace studies of this nature in muon science. An early (non-laser) example of identifying final states was provided in a chemiluminesence study of the Rydberg states of NeMu* at TRIUMF, in comparison with quantum theory [S. Baer et al., *J. Chem. Phys.*, 1993]. The only example, to our knowledge, of Mu reactivity from a *state-selected* reactant, has been recent work on the Mu +H_2(v=1) reaction rate, where stimulated Raman pumping utilizing the Nd:YAG laser at 532 nm (green) at the RIKEN/RAL Facility at ISIS was used to produce H_2 in its first vibrational state, identified by measuring the amount of "1st-Stokes" red light at 683 nm [P. Bakule et al., *J. Phys. Chem. Lett*, 2012; J. Phys. B, 2015]. These results and their comparison with rigorous quantum rate theory, as well as a proposed measurement of the Mu + CH_4(v) reaction, will be discussed.

First Evidence for the Interaction of a Free Radical, the MuC_6H_6 Radical, with a Au NP Surface in a Mesoporous Silica Enviroment.

Abstract:

Transient free radicals play important roles as reactive intermediates in heterogeneous catalyis. The μSR technique is well suited to their study since these radicals typically have $\sim \mu$s lifetimes. In recent work in the faujasitic zeolites (NaY, HY and USY), well-known heterogeneous catalysts, the Hfcc and LCR line shapes for both the Mu-butyl and Mu-cyclohexadieynl radicals exhibited a clear sensitivity to the nature of their binding sites [D.G. Fleming et al., *J. Phys. Chem.*, 2011, 2013]. This prompted our interest in the study of metal nanoparticles (MNPs) encapsulated in SBA-15 mesoporous silica, Au in particular, also well-known catalytic environments,

Grains are micron size with overlaping pore channels of ~10-15 nm in dia., into which Mu diffuses. These pores have hexaganol cross sections with Au NPs localized in the corners, thereby preventing their aggregation. The interactions of the MuC_6H_6 radical with Au NPs of ~25 and 8 nm sizes have been investigated at benzene (Bz) loadings from sub-monolyaer to several monolayers, bound to the NP sites, thereby forming the MuC_6H_6 radical at these sites.

The LF-μSR Asy(t) data has been analyzed by a two-component function. The field dependence of the fast component exibits a SE mechanism of Mu with paramagnetic centers either on the Au NPs or induced by them. [M. Dehn et al., *2014 μSR Proceedings*, pg. 012006]. The amplitde of the slow component scales with Bz loading with an enhanced dependence for the ~8 nm Au NP. Clear LCR signals are seen for multi-layer loadings for ~25 nm Au [J. Xiao et al., *2014 μSR Proceedings*, pg. 012044] but these are apparent even at a nominal monolayer loading for the ~8 nm size. More detailed results of the data analysis, still ongoing, will be presented.

Nigel Clayden (University of East Anglia)

Applications of muon spectroscopy in surfactant based soft matter

Nigel Clayden

Applications of muon spectroscopy in surfactant based soft matter will be described. The underlying requirements will be highlighted, in particular the need to tailor the system to the nature of muon spectroscopy. An introduction will be given to the most flexible technique, avoided level crossing muon spectroscopy, stressing how the fundamental experimental parameters, the hyperfine coupling constants, can be used to study surfactant based systems. Three areas will be touched upon: co-surfactant partitioning, surfactant dynamics and the exchange kinetics of small molecules. These examples illustrate how muon spectroscopy might be used in the future to investigate more applied problems. To conclude, areas of potential interest in lipid nanoparticles will be mentioned.

Martin Månsson (KTH Royal Institute of Technology)

Muons for Energy and Environmental Science

Martin Månsson

Muons are very sensitive probes of static and dynamic fields within bulk or thin film materials. During the last decade our research collaboration has developed several protocols for using μSR to study ion dynamics in energy related materials. In this talk I will briefly introduce our experimental method and its advantages compared to other techniques. I will then summarize some of our published work regarding ion diffusion in Li- and Na-battery compounds as well as hydrogen storage materials. Finally, we have recently initiated a new research project concerning clays for applications in nuclear waste management. I will introduce the general goals for our project and present very recent and novel μSR results concerning Na-ion diffusion in these compounds.

