



# Materials, Energy and Life:

Research Using Intense Magnetic Fields

Greg Boebinger

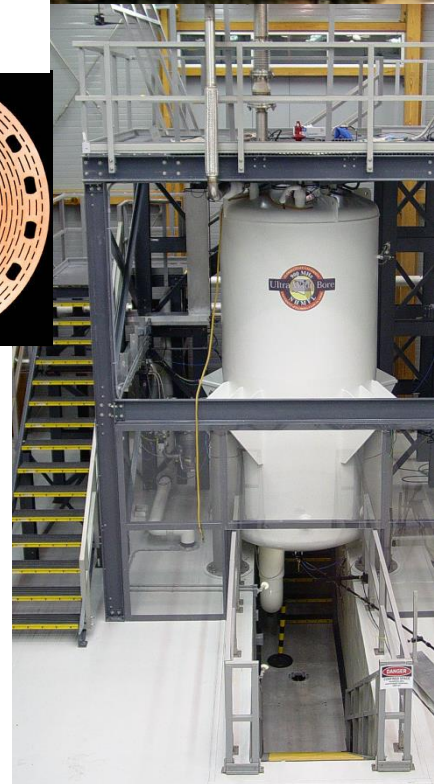
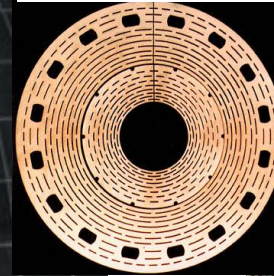
[www.magnet.fsu.edu](http://www.magnet.fsu.edu)

# National High Magnetic Field Laboratory



Florida State University

45T Hybrid DC Magnet

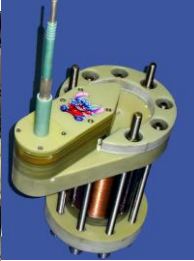


Los Alamos National Laboratory



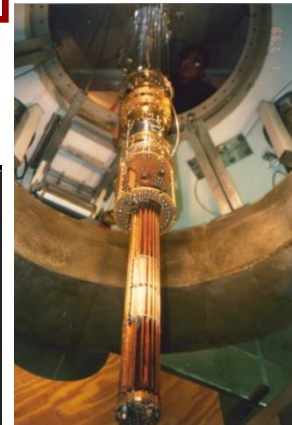
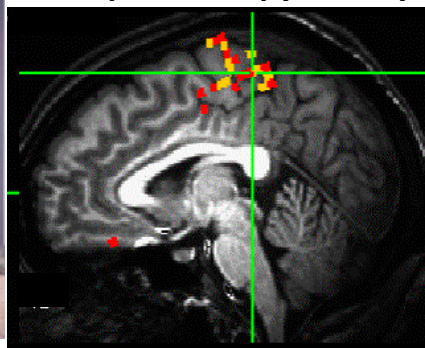
101T Pulse Magnet  
15mm bore

