



Canada's National Laboratory for Particle  
and Nuclear Physics

# Muons (and Isotopes) for Material Science

Iain McKenzie

Centre for Molecular and Materials Science TRIUMF  
Department of Chemistry SIMON FRASER UNIVERSITY

## KEK – TRIUMF Scientific Symposium

December 14<sup>th</sup>, 2017

Isotopes have broad applications in condensed matter and materials science as a low-density, very-high-signal-to-noise in situ detectors of local environments and dynamics.

$\mu$ SR and  $\beta$ NMR offer as much as *10-orders-of-magnitude improvement* in signal over conventional NMR through the combination of high polarization and beta-decay anisotropy.

## Magnetism

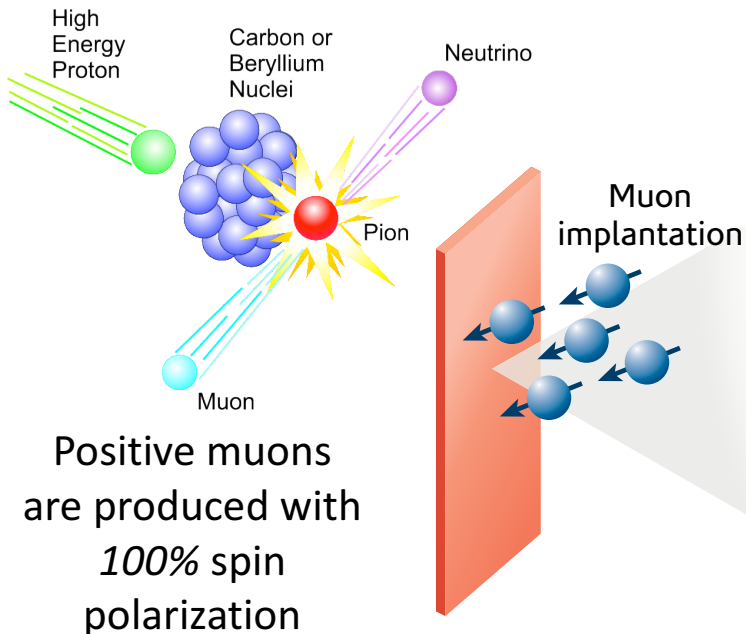
- Local fields and magnetic ordering
- Dynamics: electronic, nuclear spins
- Heterostructures and near-surface

## Superconductivity

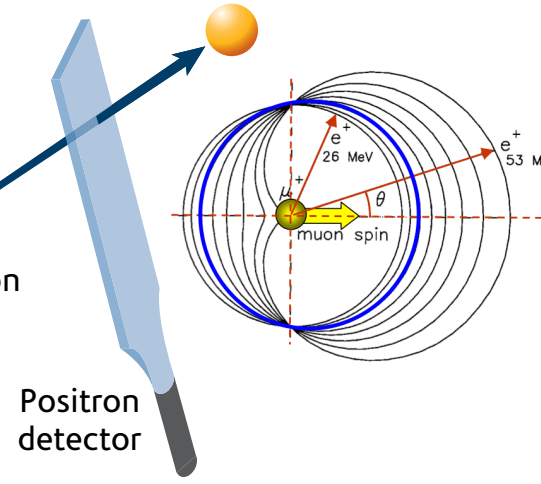
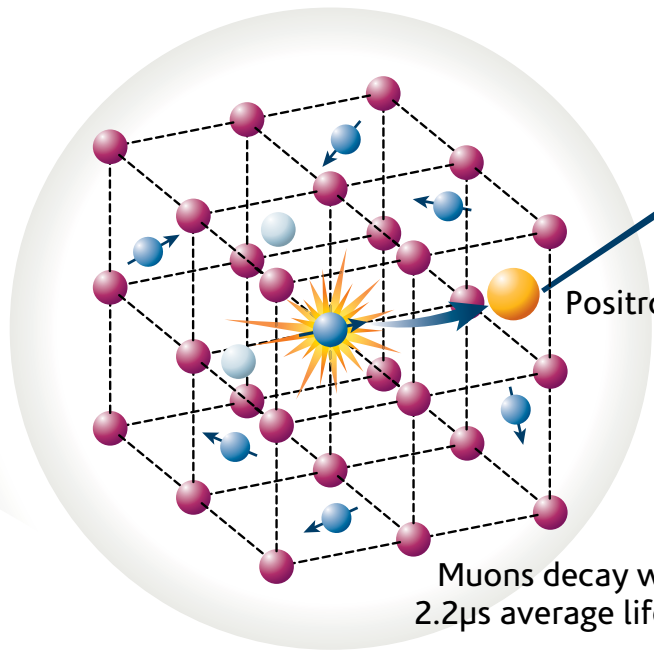
- Co-existence of SC and magnetism
- Measure magnetic penetration depth  $\lambda$  and coherence length  $\xi$

## Chemistry and Soft Matter

- Study “unobservable” H atom rxns
- Discover new radical species
- Probe ionic diffusion
- Depth dependent polymer dynamics



Positive muons are produced with **100% spin polarization**

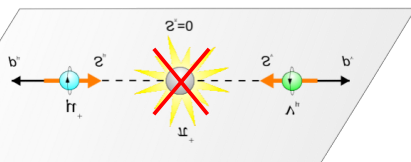
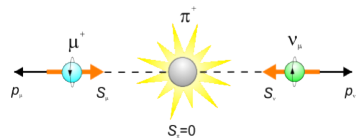


Decay  $e^+$  used to monitor time dependence of muon spin polarization

Mu<sup>+</sup> is sensitive to magnitude and fluctuation rate of magnetic field inside materials

Static field distribution  
Sensitivity:  $10^{-3} - 10^{-4} \mu_B$

Fluctuation rates  
 $10^5 - 10^9$  Hz



## 1. Bassam Hitti: Operations Manager

- i. Experimental Setup, Operations and User support
- ii. L-He Coordination
- iii. MRO Coordination
- iv. Device electromagnetic simulation (i.e. Opera)
- v. Semiconductor Solid State Physics

## 2. Gerald Morris: Deputy Manager

- i. M20 project management
- ii.  $\beta$ NMR Management & beam line coordinator
- iii. Experimental Setup and User support
- iv. CMMS Experimental Safety reviews
- v. Subsurface layer CM Physics

## 3. Donald Arseneau: IT /DAQ & Programming Management

- i. Experimental Setup and User Support
- ii. Facility IT, DAQ and programming
- iii. Spectrometer design
- iv. Common Account Assessment Management
- v. Physical Chemistry and Fundamental Kinetics

## 4. TBA: New (2018) SBQMI funded (5 Yrs.) BAE

## 5. Iain McKenzie: Outreach & User Support

- i. Outreach Planning and Implementation
- ii. Liaison with User Community
- iii. EEC Secretary
- iv. Experimental Setup and User Support
- v. Physical Chemistry of Soft Materials Structure and Dynamics of Free Radicals

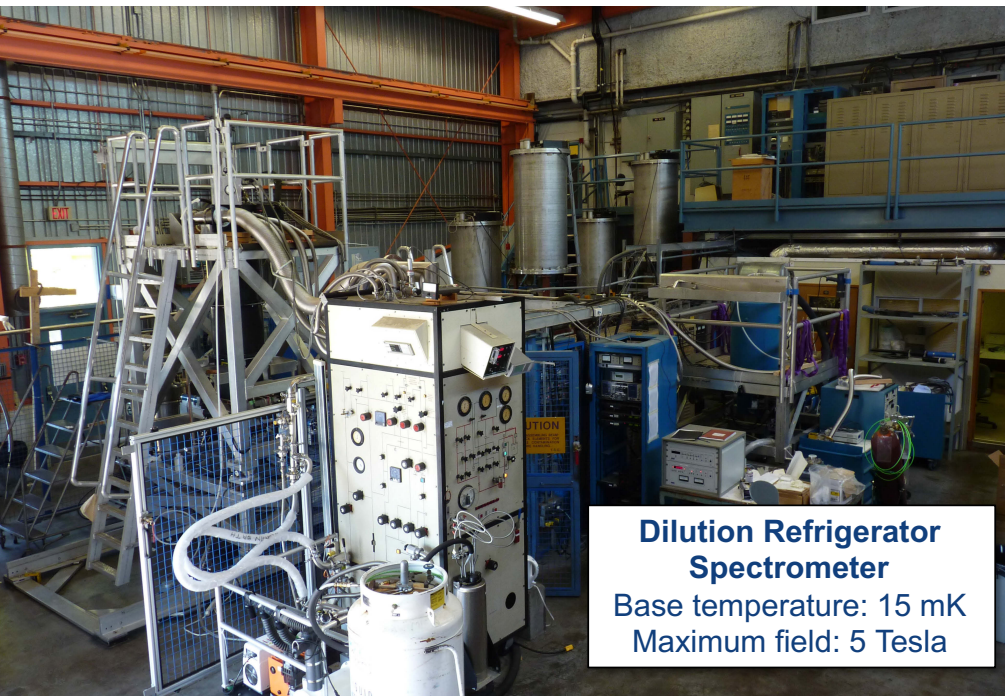
## 6. Syd Kreitzman: Manager

- i. Liaison with TRIUMF Management
- ii. M9 beamline project management (to date)
- iii. Spectrometer design coordinator
- iv. Experimental Setup and User Support
- v. MuSR Techniques ,Tools & Toys
- vi. Spin relaxation theory