Upali Jayasooriya (University of East Anglia)

Antioxidant Capacity

Jamie Peck[2], Suzie Jones[1], Martin Loftus[1], Stephen Cottrell[2] and Upali A Jayasooriya[1*]
[1] School of Chemical Sciences, University of East Anglia, Norwich NR4 7TJ, UK
[2] ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, Didcot OX11 0QX

Abstract

There are a number of methods of antioxidant capacity measurement that exist in the literature using a variety of techniques, but results from none of these techniques appear to agree with each other.* These techniques in general involve the measurement of the relative rate of quenching of a stable radical species by the material under scrutiny compared to a standard molecule, as a measure of the antioxidant capacity. The unsatisfactory nature of the extant techniques is mainly due to the following inherent problems. These methods depend on relatively stable radical species, which are inherently large, for their measurements, thus including an unquantified steric contribution to the measurement, due to the choice of different probe radicals. Secondly the standard compound used for the comparison depends on the medium of measurement whether it is aqueous or lipid. Here we present the use of Muon spectroscopy (μSR), which uses the smallest radical known, muonium, as the probe species, which eliminates both these problems. Dependence on the steric requirements of the probe molecule is eliminated due to the small size of the muonium radical probe. Being applicable to all types of liquids both aqueous and lipid, eliminates the need for the practice of using a third molecular species as a standard. The method is illustrated using our preliminary measurements on vitamins E, C and K.

* See for example: J Tabart, C Kevers, J Pincemail, J-O Defraigne, J Dommesa; Food Chemistry, 113 (2009) 1226–1233

Leander Schulz (University of Oxford)

Spintronic properties of organic spin valve devices measured with muon spin rotation

L. Schulz[1,2], L. Nuccio[3], M. Willis[3], P. Desai[3], P. Shakya[3], T. Kreouzis[3], V. K. Malik[2], C. Bernhard[2], F. L. Pratt[4], N. A. Morley[5], A. Suter[6], G. J. Nieuwenhuys[6], T. Prokscha[6], E. Morenzoni[6], W. P. Gillin[3] and A. J. Drew[1,2,3,4]

[1]*College of Physical Sciences and Technology, Sichuan University, Chengdu 610064, China*
[2]*Department of Physics and FriMat, University of Fribourg, 1700 Fribourg, Switzerland*
[3]*Queen Mary University of London, School of Physics, Mile End Road, London E1 4NS, UK*
[4]*ISIS Facilities, Rutherford Appleton Laboratory, Chilton, Didcot OX11 0QX, UK*
[5]*Dep. of Mat. Science and Eng., University of Sheffield, Mappin Street, Sheffield S1 3JD, UK*
[6]*Laboratory for Muon-Spin Spectroscopy, PSI, CH-5232 Villigen, Switzerland*

Using the spin degree of freedom for electronic applications has been the goal and - to a large extend - a dream for a large community ranging from physicists to electrical engineers. Of particular interest has always been the manipulation of the spin in materials and spintronic properties of devices, as it holds the key to potentially revolutionise the electronics industry.

I will begin with a general introduction to how we can access spintronic properties of organic-base spin valves with low-energy muon spin rotation (LE-MuSR). After a brief intermezzo about the properties of the studied devices, I will talk about results of a proof-of-principle experiment [1], where it was demonstrated that a) the depth dpendence of the spin current can be measured and b) the spin coherence length is strongly correlated to the magnetoresistive properties of the device [1].

Eventually, I will show that a modification of the sign of the spin polarisation of charge carriers that are injected across a metal-organic interface of fully functional organic-metal spin valve devices can be realised by inserting an additional simple polar layer [2]. At a microscopic level, we measured the spin current with LE-MuSR. This inversion of the spin polarisation is also observed with macroscopic magneto-transport measurements [2].

[1] A. J. Drew et al., Nature Materials 8, 109 (2009).

[2] Schulz L et al., Nature Materials 10, 39–44 (2011).