11.4T MRI Magnet  
400mm warm bore



University of Florida

Advanced Magnetic Resonance Imaging and Spectroscopy Facility

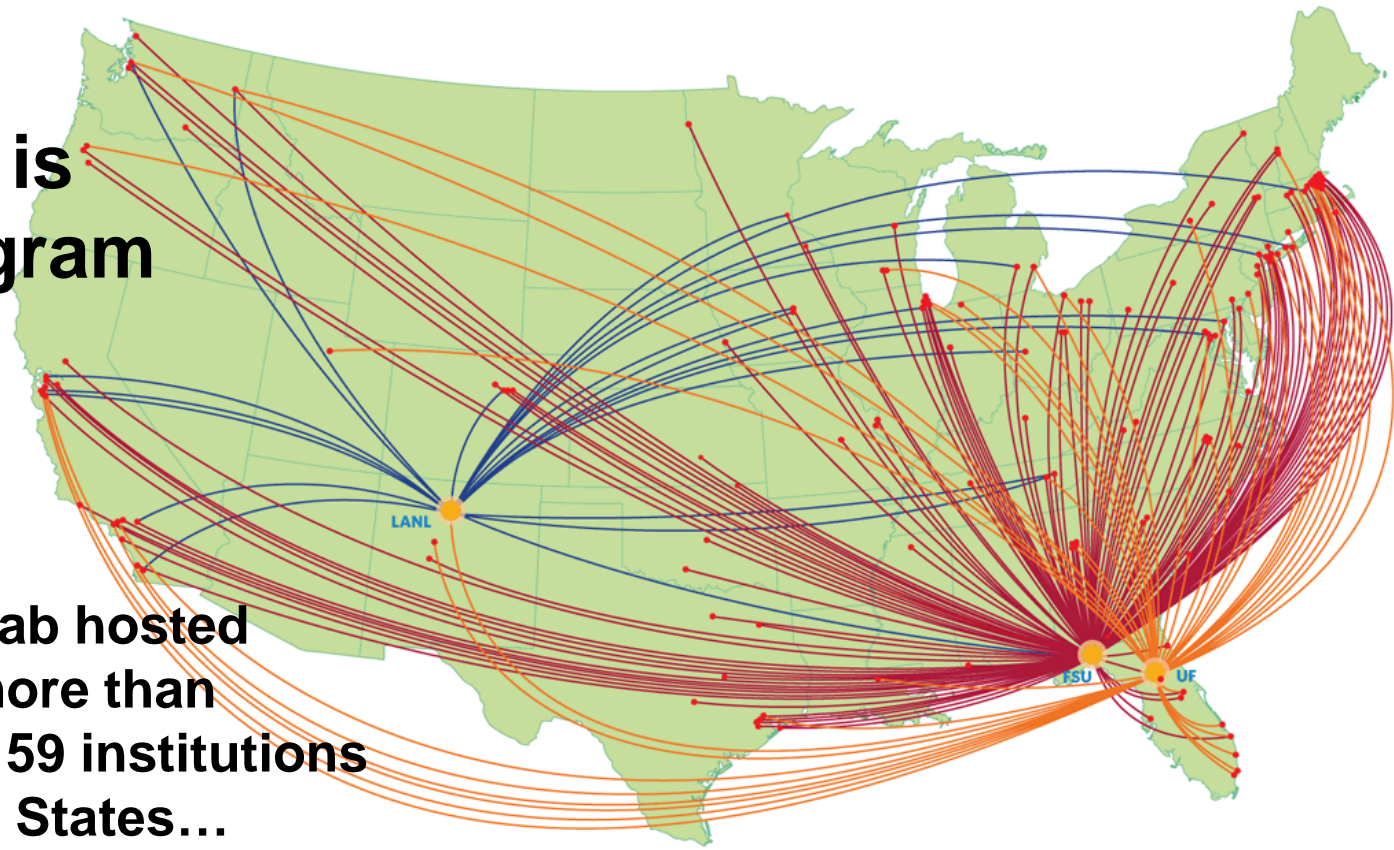


High B/T Facility  
17T, 6weeks at 1mK

900MHz, 105mm bore  
21T NMR/MRI Magnet

# The MagLab is its User Program

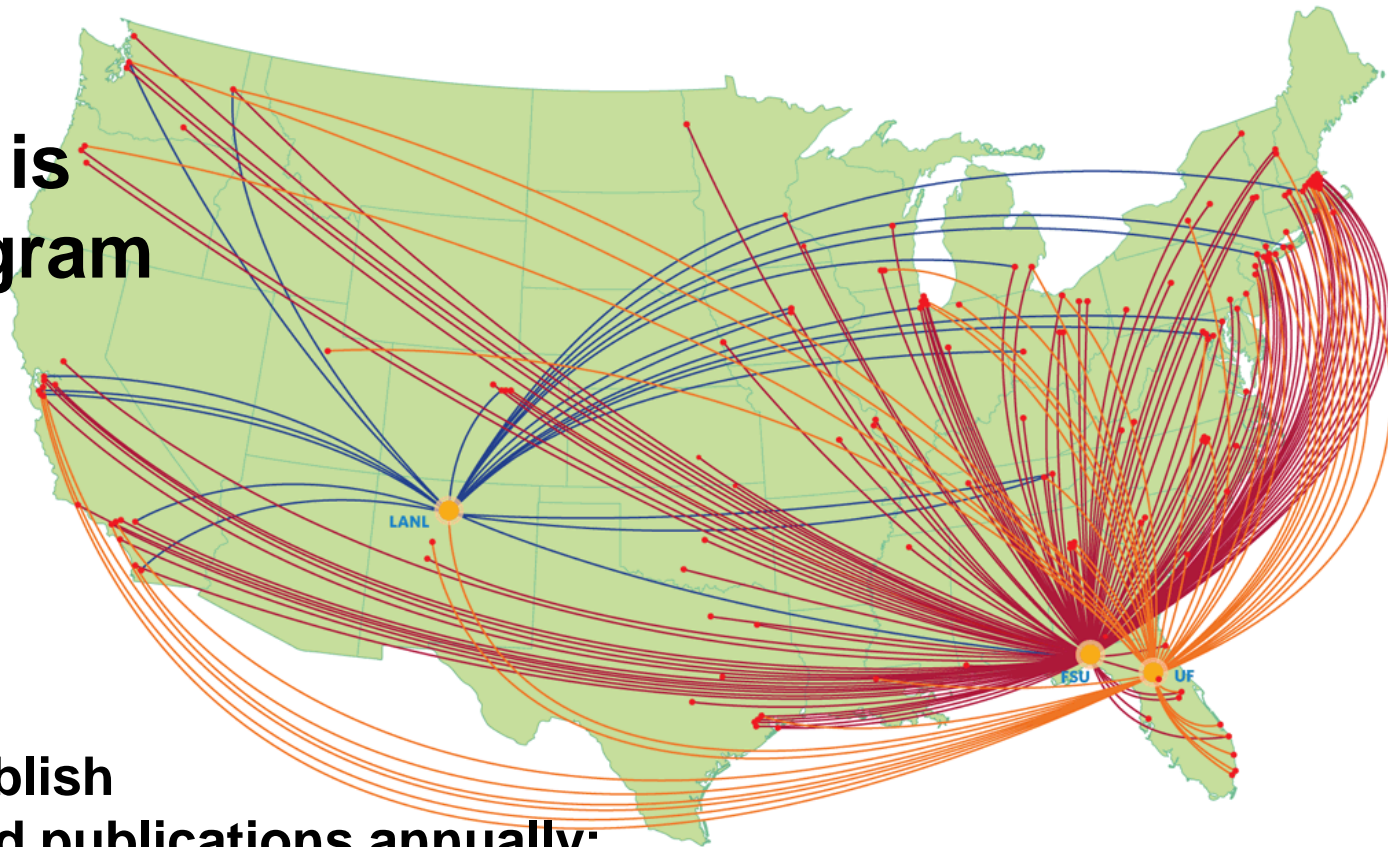
In 2012, the MagLab hosted experiments by more than 1350 users from 159 institutions across the United States...



...and a total of 277 institutions throughout the world.



# The MagLab is its User Program



MagLab users publish  
about 440 refereed publications annually:

## 2009-2013 Publications

**2200** Total Publications

**28** *PNAS*

**63** *Nature Journals*

**147** *Physical Review Letters*

**318** *Physical Review B*

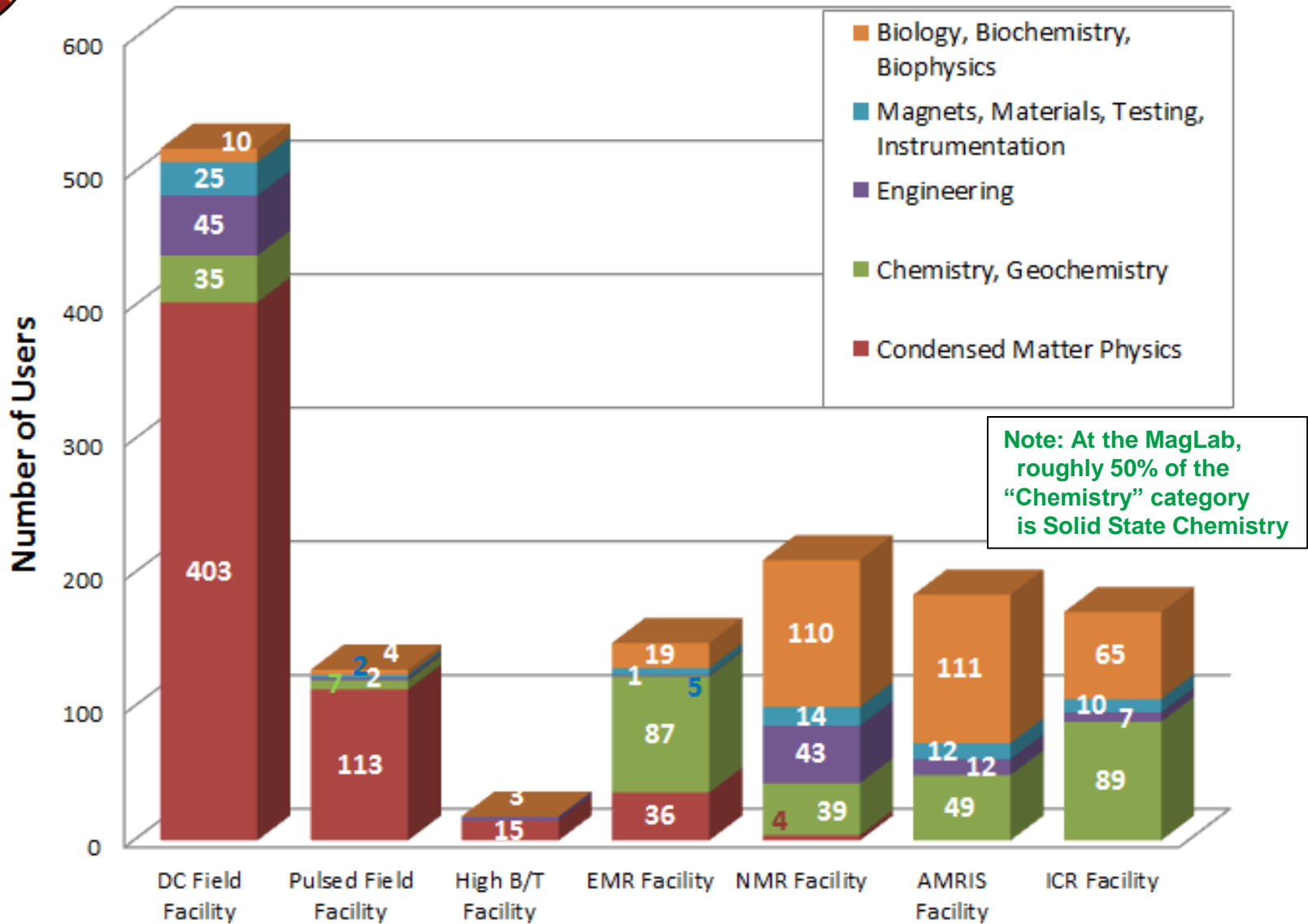
**47** *PRB (Rapid Comm)*

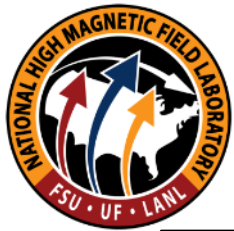
**59** *JACS*



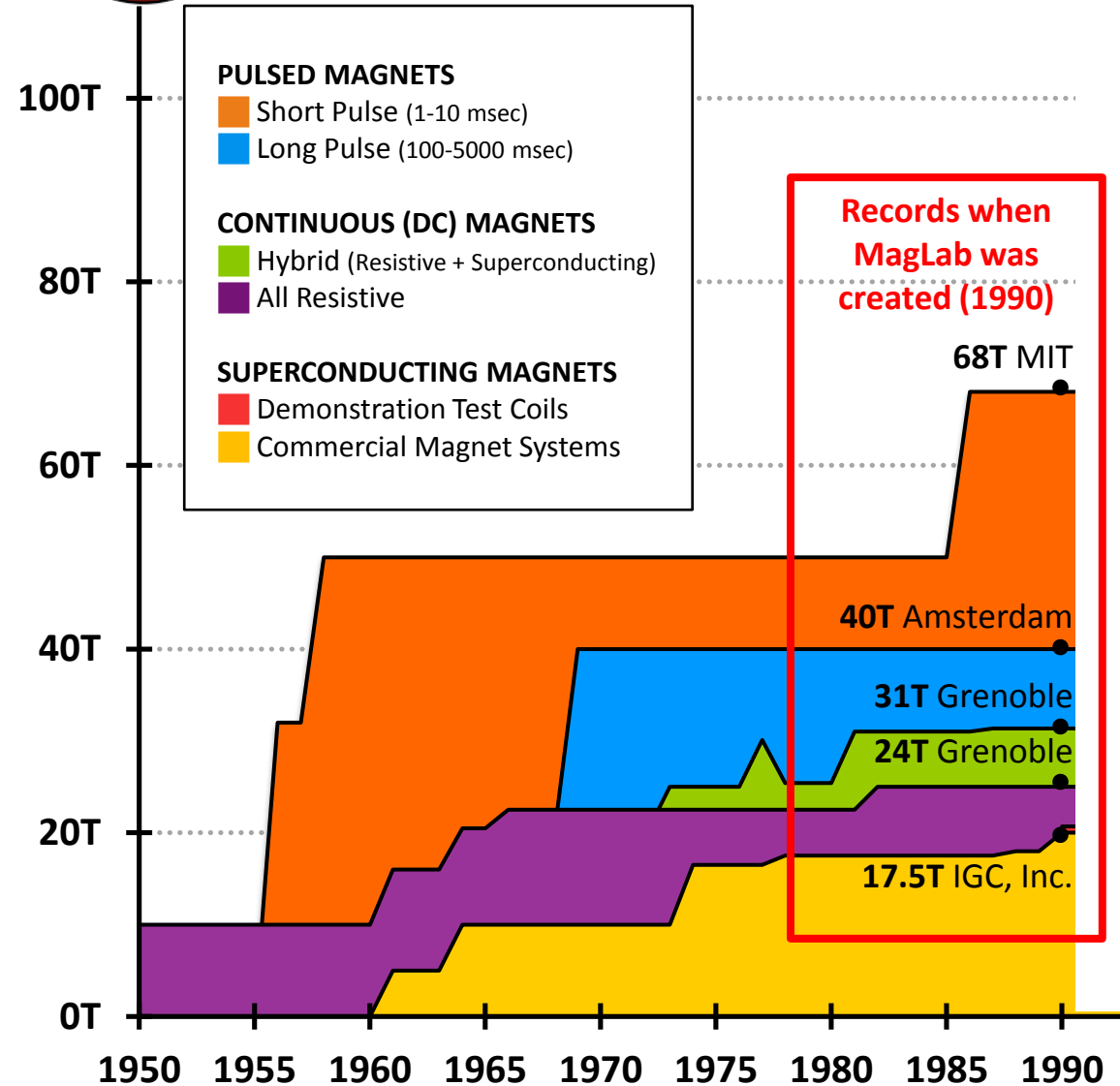


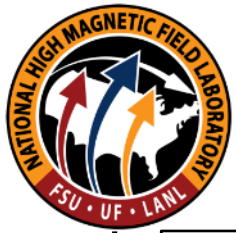
## 2013 MagLab Users by Discipline for Each Facility



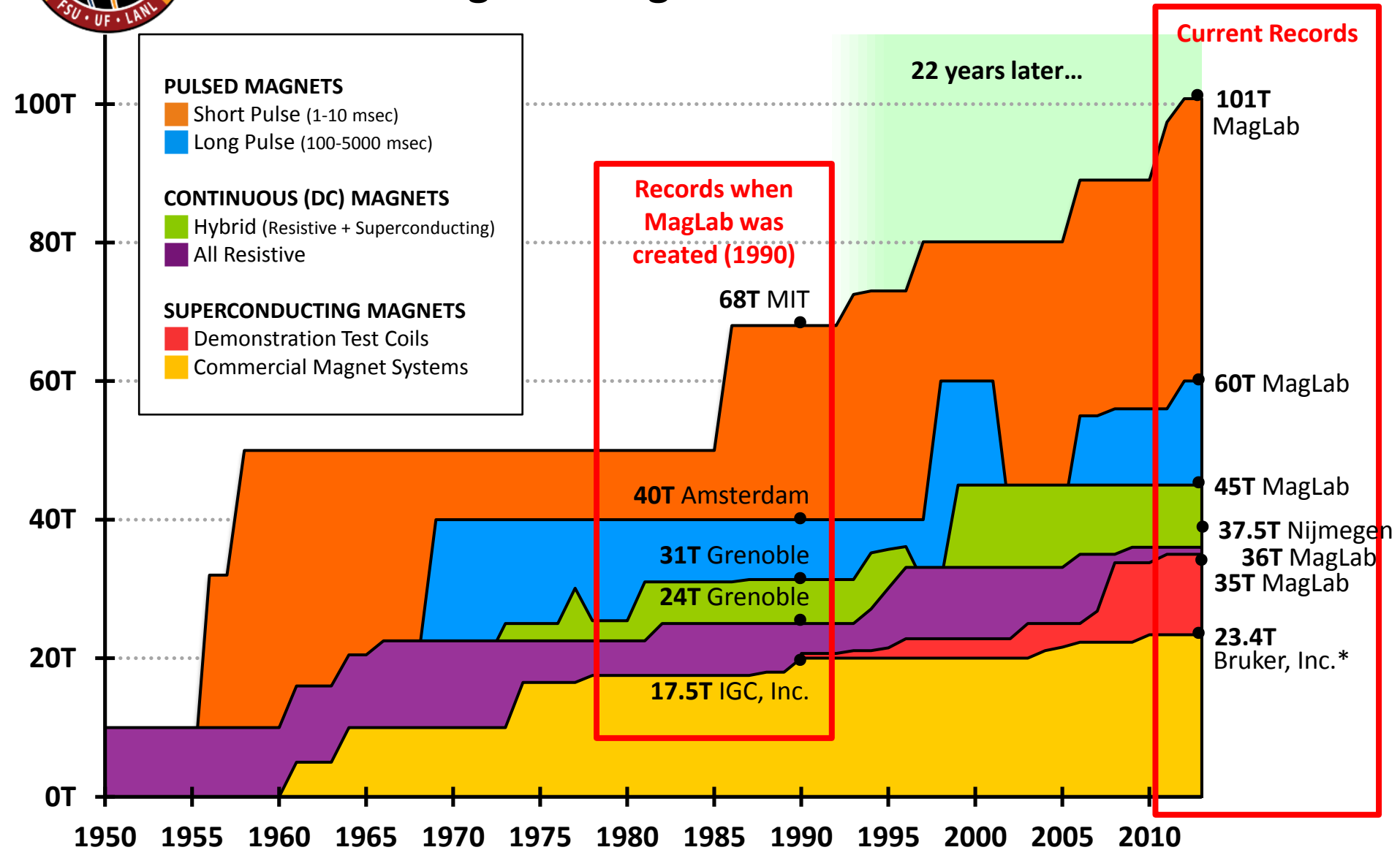


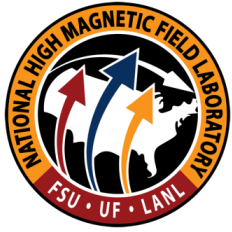
# MagLab Technology Leads the World for Highest Magnetic Fields Achieved