## Facility Technicians:

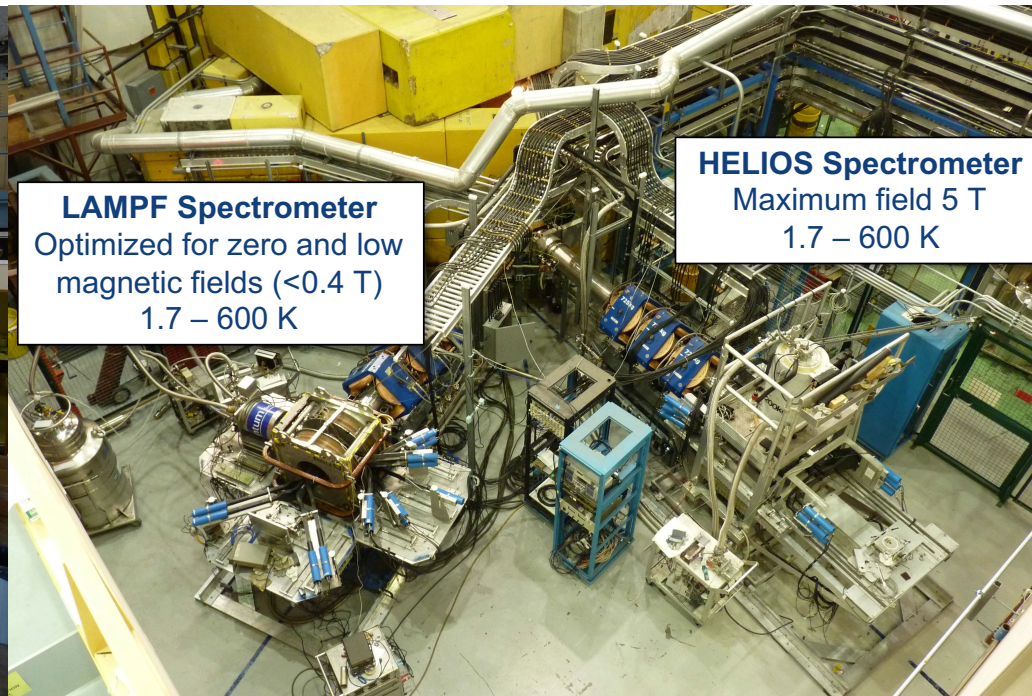
1. Rahim Abasalti: High Vacuum Specialist
2. Mike McLay: Design Technologist
3. Deepak Vyas: Millwright & Work Area Safety Coordination
4. Collin Dick: Liquefier Technician (cryogenics group)

## M15



**Dilution Refrigerator  
Spectrometer**  
Base temperature: 15 mK  
Maximum field: 5 Tesla

## M20D

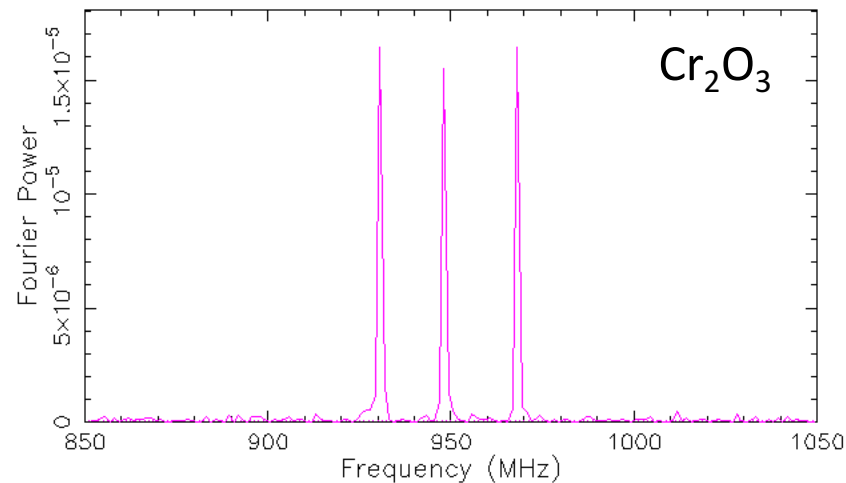
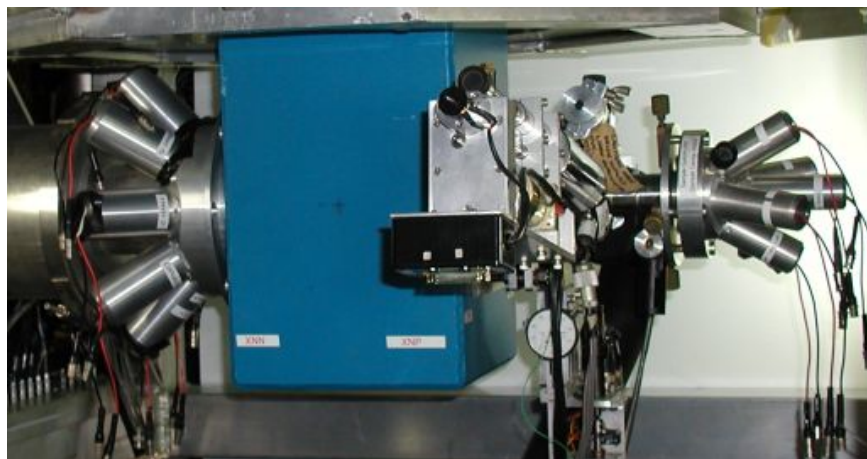


**LAMPF Spectrometer**  
Optimized for zero and low  
magnetic fields (<0.4 T)  
1.7 – 600 K

## M20C

**HELIOS Spectrometer**  
Maximum field 5 T  
1.7 – 600 K

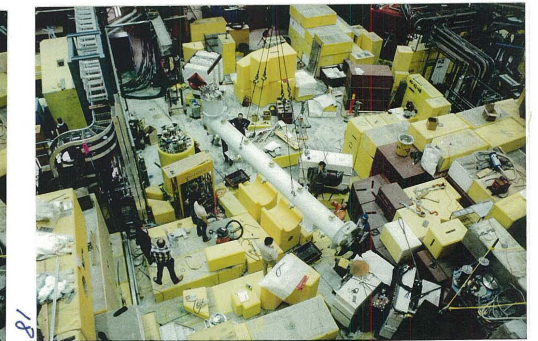
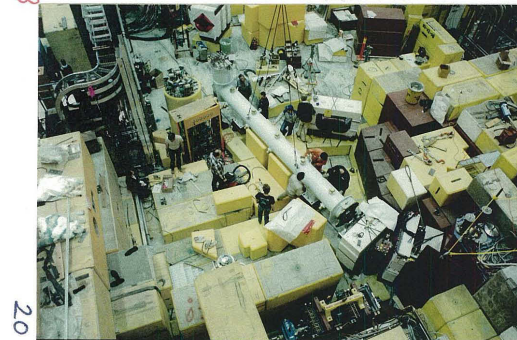
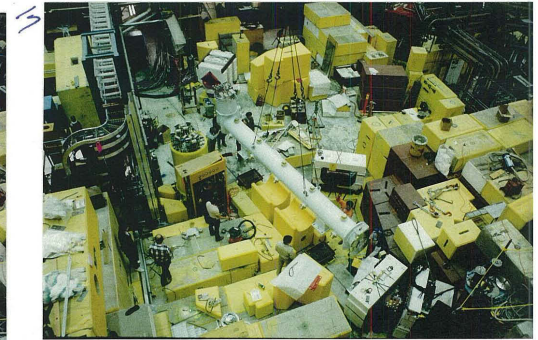
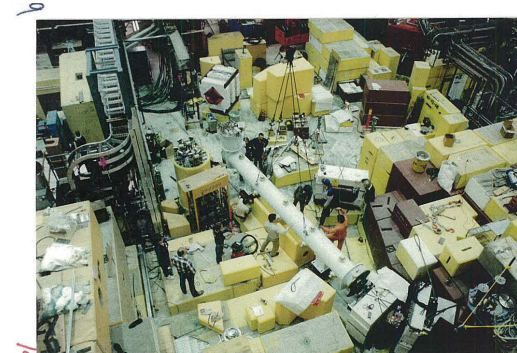
- 7 T replacement for HiTime with improved field homogeneity (10 ppm over 1 cm diameter disk  $\pm 3$  mm in z) and alignment (within  $0.25^\circ$  of physical bore).
- \$300k awarded for magnet and  $^3\text{He}$  cryostat from NSERC RTI - J. Sonier (SFU) + G. M. Luke (McMaster) + contributions from facility users



High homogeneity + unique detector design → amazing high frequency / field spectra



In 1988 the KEK MSL Group (Yamazaki, Nagamine et al) were responsible for the procurement and installation of M9B



- Toshi Yamazaki
- Tomo Uemura
- Ryu Hayano
- Jun Imazato
- Nobu Nishida
- Ken Nagamine (not pictured)



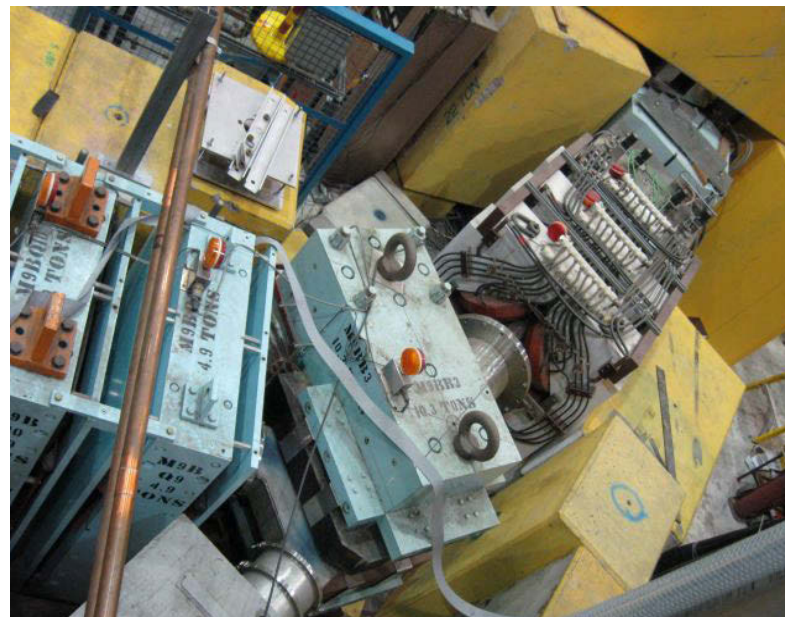
As they overlooked M9B Erich Vogt explained to the Prime Minister why having an operational muon decay channel is so important to a Laboratory that does Muon Science.