Ke Wang (Queen Mary University of London)

The magnetic field dependent crossover between hyperfine and spin-orbit interactions in organic semiconductors

Ke Wang

Identifying the individual contribution of spin-orbit coupling (SOC) and hyperfine interaction (HFI) to electron spin relaxation (eSR) is a big issue in organic spintronics. Measuring the electron spin relaxation rate (eSR) as a function of temperature, magnetic field, and targeted chemical substitution can differentiate between the individual contributions, which requires reliable method. The so-called avoided level crossing muon spin resonance (ALC-μSR) is an extraordinarily sensitive probe of dynamics in organic molecules, including the electron spin relaxation rate [1][2]. In the ALC field region where the HFI from nuclear spins is decoupled, the predominant mechanism of eSR is evidently SOC in organic molecules [2].

In order to achieve a full picture of field-dependent eSR, the off-resonance muon spin relaxation as a function of magnetic field can be used to obtain the electronic dynamics, though it is difficult to interpret and model, as all types of dynamics from all muonium states in the system contribute. Here we present the muon relaxation rate as a function of magnetic field, for both hydrogenated (H) and deuterated (D) pentacene, to try to disentangle the various mechanisms at play. From our data, at lower intermediate fields, there is a significant difference in the muon spin relaxation rate, is suggesting that all HF relaxation processes directly or indirectly contribute to the electron spin relaxation. Meanwhile, it is clear that above a modest field, the muon's relaxation rate is identical within the experimental error for the H and D pentacene, suggesting only SOC is present. To fully understand the underlying mechanisms of muon relaxation at low fields, we performed simulations with the software QUANTUM [3]. The simulation shows consistent results to the B-field dependent crossover feature of the HFI and SOC. The temperature-dependence of the muon relaxation rate is also able to validate the simulation model, with the explanation from the DFT on the molecular vibrational modes. By putting all these together we are developing a comprehensive understanding of HFI and/or SOC mediated eSR in organic spintronics.

[1] L. Schulz et al., Phys. Rev. B 84, 085209 (2011)

[2] L. Nuccio et al., Phys. Rev. Lett. 110, 216602 (2013)

[3] J. S. Lord, Physica B 374, 472 (2006).

Tom Lancaster (University of Durham)

Muon sites and spin dynamics in the one-dimensional molecular spin chain $Cu(pyz)(NO_3)_2$

Tom Lancaster

We discuss the results of our recent measurements of spin dynamics in the one-dimensional molecular spin chain $Cu(pyz)(NO_3)_2$, along with density functional theory calculations of the probable muon sites. It has been suggested that muons are not innocent probes of magnetism in systems such as these and we assess the proposed muon sites in terms of their influence on the local environment. Our measurements of diffusive spin transport turn out to provide a consistency check with the muon site calculations and we argue that the muon site sensitive to the magnetism of the system makes the muon effectively an innocent probe.

Franz Lang (University of Oxford)

A DFT+μ study of Pr-based pyrochlores: the effect of muon-induced distortions in quantum spin ice

Franz Lang

Muon spin relaxation (MuSR) is a powerful technique to investigate local magnetic structures and although it has been successfully applied to probe magnetic order, spin freezing and spin dynamics, etc., it has been a long standing question whether muons are a completely passive probe or can sometimes influence measurements through strongly perturbing their local environments. We have identified an experimental scenario in which indeed the MuSR observations reflect the response of a compound to the presence of the muons, rather than its intrinsic behaviour. I will present how we utilized density functional theory (DFT) calculations in the quantum spin ice candidates $Pr_2B_2O_7$ (B=Sn, Zr, Hf) to explain the detected static distribution of magnetic moments through a muon-induced splitting of the non-Kramers ground state of the Pr ions close to the muons. I will discuss the relevance of our observations to muon experiments in other magnetic compounds and how DFT calculations can in general be used to characterise the local environment implanted muons experience. Further information can be found in F.R.Foronda *et al*. PRL 2015.

Alex Amato (Paul Scherrer Institute)

The Non-Centrosymmetric Helical Magnet MnSi: a μSR Study

Alex Amato
Paul Scherrer Institute

I will present a precise TF and ZF μSR study of the non-centrosymmetric cubic system MnSi. The temperature, angular and field dependences of the muon-Knight-shift allow us to precisely determine the muon-stopping localization (4a site of the P213 crystallographic structure). The knowledge of the muon-site is also used to unravel the details of the field distribution measured below the magnetic transition temperature T_C. In particular the helicity of the helimagnetic state could be confirmed.