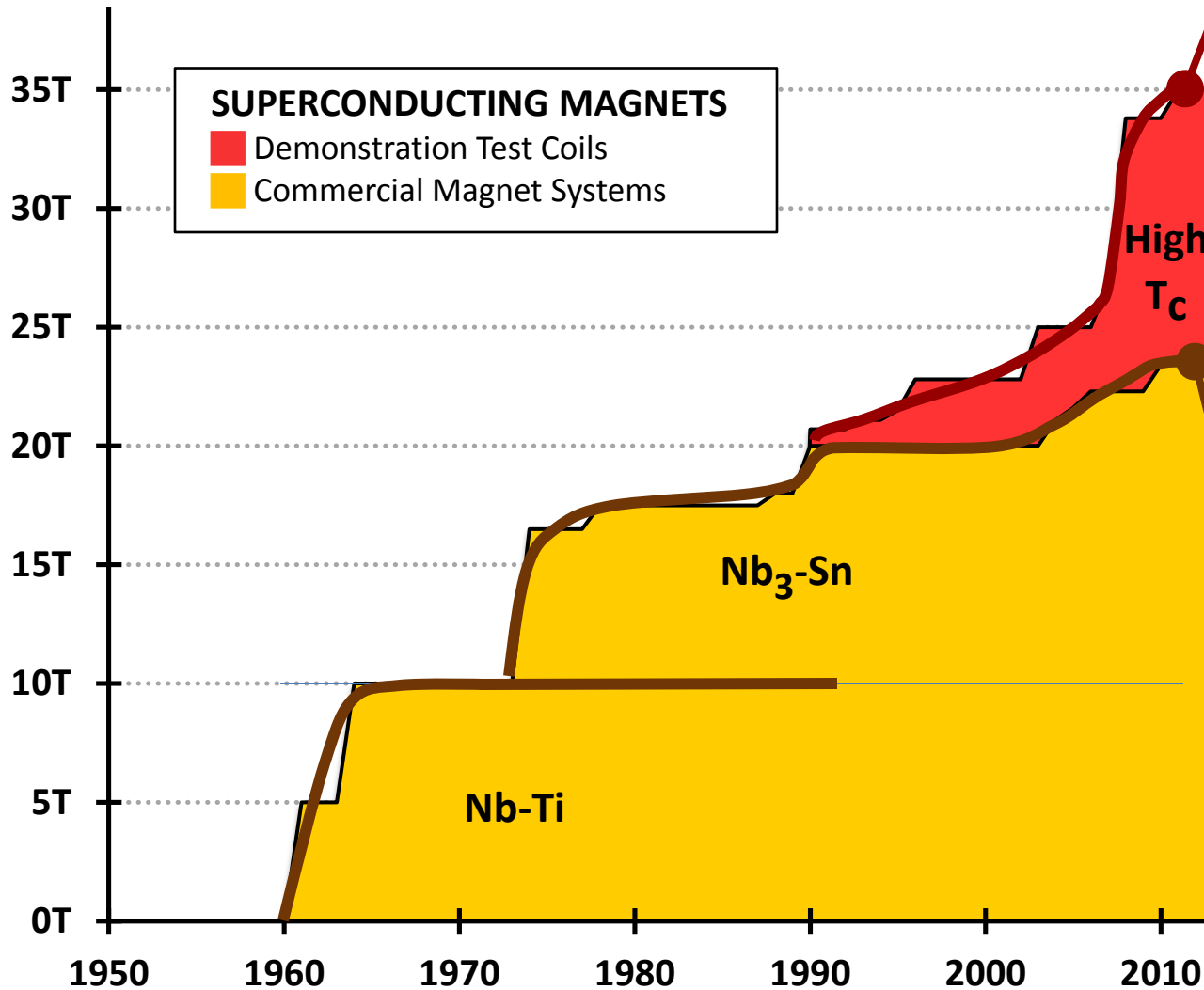
# MagLab Technology Leads the World for Highest Magnetic Fields Achieved





# Superconducting Magnet Technology

Watching a revolution in real time



35 T Proof-of-Principle Demo  
(4T HTS Test Coil in a  
31T Background Magnetic Field)



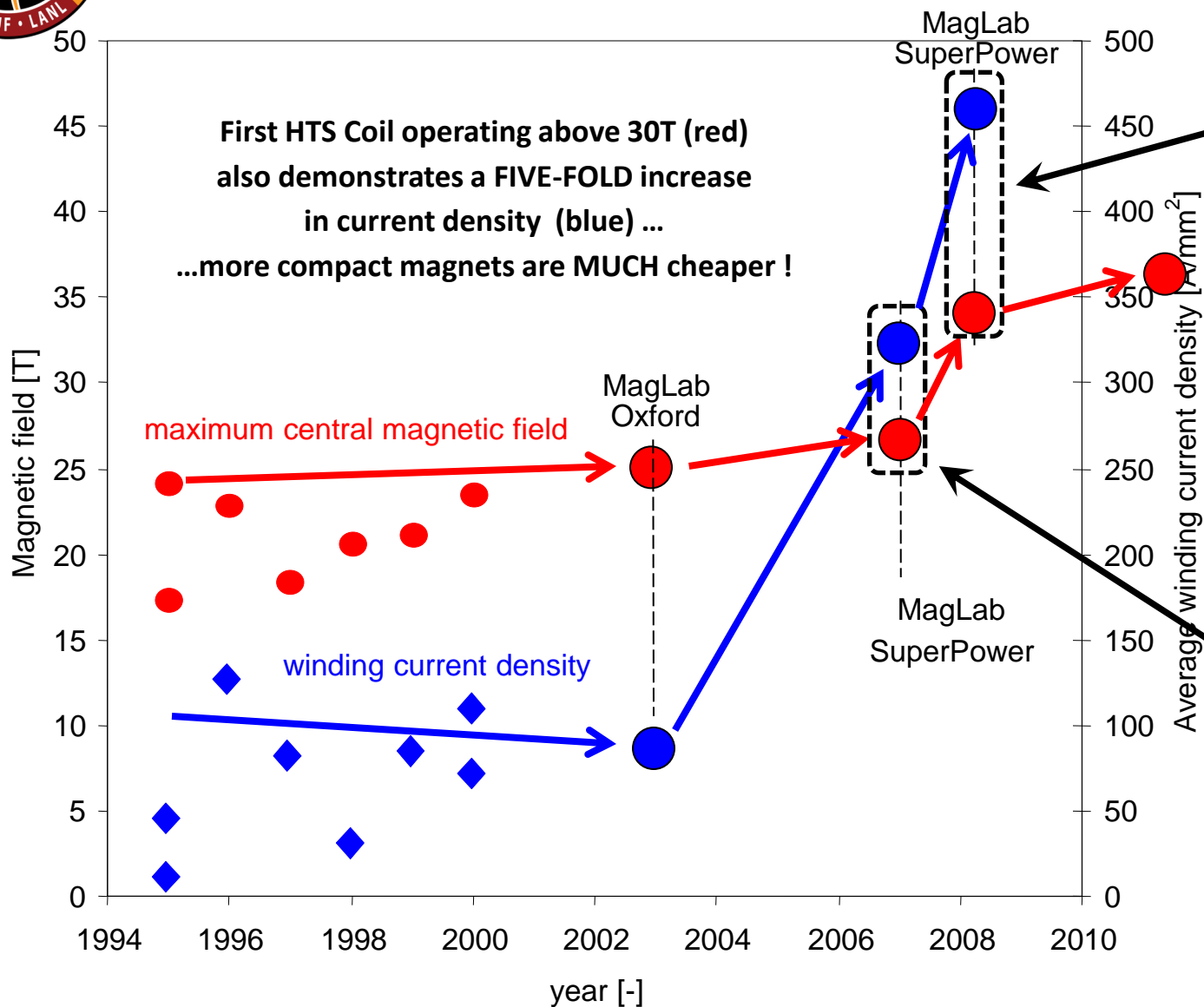
∅ 39 mm

23.5 T (1GHz NMR) Nb<sub>3</sub>-Sn  
Superconducting Magnets  
(Manufactured Commercially)

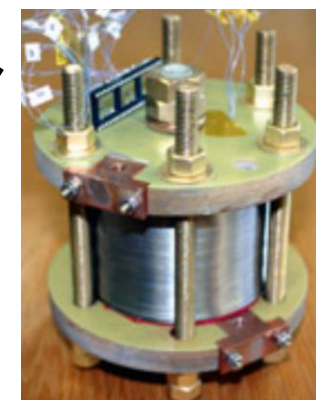




# A Decade of MagLab Collaborations on High-Tc Test Coils



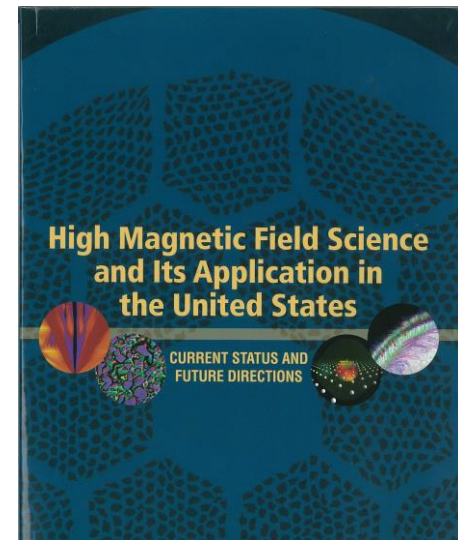
$\phi$  39 mm



$\phi$  87 mm



# The 2013 National Research Council “MagSci” Report is extremely supportive of the MagLab



## EXECUTIVE SUMMARY:

Continued advancement in high-magnetic-field science requires substantial investments in magnets with enhanced capabilities.

The NHMFL in the United States is presently considered to be the world leader in both advancing magnet technology and high-field science.