Toshiki Kaifu, the Japanese Prime Minister, visits TRIUMF and is greeted by Stan Hagen (left, Minister of Advanced Education), Bill Vander Zalm (B.C. Premier), and Erich Vogt (Director of TRIUMF).





**M9A: Surface  $\mu^+$** 

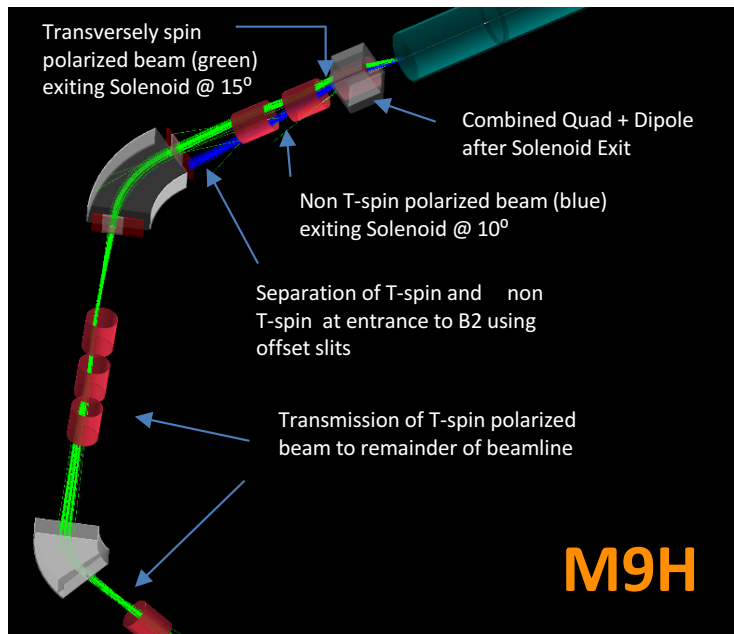
**M9B: High momentum SR  $\mu^\pm$** 


**Not operational since 2012 due to M9-T2 vacuum leak**

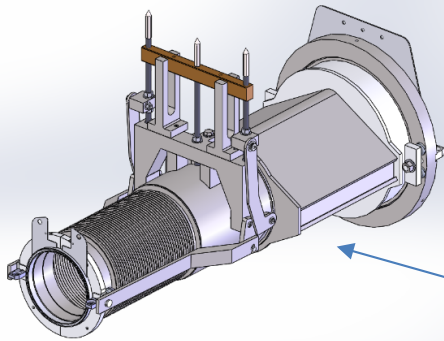
## Multi-Institutional CFI Proposal *Approved Nov. 2017*

- Replace M9B with M9H
  - Upgraded beam line including new persistent coil solenoid
  - New spectrometer for high pressure, high field studies in a DR
- M9-T2 repair + M9A completion + 3T spectrometer

CFI	4,290,724
Total Prov. Funding	4,290,724
Vendor Discounts	951,699
TRIUMF Contribution	1,193,662
<b>Total Project</b>	<b>10,726,809</b>

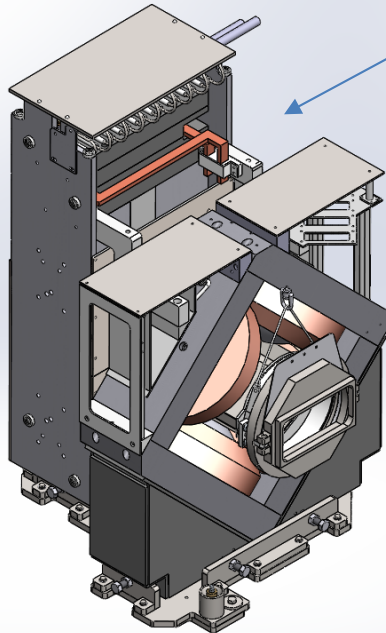
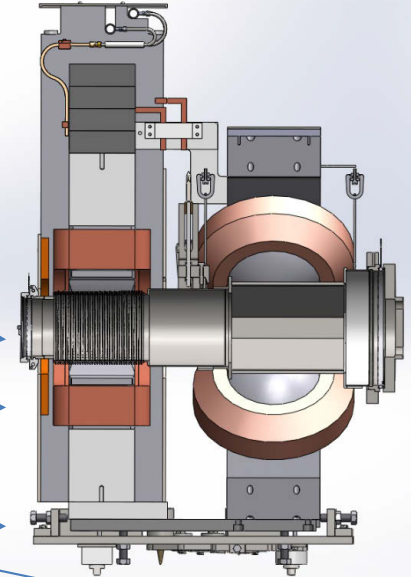


- One of a kind beams on M9H; i.e. spin-rotated decay muons and high flux  $\mu^-$ .
- Unique physical parameter space (high pressures + ultra-low temperature + high magnetic fields on M9H)
- M9A to focus on highly efficient sample characterization for the increasingly important broad non-expert (in  $\mu$ SR) user community.



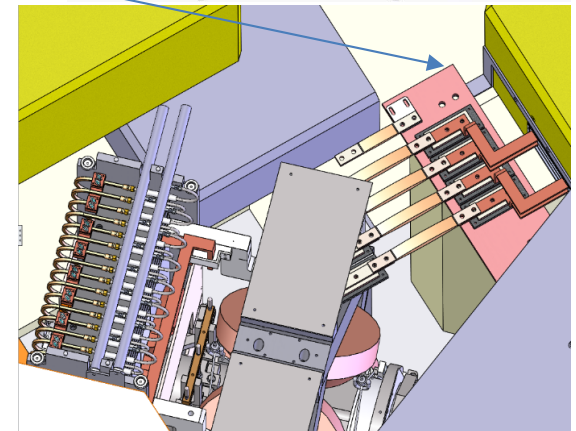
The required elements to repair the M9-T2 front end are being developed & new engineer is here!

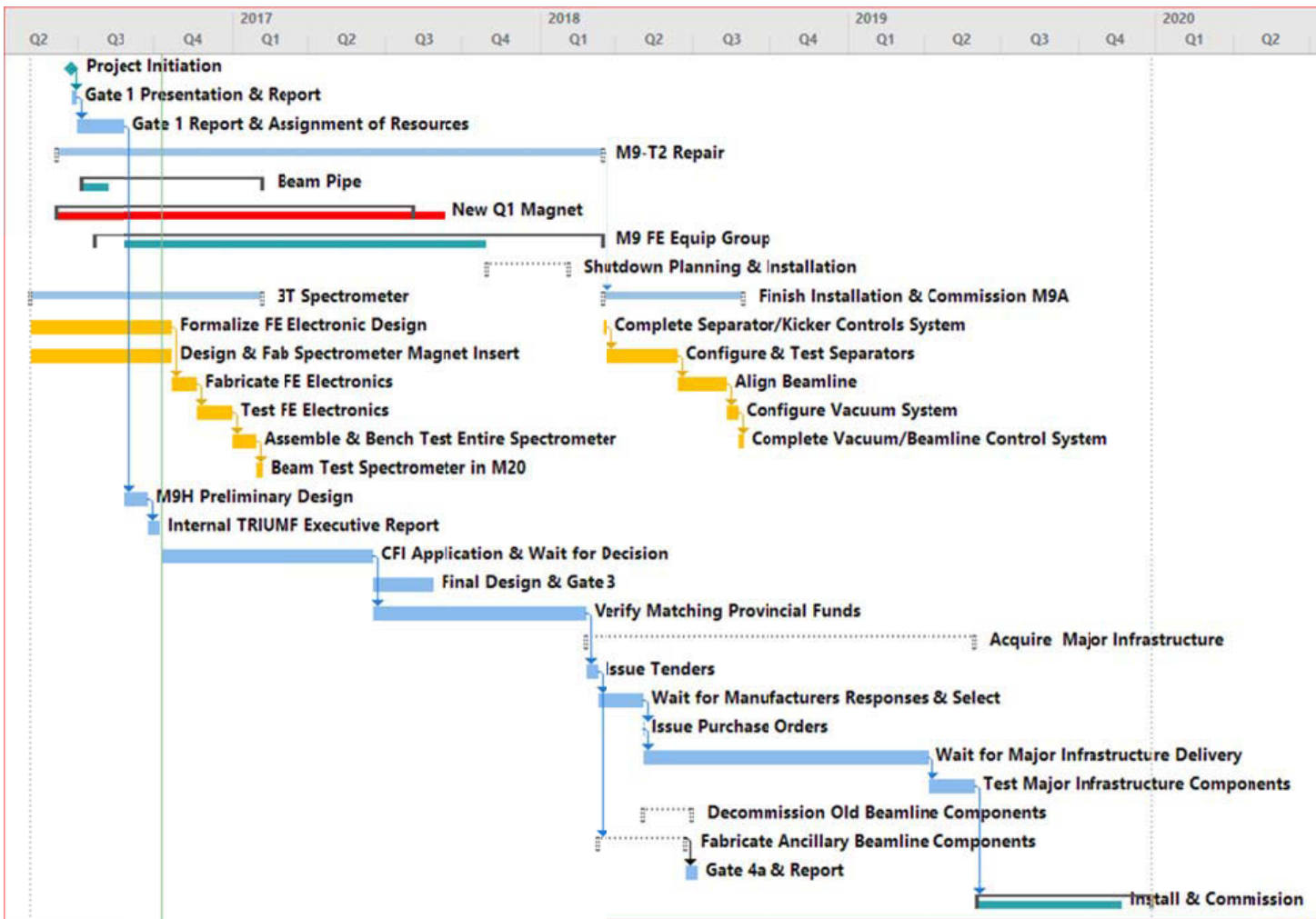
- Retractable beam pipe
- New Q1
- Field Adjustable Q1Q2 base
- Removable service stand