This work is a first step towards a quantitative study of the skyrmion phase by μSR and is the result of a collaboration between PSI, CEA Grenoble, University of Parma, University of Cagliari and Babes-Bolyai University.

Alan Drew (Queen Mary University of London)

Applications of photomusr – a local probe investigation of excitons

Dr. A. J. Drew, Queen Mary University of London
(A.J.Drew@qmul.ac.uk)

Organic semiconductors fall into a class of materials that shows significant potential for future applications and as a result, the field is becoming extremely topical. This is due to their ease of processing, low cost, highly tuneable electronic properties, favourable mechanical properties and long spin coherence times. However, there is a lack of suitable techniques that can yield information on intrinsic spin and charge carrier dynamics in organic materials. This is ever more true for organic semiconductors in the excited state. Muon spin spectroscopy is a technique that has rarely been applied to study excitonic problems in inorganic systems, yet it's local nature is ideally suited to studying them [1,2]. Therefore, I will discuss a some recent results on exciton dynamics in TIPS-Pentacene, using the newly commissioned photo-musr setup on the ISIS HiFi spectrometer.

In particular, the application of photomusr to study excitonic dynamics relies on one of the more exotic methodologies available to the muon technique - avoided level crossing (ALC) spectroscopy. It has already been shown that it can be used to probe the spin dynamics in organic semiconductors on a molecular lengthscale [3-5]. I will therefore briefly introduce this application of muons, using the temperature and mass-dependence of electron spin relaxation rates as examples [4,5].

I will then show how laser excited ALC spectroscopy [2] can offer unique insight into exciton dynamics of organic molecules. I will demonstrate that muons are sensitive to the presence of triplet excitons, and in particular, their role in the photochemical reactions of TIPS-Pentacene. Indeed, being sensitive to excitons with carbon specifity, I will argue that muons have the potential to offer insight into many fundamental biological and chemical processes.

[1] L. Nuccio et al., J. Phys. D: Appl. Phys. 47, 473001 (2014)
[2] K. Yokoyama et al., Phys. Script. 88, 068511 (2013)
[3] A. J. Drew et al., Phys. Rev. Lett. 100, 116601 (2008)
[4] L. Schulz et al., Phys. Rev. B 84, 085209 (2011)
[5] L. Nuccio et al., Phys. Rev. Lett. 110, 216602 (2013)

Harry Tom (University of California, Riverside)

Muon probing of spin-polarized conduction electrons in semiconductors

Harry W. K. Tom, Physics and Astronomy, University of California, Riverside, USA

The spin polarization and dynamics of conduction electrons in semiconductors is of increasing scientific and practical interest in next generation electronics. Research in "spintronics" materials and devices is motivated by the potential to use spin and charge or even purse spin currents to carry electronic information and integrate to memory better than charge-based electronics. Spin-dynamics in direct bandgap semiconductors has been largely pioneered by time-resolved optical measurements where optical selection rules allow straightforward access to spin-polarized carriers. But in indirect bandgaps semiconductors like Silicon, muons are a potentially unique probe of spin-polarized carriers. For example, electrons bound to implanted muons in triplet muonium (muon spin up+electron spin up) can exchange with co-polarized (spin up) or counter-polarized (spin down) conduction electrons to either preserve the triplet muonium polarization and muon polarization or increase triplet-singlet muonium conversion and increase the muon depolarization rate. To test this, we performed experiments in n-GaAs in which circularly polarized light introduced spin-polarized electrons and holes and we found a large spin-dependent effect on the depolarization rate of muons at T-Mu- sites. We have recently performed similar experiments in Si and I will discuss some of those preliminary results.

Stephen Cottrell (STFC)

New Science with Radio Frequency Techniques

Stephen Cottrell

Perhaps because of their inherent complexity and the short muon lifetime, very few muon experiments currently exploit radio-frequency (RF) methods, and many of the pulsed excitation techniques now regarded as essential to modern NMR spectroscopy have never been tested.