Magnet projects must include materials development and magnet component test-bed facilities

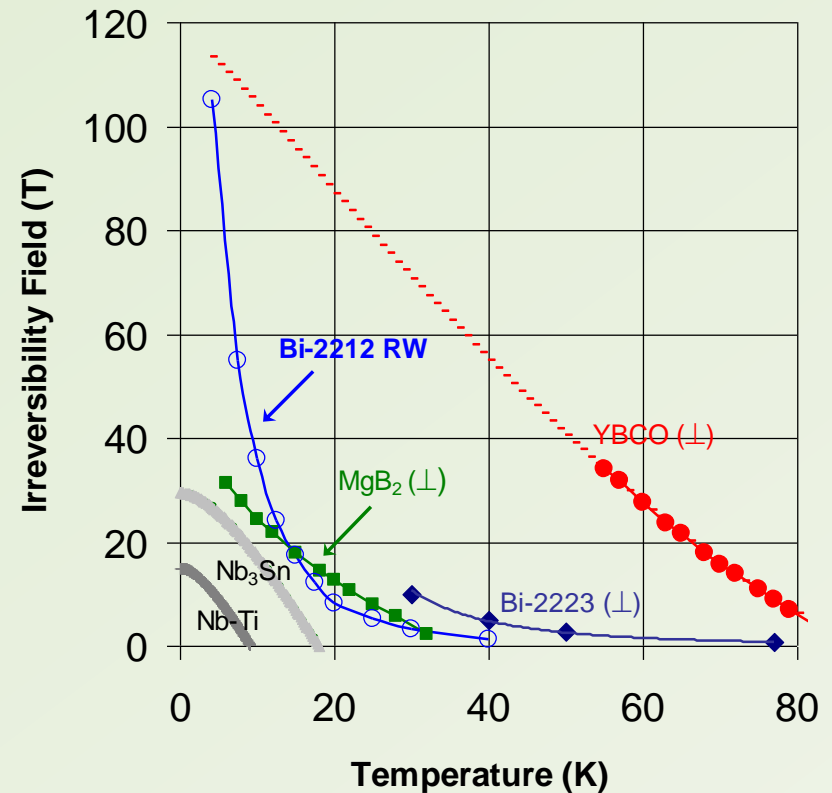
**Most MagSci magnets require HTS materials and technology development**

### MagSci Recommended Magnet Projects

- 1: 30-37 T (1.3 – 1.6 GHz) NMR Magnet
- 2: 150 T (msec) pulse for thermal transport & optical experiments
- 3a: 40 T pulse, 30 sec rep rate for neutrons and/or x-rays
- 3b: 40 T HTS SC magnet for neutrons (and/or x-rays)
- 3c: 25-35T Series Connect Hybrid for neutrons and/or x-rays
- 4: Regional 32 T – 40T SC facilities (including at the MagLab)
- 5: 60 T hybrid magnet
- 6: 20 T large-animal & human MRI
- 7: Axion & other detectors, fusion, **particle accelerators**, radiotherapy.

# An important sidebar.....

- Higher  $T_c$  superconducting magnets are a **persistent dream** of the condensed matter community.....
- Cuprates can superconduct up to 130 K
  - Applications in liquid nitrogen at 77 K are still very rare
  - More than 95% of all superconductor sold is still Nb-Ti with  $T_c$  of 9 K
- Applications are determined by high  $J_c$ ,  $J_e$  and  $H_{irr}$  rather than by high  $T_c$
- Conductors of exotic materials are **difficult!**



The dream: escape from bottom left corner to the upper and the right.....

# ITER has made tonnage breakout for Nb<sub>3</sub>Sn – both CERN and the MagLab are assisting ITER

## SUPERCONDUCTIVITY IN Nb<sub>3</sub>Sn AT HIGH CURRENT DENSITY IN A MAGNETIC FIELD OF 88 kgauss

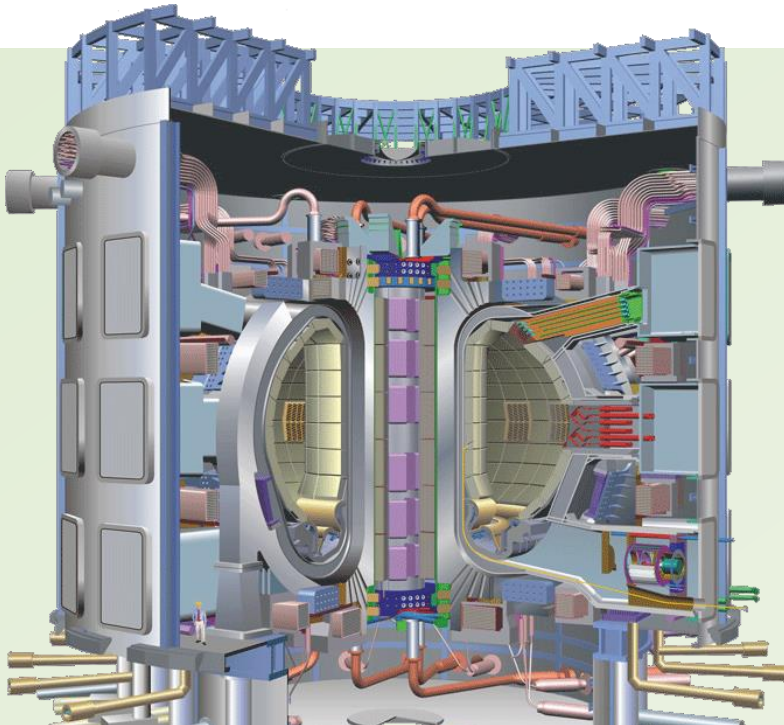
J. E. Kunzler, E. Buehler, F. S. L. Hsu, and J. H. Wernick  
Bell Telephone Laboratories, Murray Hill, New Jersey  
(Received January 9, 1961)

We have observed superconductivity in Nb<sub>3</sub>Sn at average current densities exceeding 100 000 amperes/cm<sup>2</sup> in magnetic fields as large as 88 kgauss. The nature of the variation of the critical current (the maximum current at a given field for which there is no energy dissipation) with magnetic field shows that superconductivity extends to still higher fields. Existing theory does not account for these observations. In addition

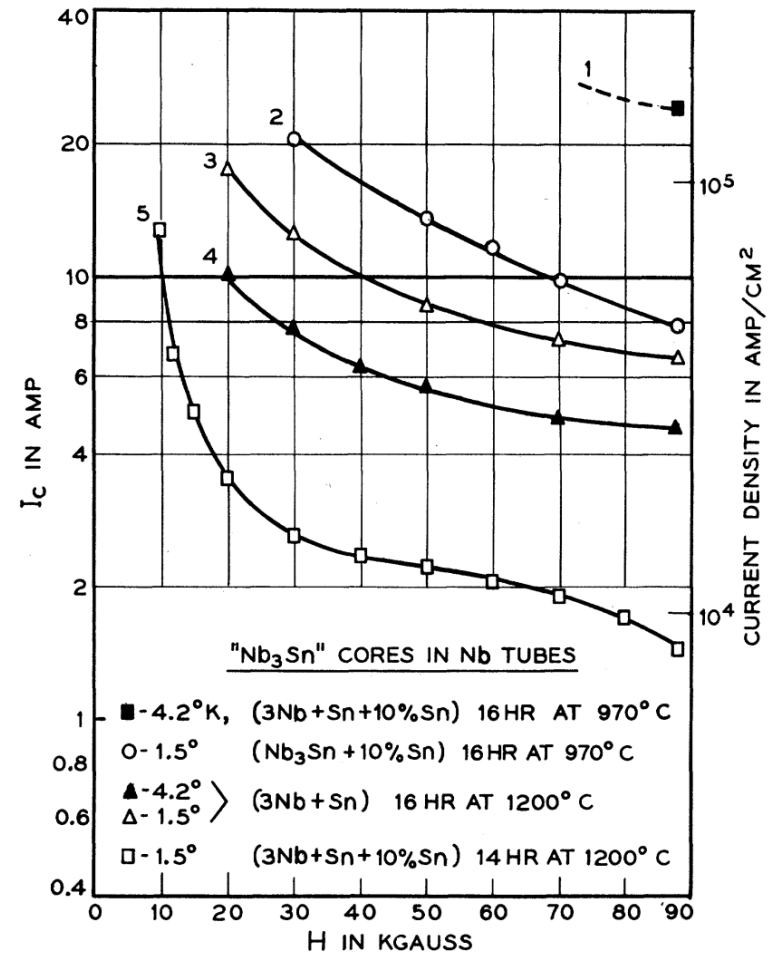
to some remarkable implications concerning superconductivity, these observations suggest the feasibility of constructing superconducting solenoid magnets capable of fields approaching 100 kgauss, such as are desired as laboratory facilities and for containing plasmas for nuclear fusion reactions.<sup>1,2</sup>