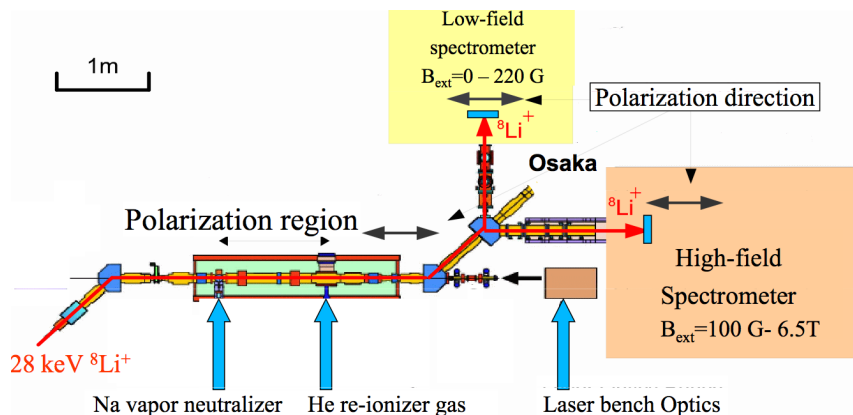
Foremost in mind are:

- 1) safety (reduced dose) for installation and maintenance.
- 2) Utility and practicability for remote handling
- 3) Capability to withstand high neutron doses  $>5E22$  n/m<sup>2</sup> over 15 years.

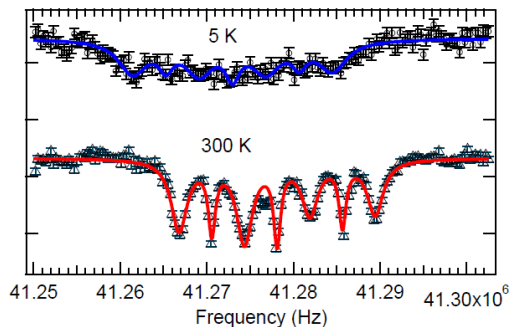




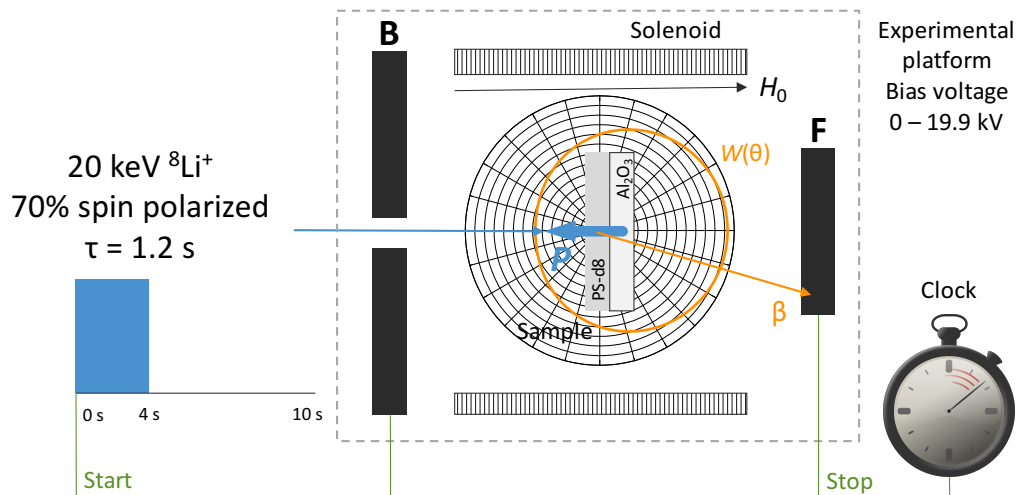
## High spin polarization from optical pumping



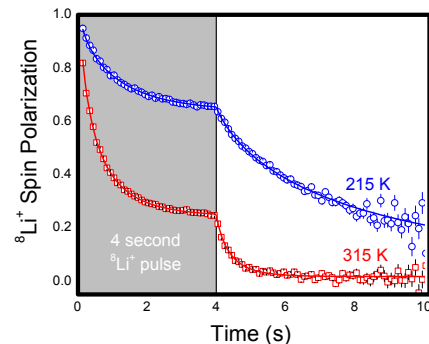
Resonance techniques used to study interaction of  $^8\text{Li}^+$  with local environment

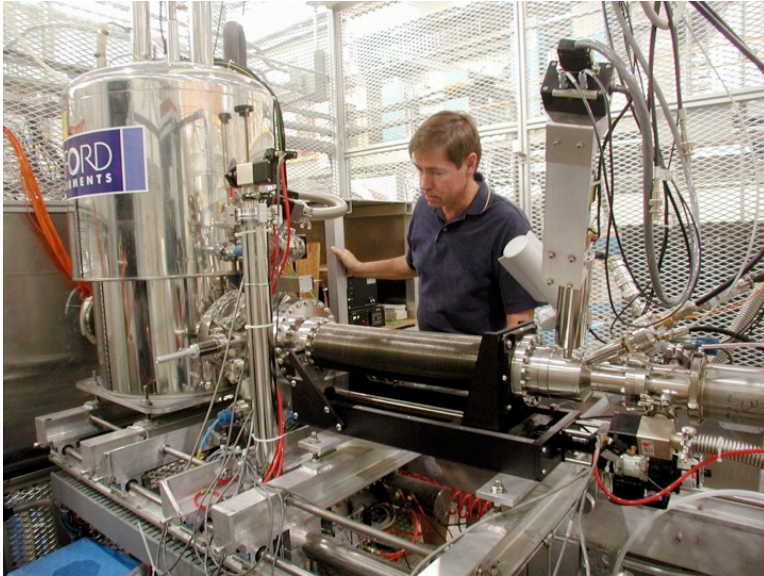


## Magnetic resonance with depth resolution



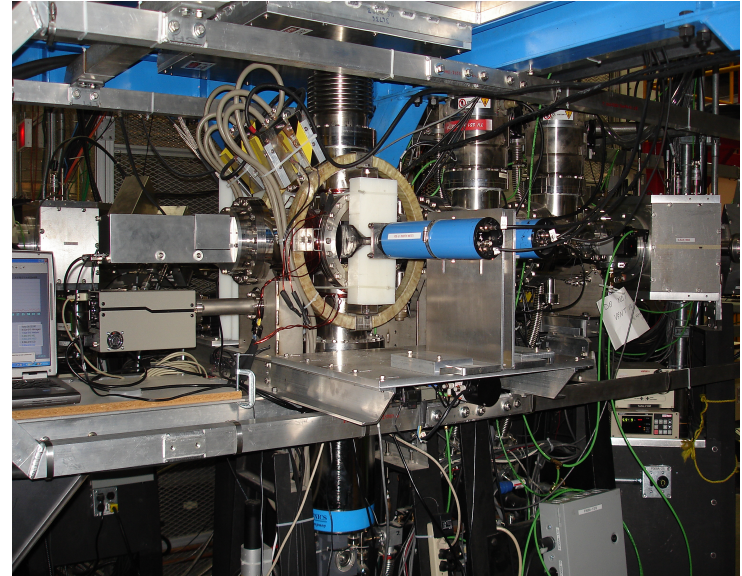
Relaxation methods used to study dynamics of  $^8\text{Li}^+$  and the local magnetic field