This talk will introduce a number of pulsed muon spin resonance (μSR) techniques, and show how they can be used to extend the scope of information obtained from muon spectroscopy. The application of 90º pulse, spin-echo and spin-locking sequences will be considered, and the unique information obtained from double resonance experiments examined. The talk will conclude with an extended example, where the rate constant for hydrogen abstraction by Mu in propane is measured in the gas phase. In this case, RF techniques provide a unique method for following this slow reaction, the results contributing to the extended study of kinetic isotope effects.

Adrian Hillier (STFC)

Bulk non-destructive elemental analysis using muons

Adrian Hillier[(1)], Don Paul[(2)] and K. Ishida[(3)]

(1) ISIS facility, STFC Rutherford Appleton Laboratory, Harwell Science and Innovation Campus, Oxfordshire, OX11 0QX, UK
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Elemental analysis is a process in which a sample is analysed for its composition. Often this is accomplished by destructive and damaging techniques. Clearly, such techniques are not desirable for valuable items (either scientific or monetary). A non-destructive, non damaging elemental analysis would be an extremely useful tool. Using negative muons, which emit a characteristic X-ray, could be such a tool.

Negative muons are like heavy electrons and replace an electron in the outer shell of an atom then travel to near the nucleus through the modified energy states of the atom. Each transition on this path produces an x-ray which is characteristic of the atom, which absorbed the muon, hence allowing this spectrum to reflect the atomic species (see Figure 1). The sensitivity of this technique is such that even light atoms can be detected and further the technique is open to be used as a depth analysis tool, since by varying the energy of the incident muon beam it is possible to change the depth of implantation for the negative muon. A significant advantage of muonic X-rays over those of electronic X-rays is the higher energy (0.1-6MeV). These high energy muonic X-rays are emitted from the bulk of the samples without photon self-absorption and can be simply detected by a semiconductor detector. In addition, this technique will not activate the sample, unlike prompt gamma-ray analysis by neutron irradiation. Over the years there has been sporadic use of negative muons as an elemental analysis tool, and a wide-ranging number of materials have been investigated, including Japanese coins[1], spinal columns[2], pig fat[3], tissue analysis[4] and ancient Chinese mirrors[5].

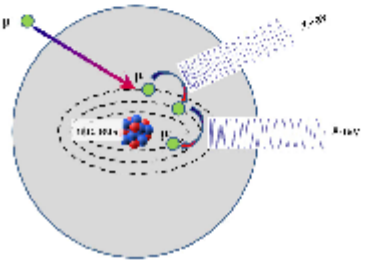

Figure 1: A schematic diagram which shows the μ^- capture and X-ray emission process.

ISIS pulsed neutron and muon facility, UK is a primary high-flux source of pulsed muon beams. In this talk we will review the results in soft-matter, the latest developments and the possible uses for the future.

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Steve Bramwell (University College London)

Wien Effect for Magnetic Monopoles in Spin Ice

Steve Bramwell

In principal, the defining signature of emergent magnetic monopoles in spin ice is the so-called Wien effect: the magnetic field-enhanced quasiparticle production from the monopole vacuum. An early and spectacular confirmation of the Wien effect by MuSR became controversial, but also highlighted flaws in the standard MuSR method when applied to dense magnetic oxides. More recently, the Wien effect has been definitively confirmed by other methods. Here I review these developments with the aim of identifying issues and opportunities in MuSR, as applied to magnetic monopoles in spin ice.

Steve Blundell (University of Oxford)

What do muons do inside spin ice?

Steve Blundell

The behaviour of muons in spin ice has attracted some controversy, and unfortunately this has become entwined with a question about whether monopoles are the appropriate excitation in spin ice and whether the non-equilibrium transport of monopoles can be studied using an analogy with electrolytes. My view is that the realisation of monopoles in spin ice and the study of emergent magnetolytes are both hugely important advances in this field, but the early 'demonstration' of monopole transport using muons needed correction. I will describe some recent results that have advanced our understanding of what muons do inside spin ice.

Nicola Morley (University of Sheffield)

Muon studies of polymers

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Understanding the electronic spin relaxation (eSR) of organic semiconductors is important, as they are used in a wide range of applications including OLEDs, transistors and spin-valves. Conjugated polymers in general have higher mobilities compared to small molecules, due to their long chains, which mean they have less structural discontinuities and grain boundaries. Another useful property is their long spin relaxation rate, due to low spin-orbit coupling and hyperfine coupling strength. One method to measure the eSR is to use muon spin relaxation and avoided level crossing (ALC) resonance spectroscopy.