The highest values of critical magnetic fields previously reported for high current densities

89

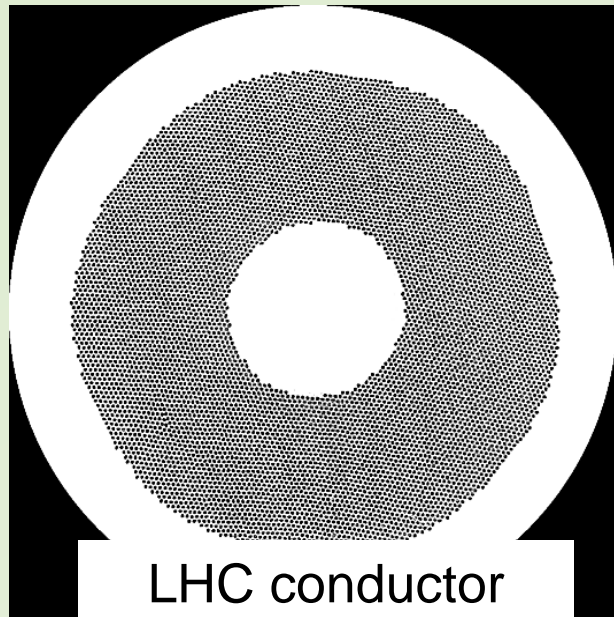


ITER uses 600 tonnes of Nb<sub>3</sub>Sn

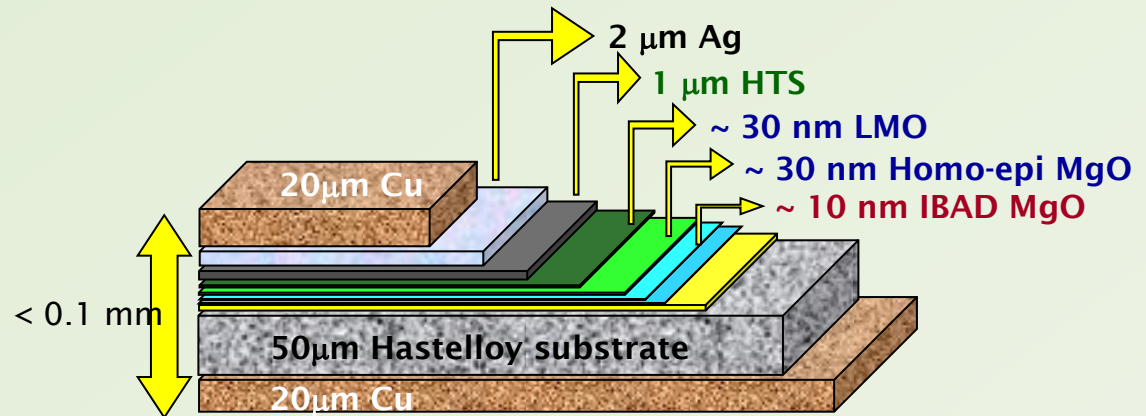


Phys Rev Letts 6, 89 (1961),  
submitted January 9, 1961,  
published February 1, 1961!

# HTS Magnet Conductors in 2012



Nb47Ti conductor- thousands of 8  $\mu\text{m}$  diameter Nb47Ti filaments in pure Cu (0.8 mm dia.), easily cabled to operate at 10-100 kA



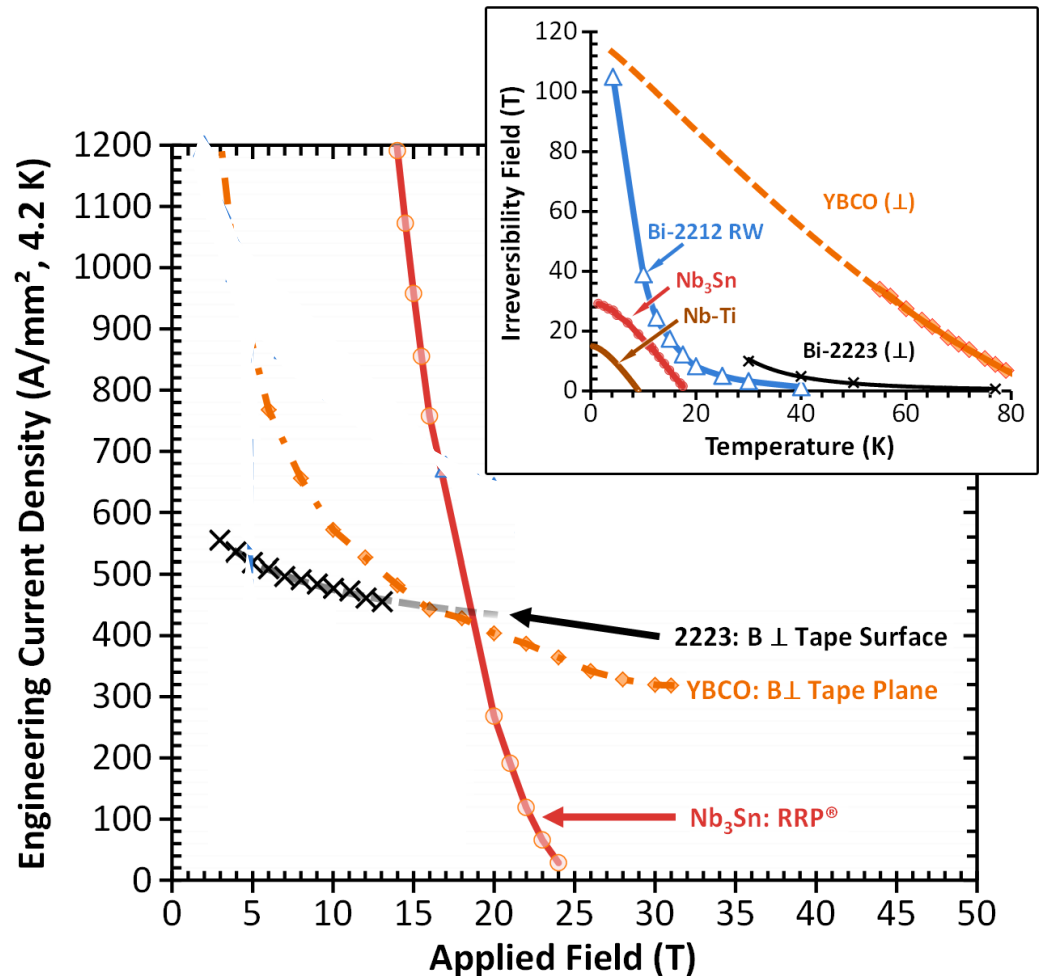
**2. REBCO coated conductor – extreme texture (single crystal by the mile) – for maximum GB transparency (2007)**

**1. Bi-2223 – the first HTS conductor – uniaxial texture developed by deformation and reaction (1995- today)**



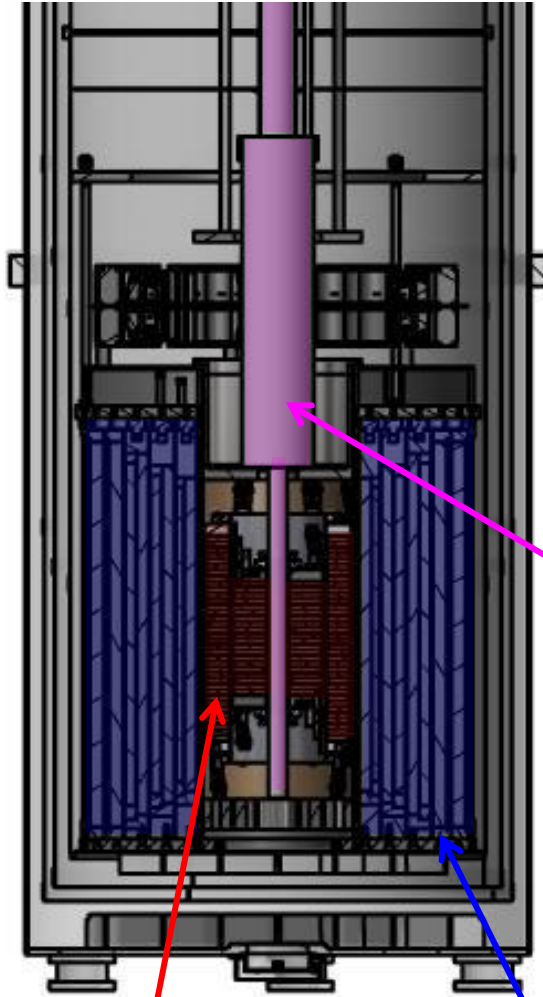
# An important sidebar.....