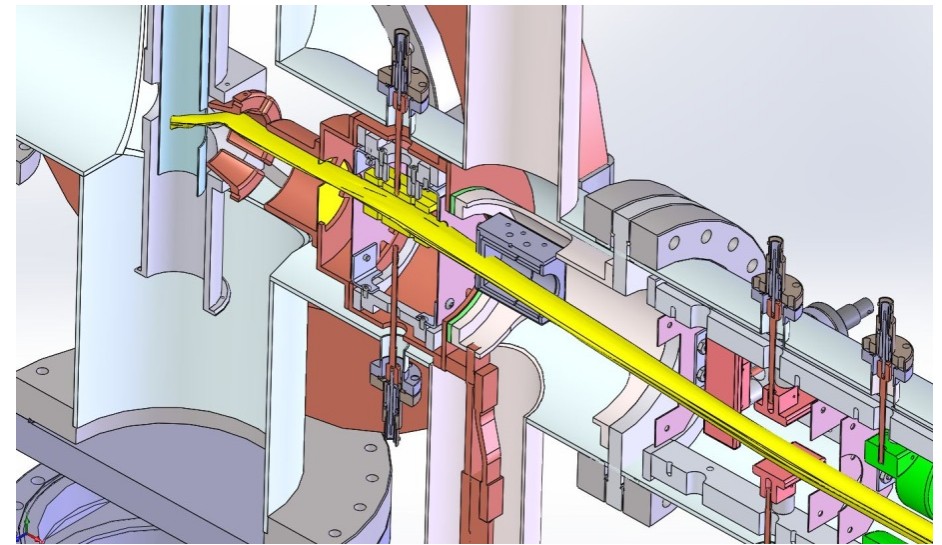
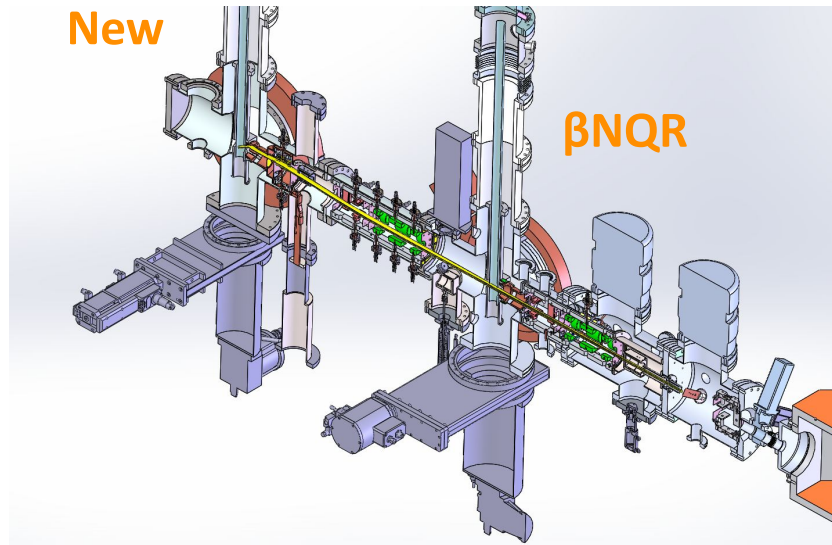


**$\beta$ NMR: High Field (9 T) Spectrometer**

- $^8\text{Li}^+$  implanted at energies between 0.1 and 28 keV.
- Near-surface probe up to hundreds of nm.
- Temperature range 5 – 320 K.



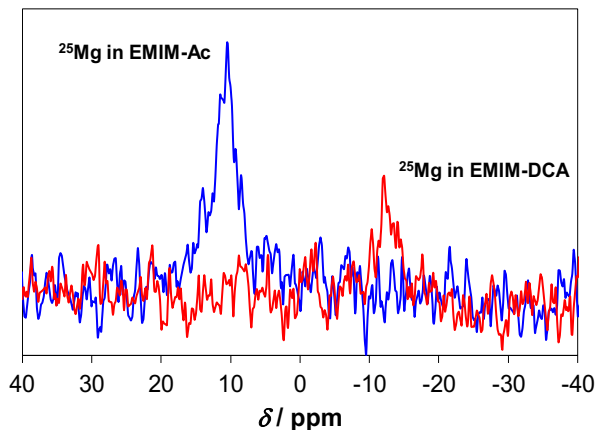
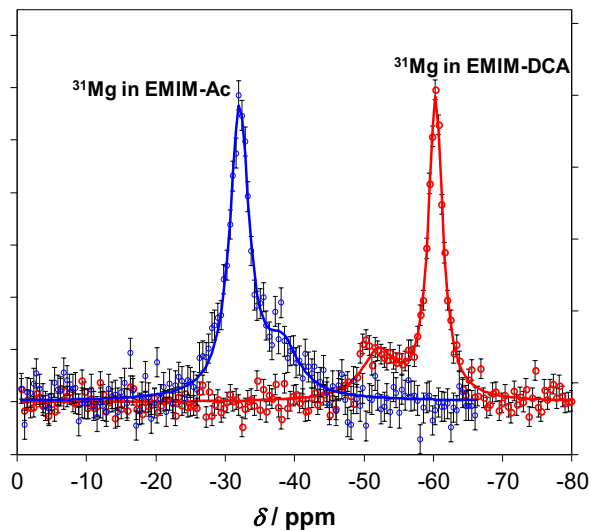
**$\beta$ NQR: Low (20 mT) and Zero Field Spectrometer**



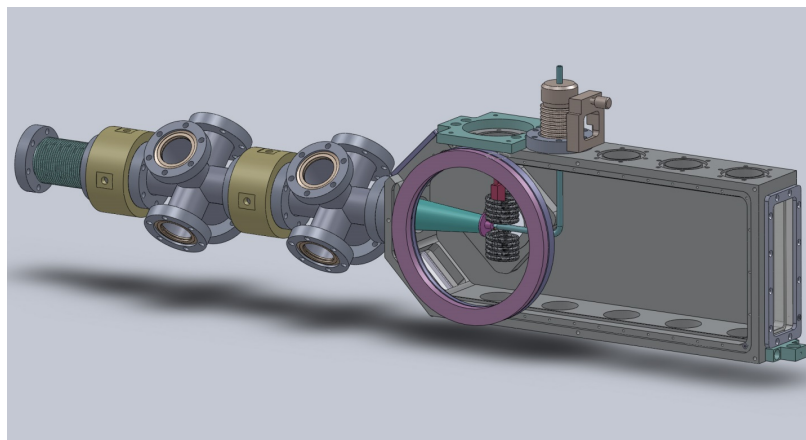
Extremely flexible new  $\beta$ NMR spectrometer

- 0 – 0.22 T (magnetic field between  $\beta$ NMR and  $\beta$ NQR)
- 300 mK – 300 K (lower temperatures than  $\beta$ NMR and  $\beta$ NQR using  $^3\text{He}$  cryostat)

Measure field penetration profiles in Nb cavity materials relevant to advanced superconducting RF accelerator research



- $^{31}\text{Mg}$  ( $I = 1/2$ ) will be used to study the local chemical environment of magnesium in biologically important contexts, e.g. where Mg is part of an enzyme.
- Superior to conventional NMR with  $^{25}\text{Mg}$ .
- Experiments performed on ionic liquids.
- New spectrometer for liquid samples under construction.





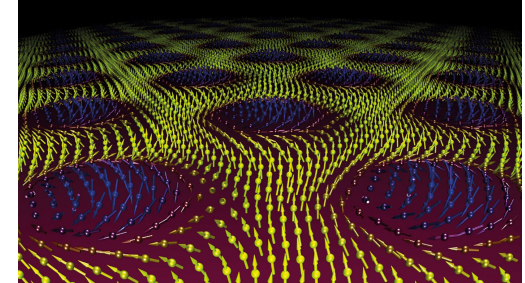
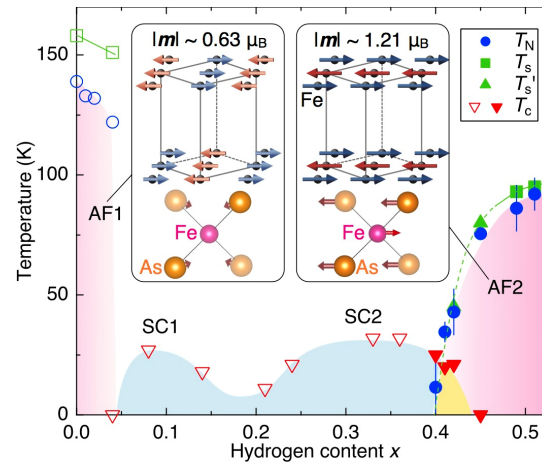
Exp.	Title	Investigators
M1459	Mechanism of hydrogen-induced vacancy formation in PdAg alloy studied by Muon Knight shift measurements	M. Mihara
M1497	$\mu$ SR investigation of stable open-shell singlet molecules	S. Ito
M1647		no
M1672		hita
M1678		azaki
M1711		
M1712		no
M1734	Transition between localized- and itinerant-electron states in the solid-solution system of $\text{CaCu}_3\text{Ti}_{4-x}\text{Ru}_x\text{O}_{12}$	J. Sugiyama
M1738	$\mu$ SR study for magnetic polarization on apical oxygen in Ruddlesden Popper series	W. Higemoto

**Japanese-led experiments  
received 20% of delivered  
beam in 2017**

# Recent Scientific Highlights

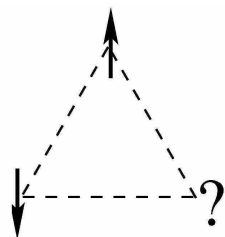
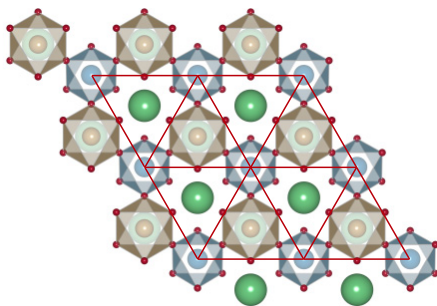


- Magnetic materials underpin much of modern technology
- Advances in such technology require new materials and greater understanding of existing ones.