This research has studied a series of polymers all of which have the same backbone (Fig. 1 inset), but have different side chain arrangements and lengths. The polymers studied were poly(3-butylthiophene-2,5-diyl) (P3BT), poly(3-hexylthiophene) (P3HT) and poly(3-octylthiophene-2,5-diyl) (P3OT). The P3HT was also studied in two different forms regio-regular (RR-P3HT) and regio-random (RRa-P3HT), with the only difference being the arrangement of the side chains either side of the backbone. Using ALC resonance spectroscopy, it was determined that P3BT, RRa-P3HT and P3OT all have similar behaviour to small organic molecules (Fig.1), thus the eSR were determined. While the ALC resonances for RR-P3HT were measured to be much larger than expected at 300K (Fig. 1a). Further research was carried out, which determined that the large increase in magnitude was due to the magnetic impurities in the polymer left over during the synthesis process.

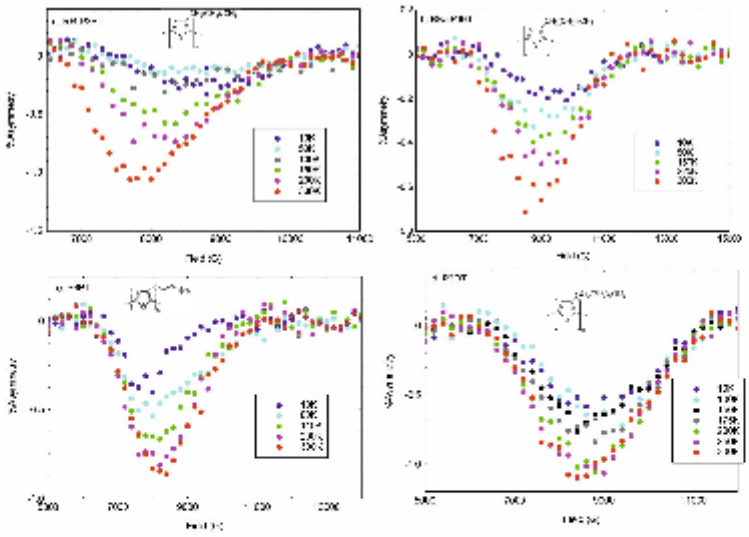

Figure 1. The ALC resonances of a. RR-P3HT, b. RRa-P3HT, c. P3BT and d. P3OT. Insets: Polymer structure

Joseph Wright (University of East Anglia)

Probing the [FeFe]-hydrogenase subsite using muon spectroscopy

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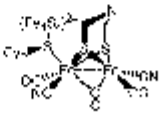
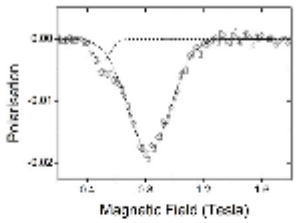
In the drive to replace fossil fuels with sustainable alternatives, achieving the reversible interconversion of protons and dihydrogen is a crucial target. The reaction can be carried out readily using platinum-based systems, but the cost and availability of this precious metal preclude scaling such approaches. In nature, the [FeFe]-hydrogenase enzymes have evolved to perform the very same task at rates that rival platinum electrodes.[1] These systems feature a large protein component in addition to a core bioinorganic unit, the {2Fe2S} subsite (right). 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 (left) allows us to understand key reactivity of iron hydrides on a timescale as short as one second.[2,3] 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 (right), with density functional theory (DFT) assignment strongly implicating competing bridging and terminal binding. This unique insight opens up the possibility of new reaction pathsways in both models and the enzyme as well as demonstrating the wider importance of muon techniques in studying reactive organometallic systems.



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Posters

Thomas Loe (STFC)

Developing muon e-learning tools

Tom Loe

As part of the SINE 2020 project, e-learning materials about muons will be produced. This will build upon the virtual neutrons for teaching platform currently nearing completion. We intend to make some short courses focusing on specific aspects of the muon technique that can be used individually or in combination, tailored to the needs of the learner. These can complement the existing ISIS muon training school.