- Applications are determined by high  $J_c$ ,  $J_e$  and  $H_{irr}$  rather than by high  $T_c$
- Conductors of exotic materials are difficult!





# High-Tc Superconducting Magnet Technology: Building a 32T All-Superconducting REBCO Magnet



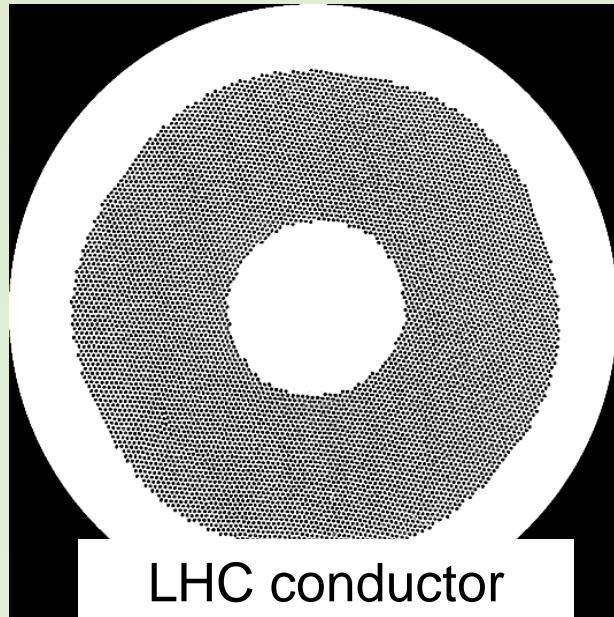
Dilution refrigerator

15 T  
250 mm bore  
LTS magnet

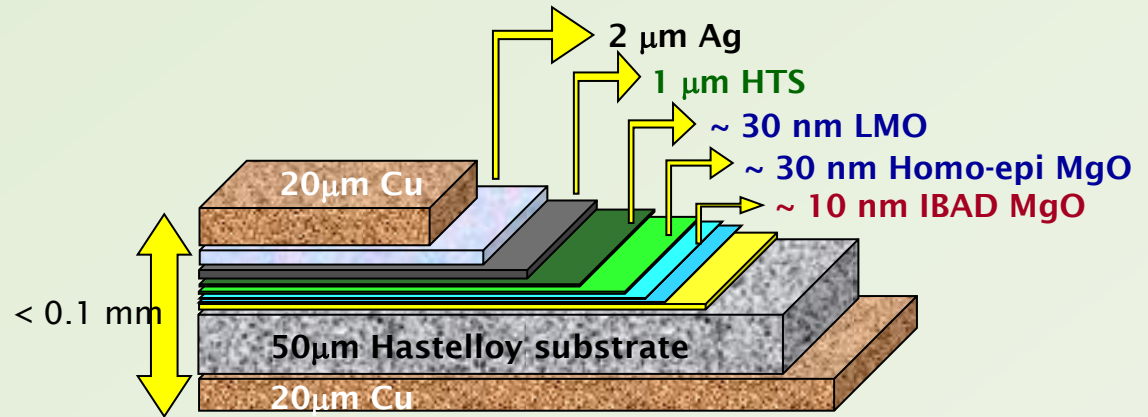
17 T / 32 mm bore REBCO coils



# HTS Magnet Conductors Now



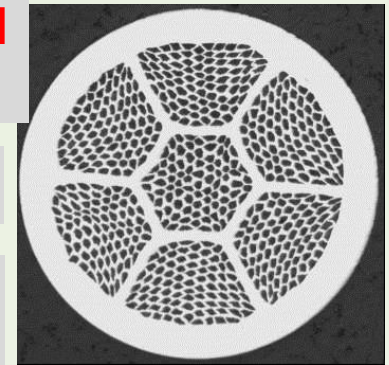
Nb47Ti conductor- thousands of 8  $\mu\text{m}$  diameter Nb47Ti filaments in pure Cu (0.8 mm dia.), easily cabled to operate at 10-100 kA



4. REBCO coated conductor - extreme texture (single crystal by the mile) - for maximum GB transparency (2007)

3. Bi-2212 - high  $J_c$  without macroscopic texture (2012)!

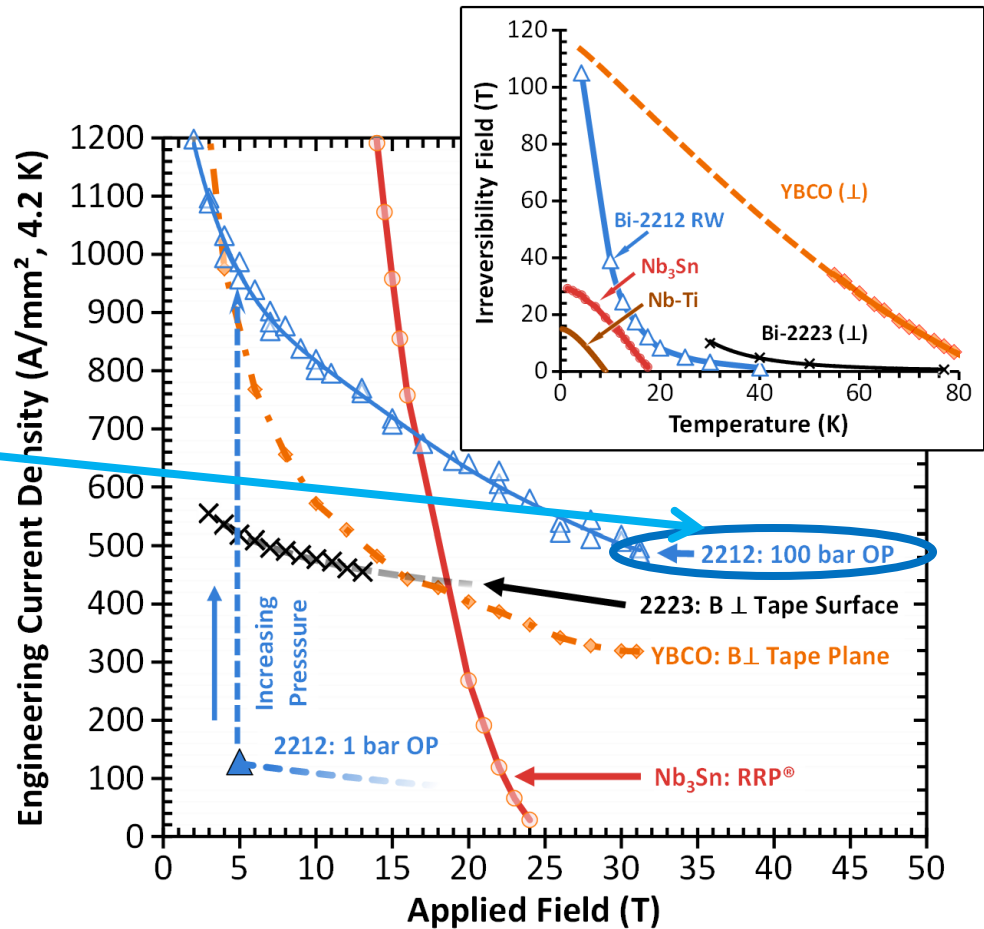
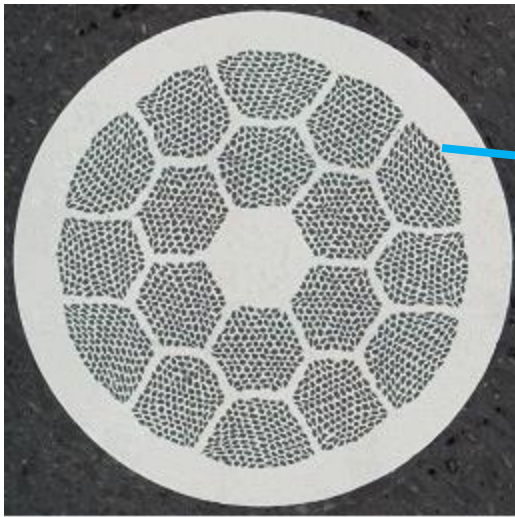
1. Bi-2223 - the first HTS conductor - uniaxial texture developed by deformation and reaction (1995- today)