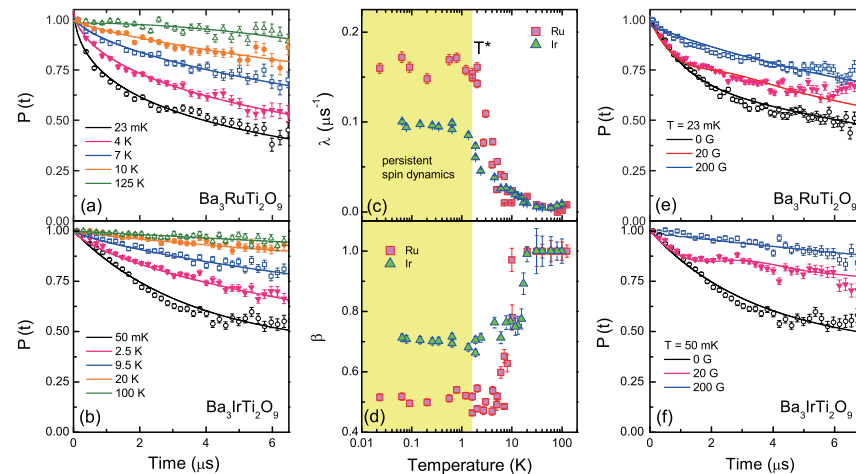
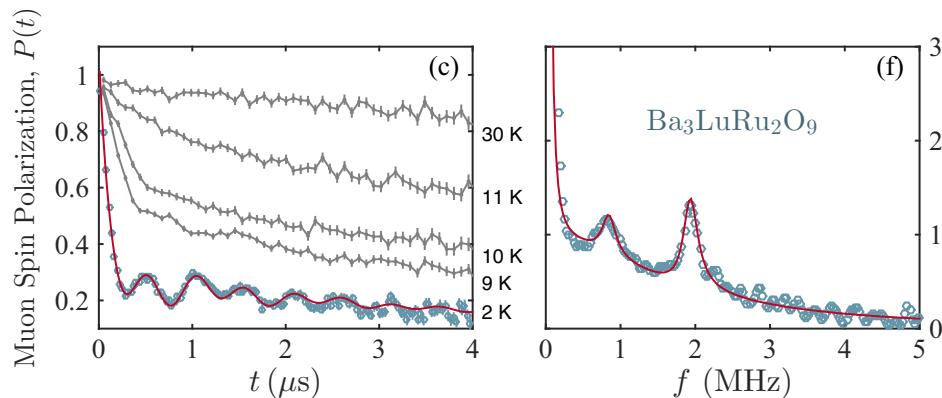
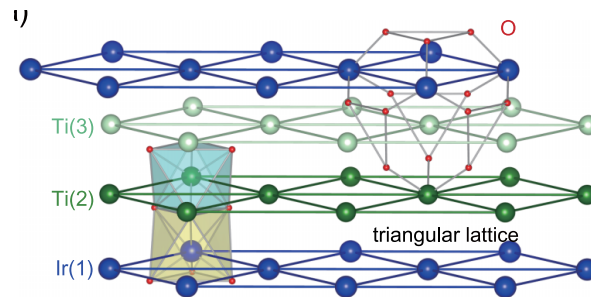
- Magnetic moments order into a pattern controlled by the symmetry of the material and the interactions between the atoms.
- Magnetic moments within materials also fluctuate and this gives a further window on how they are interacting.
- Determine magnetic phase diagrams and characterize novel magnetic states.

$\text{Ba}_3\text{LuRu}_2\text{O}_9$

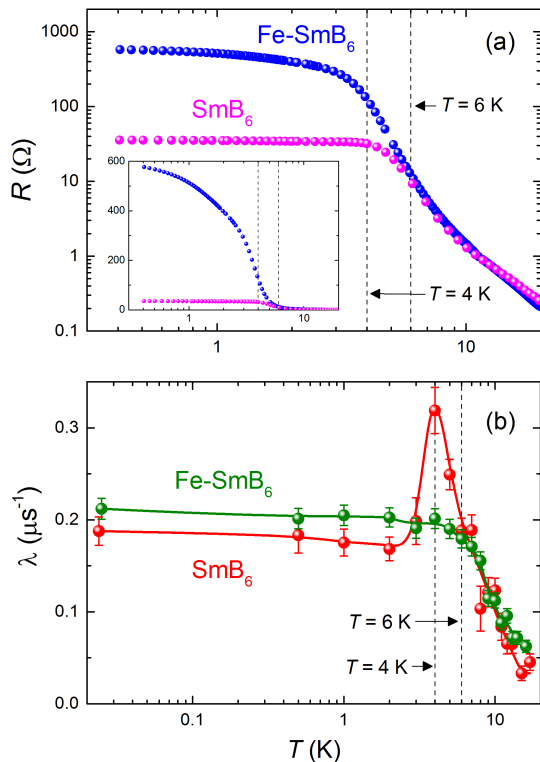


Frustration on  
triangular lattice

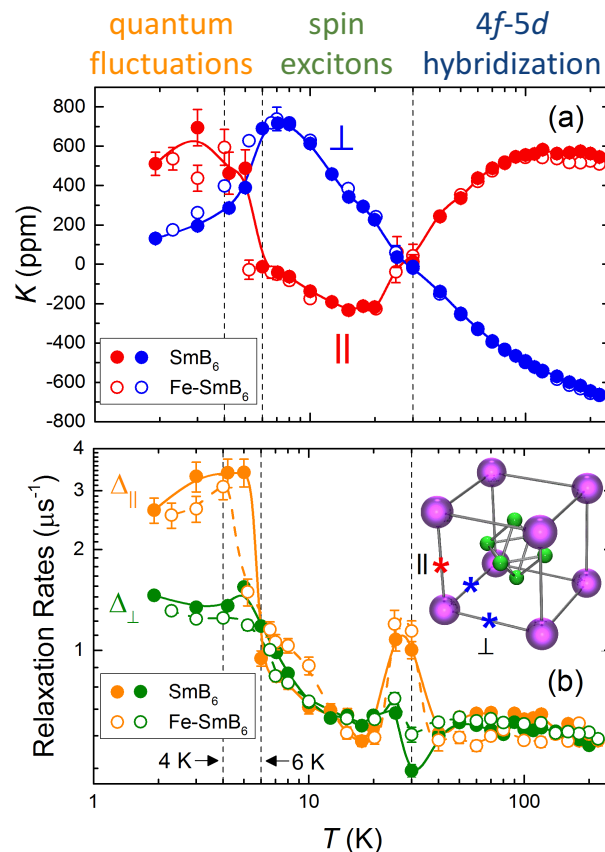
$\text{Ba}_3\text{IrTi}_2\text{O}_9$

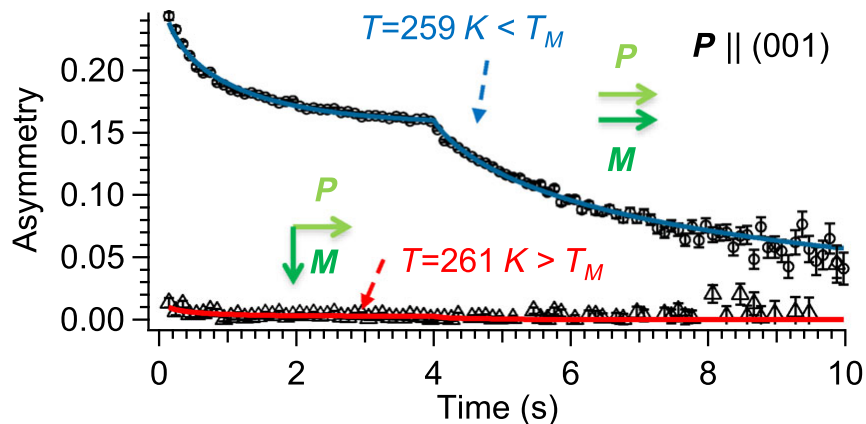


ZF- $\mu$ SR: Quantum spin fluctuations below 4 K  
 - Predicted low-energy spin exciton branch



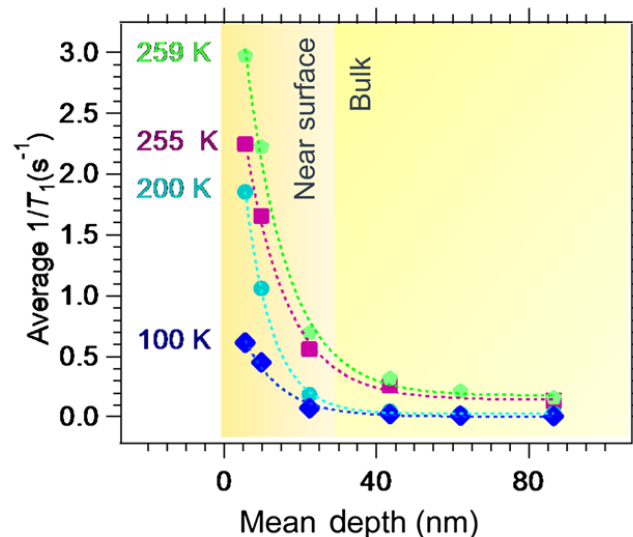
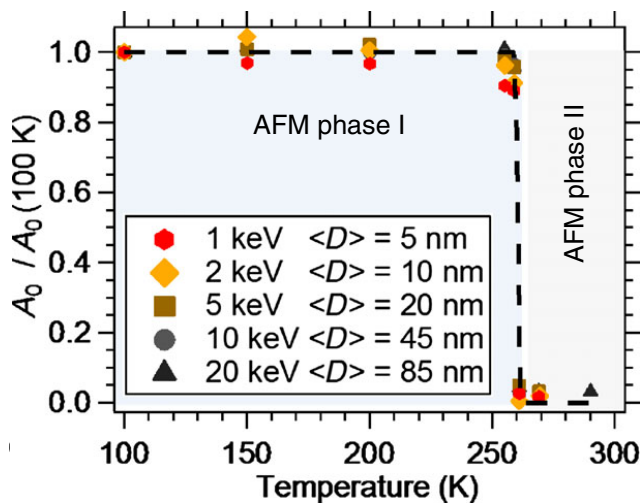
High TF- $\mu$ SR: Partially Kondo-compensated  
 Sm-4*f* sub-lattice

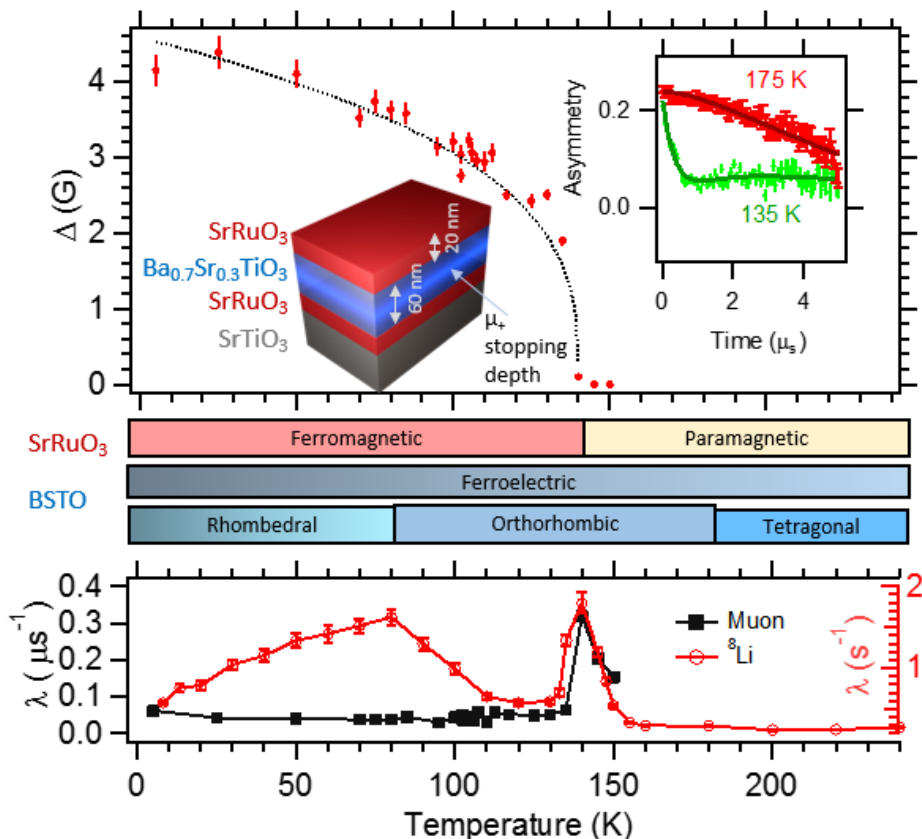




- Depth dependence of the Morin spin reorientation in  $\alpha\text{-Fe}_2\text{O}_3$
- Surface-localized dynamics decay with characteristic length of 11 nm, indicating presence of soft surface magnons.

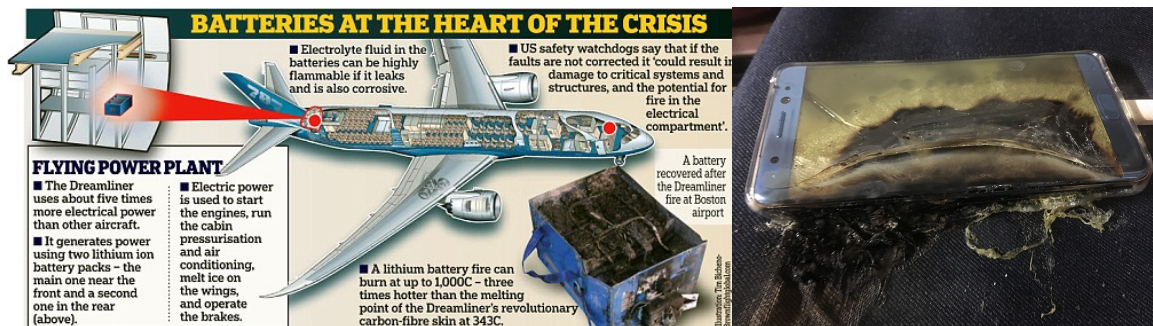
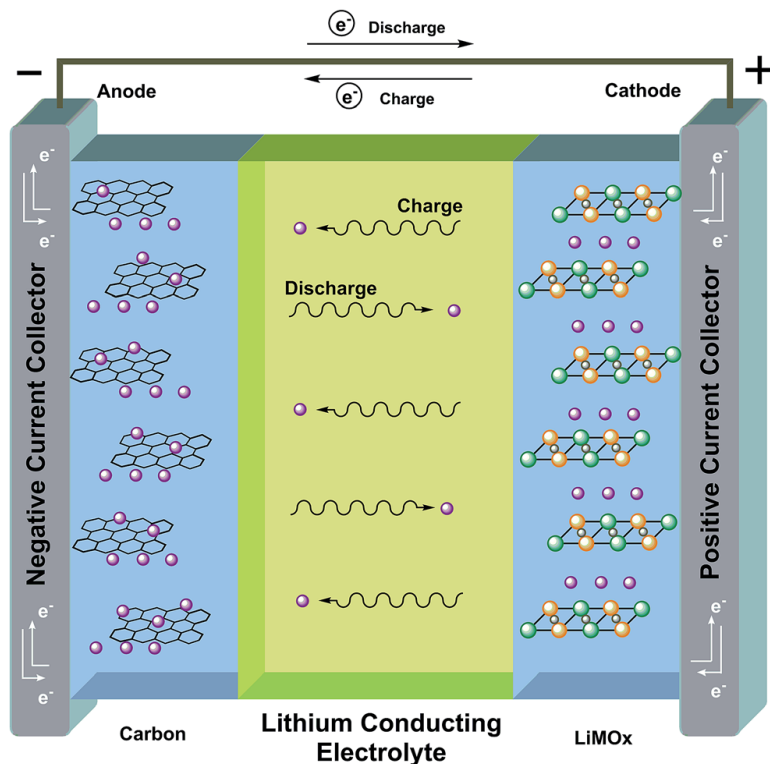
Cortie *et al.* *PRL* **2016**, **116**, 106103





- The muon which is a  $I = 1/2$  particle and detects only the magnetic dynamics.
- <sup>8</sup>Li<sup>+</sup> has  $I = 2$  and thus a finite electric quadrupole moment  $q = 31.4$  mb.
- For instance, in the case of multiferroic structures containing a ferroelectric Ba<sub>0.7</sub>Sr<sub>0.3</sub>TiO<sub>3</sub> and ferromagnet SrRuO<sub>3</sub>, this dual-sensitivity allows us to detect both the ferromagnetic and ferroelectric dynamics.

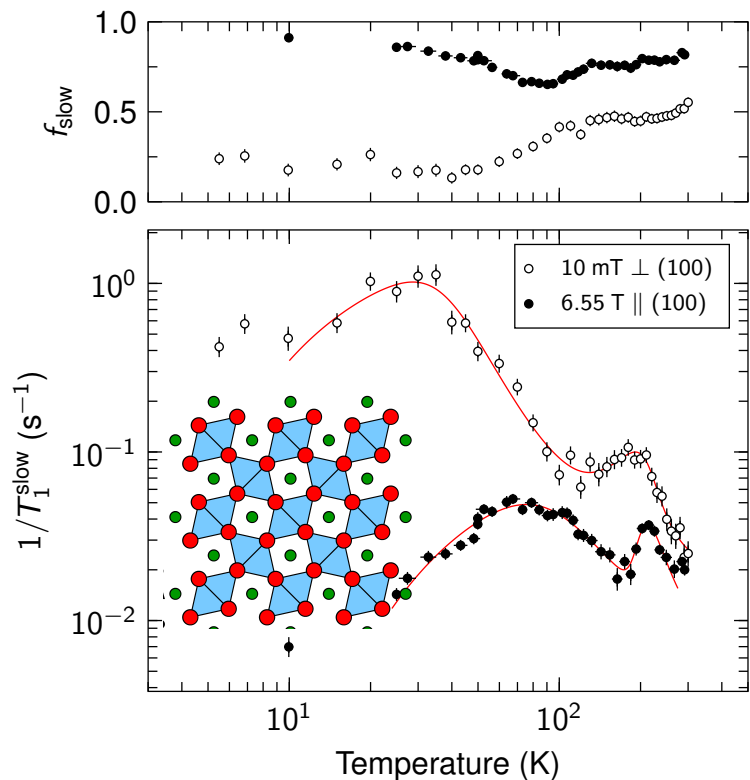
Present rechargeable batteries use electrolytes with organic solvents. Solid state batteries (SSB) are highly desirable for *safety considerations* but also for *performance and lifetime*.



The key issue in future materials developments for SSB is to understand the ion diffusion processes in the solid state at an atomic level, opening the door for tailored materials and improved device performance.

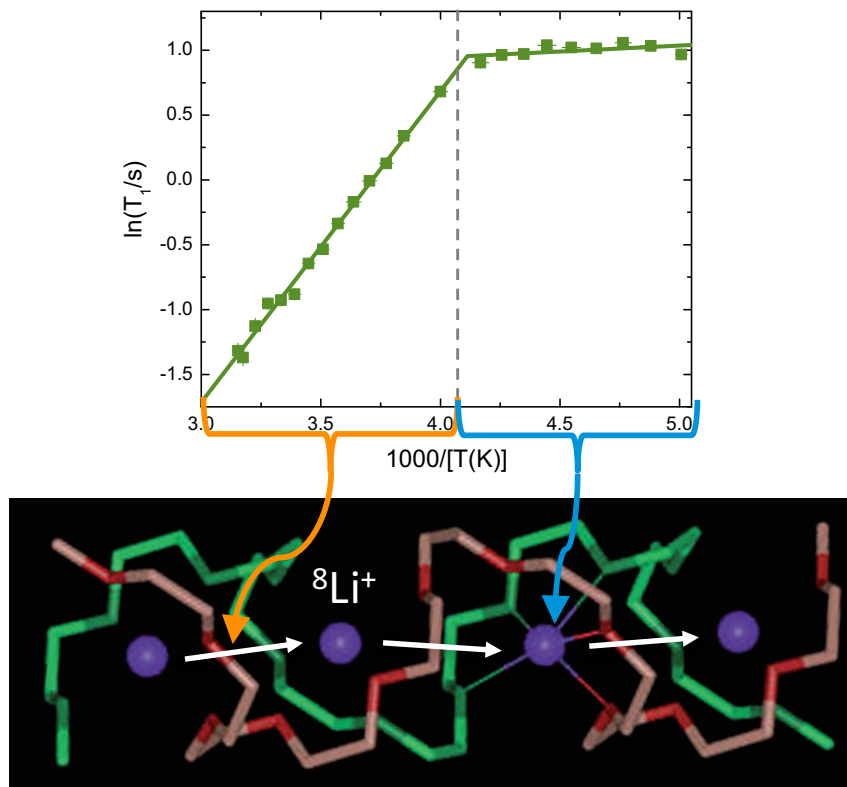


## Rutile $\text{TiO}_2$

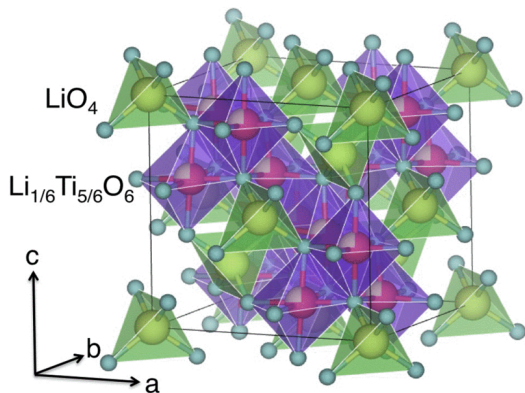


R. M. L. McFadden et al. *Chem. Mater.* **2017**, accepted

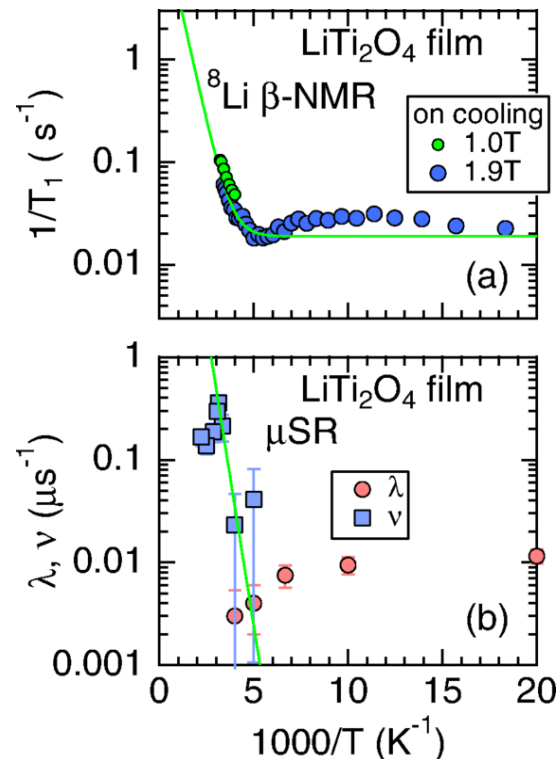
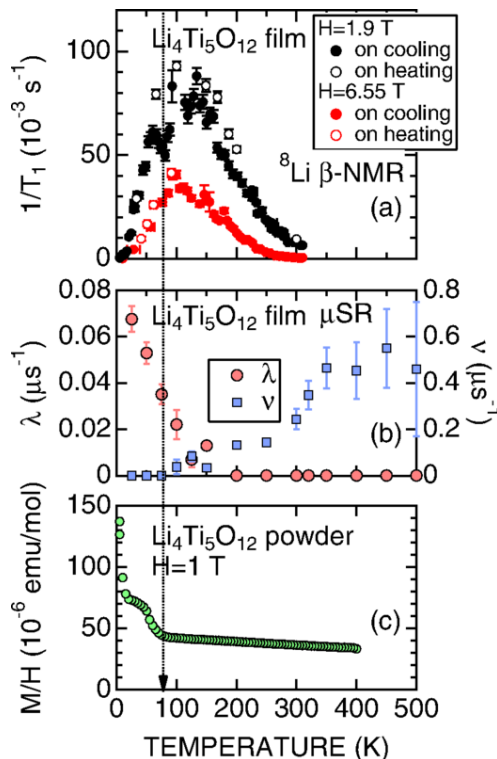
## Polymer electrolyte Poly(ethylene oxide)

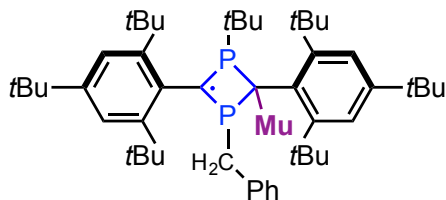
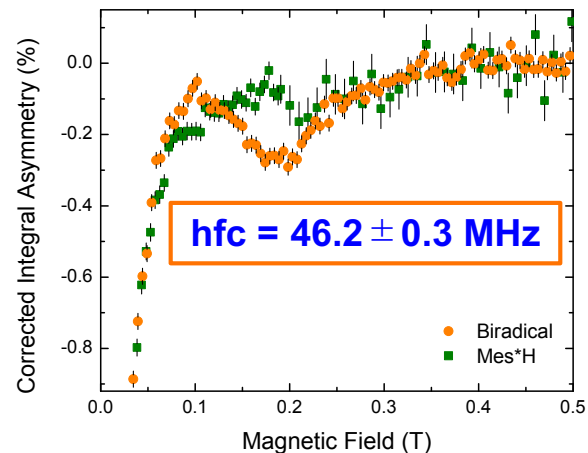
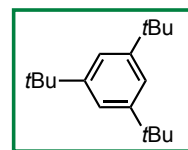
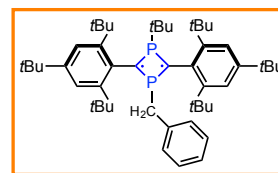
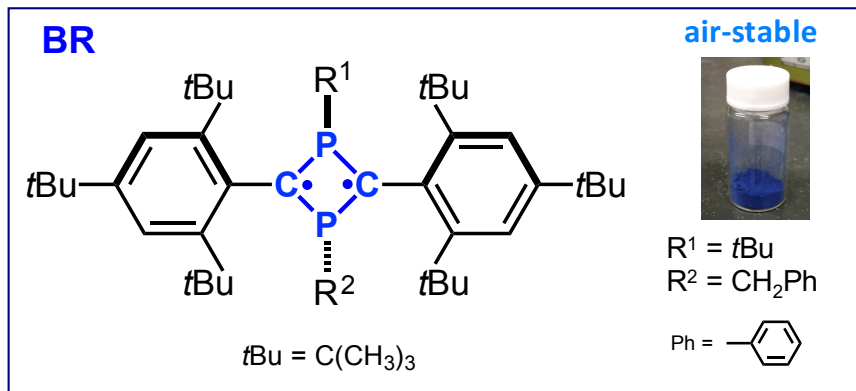


I. McKenzie et al. *J. Chem. Phys.* **2017**, 146, 244903

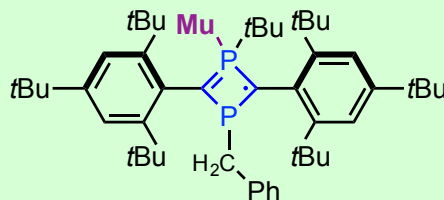


- $\text{Li}^+$  starts to diffuse in  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  above 100 K with an activation energy of 0.11(1) eV.
- $\text{Li}^+$  diffusion occurs in  $\text{LiTi}_2\text{O}_4$  above 200 K with an activation energy of 0.16(2) eV.

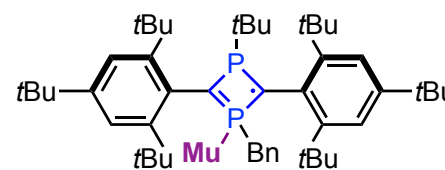




$E_{\text{rel}} = 0.0 \text{ kcal mol}^{-1}$   
 $\text{hfc} = 6.7 \text{ MHz}$



$E_{\text{rel}} = 15.3 \text{ kcal mol}^{-1}$   
 **$\text{hfc} = 51.5 \text{ MHz}$**



$E_{\text{rel}} = 20.0 \text{ kcal mol}^{-1}$   
 $\text{hfc} = 394.4 \text{ MHz}$       UBP86-D/TZ2P

***Aryl-attack structures are completely excluded.***

***Mu predominantly adds on the skeletal phosphorus.***



Canada's national laboratory for  
particle and nuclear physics

Laboratoire national canadien pour  
la recherche en physique nucléaire  
et en physique des particules

TRIUMF: Alberta | British Columbia | Calgary |  
Carleton | Guelph | McGill | Manitoba | McMaster |  
Montréal | Northern British Columbia | Queen's |  
Regina | Saint Mary's | Simon Fraser | Toronto |  
Victoria | Western | Winnipeg | York

Thank You!  
Merci  
どうもありがとうございます