# Bi-2212 – developed by NHMFL, DOE-HEP labs and Oxford Superconducting Technology (OST) – twisted, round, filamentary conductor fully competitive with any other HTS in $J_E$

- Fine filament twisted conductor is ideal for **high homogeneity NMR and accelerator magnets**



From the cover of the MagSci report

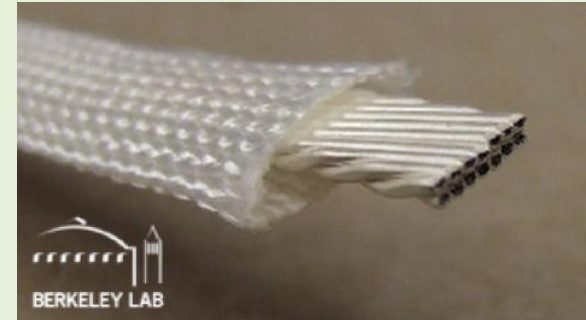
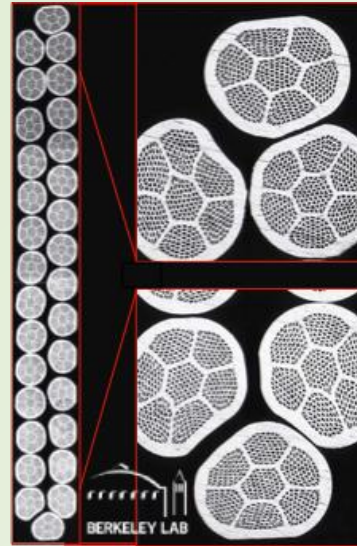
(DCL et al. arXiv 1305.1269 – to appear Nature Materials 2014)

Bi-2212 conductor support by DOE-OHEP: an outcome of Bismuth Strand and Cable Collaboration (BSCCo)

# Large magnets are better protected when cabled: Substantial R&D required to develop HTS cabling technologies

🌀 Cables vital for 60 T hybrid at the NHMFL, an LHC energy upgrade and a neutrino machine based on a Muon Collider at Fermilab

🌀 Easy path to 2212 cables through the standard Rutherford cable



Bi-2212 Rutherford cables (Arno Godeke LBNL) with mullite insulation sleeve

REBCO coated conductor cable wound in many layers helically on a round form



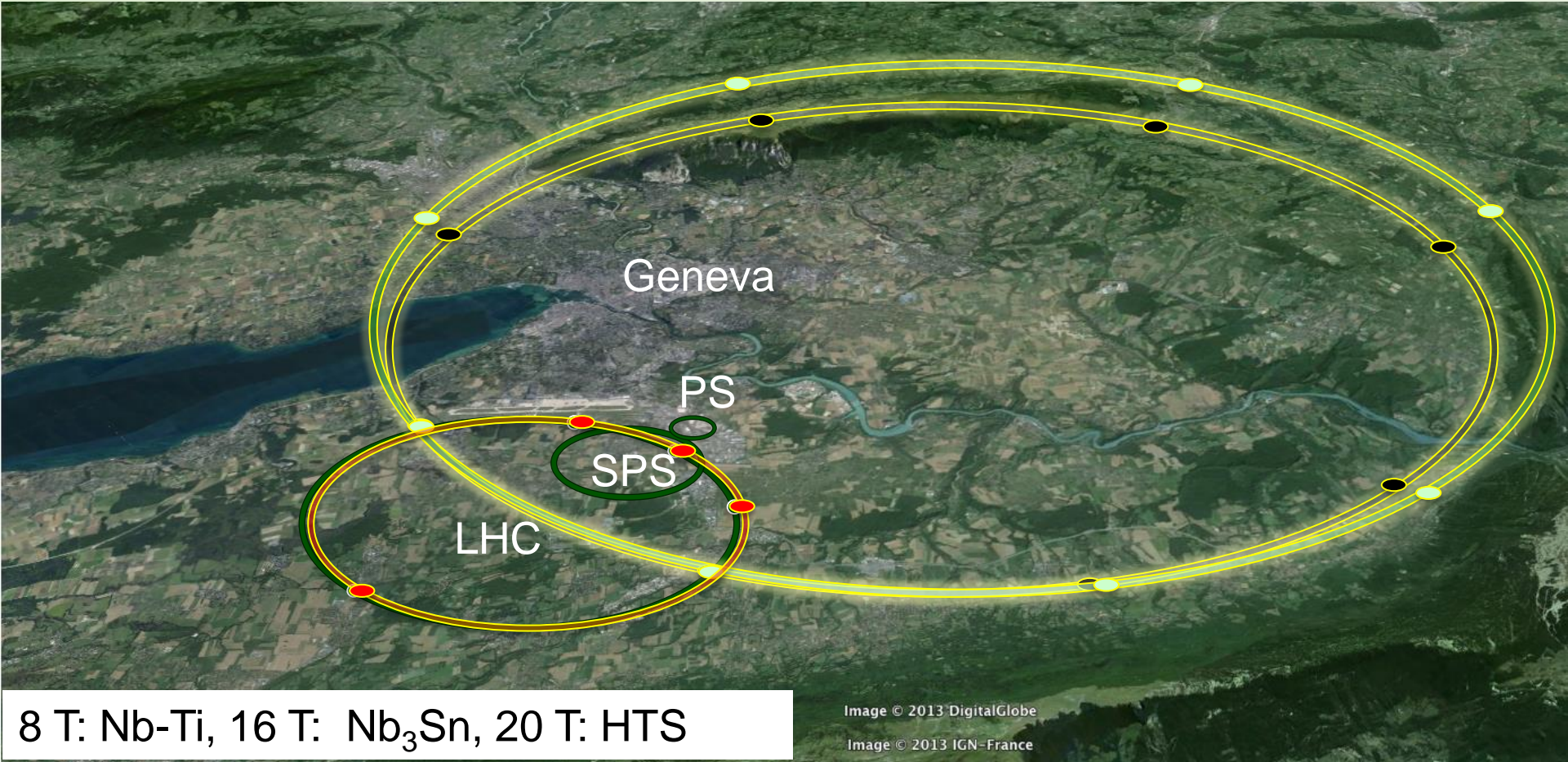
Other variants too: e.g. Roebel cable



Advanced Conductor Technologies LLC  
www.advancedconductor.com  
Danko van der Laan

🌀 REBCO cables are harder (Coated Conductor is a single filament) – but possible (IRL, KIT, CORC, twisted stack (MIT))

# Size and field trade off for the LHC



8 T: Nb-Ti, 16 T: Nb<sub>3</sub>Sn, 20 T: HTS

LHC  
27 km, 8.33 T  
14 TeV (c.o.m.)

HE-LHC  
27 km, **20 T**  
33 TeV (c.o.m.)

VHE-LHC  
80 km, **20 T**  
100 TeV (c.o.m.)

VHE-LHC  
100 km, **16 T**  
100 TeV (c.o.m.)



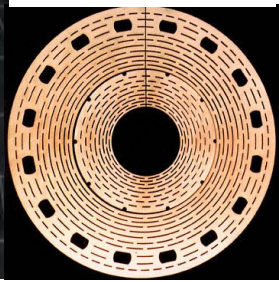
## High Magnetic Fields and Materials

# National High Magnetic Field Laboratory



Florida State University

45T Hybrid DC Magnet

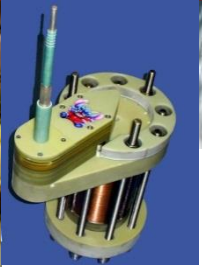


1.4 GW Generator

Los Alamos National Laboratory



101T Pulse Magnet  
10mm bore

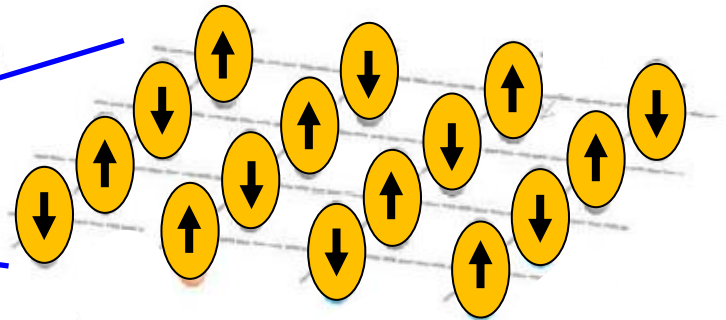
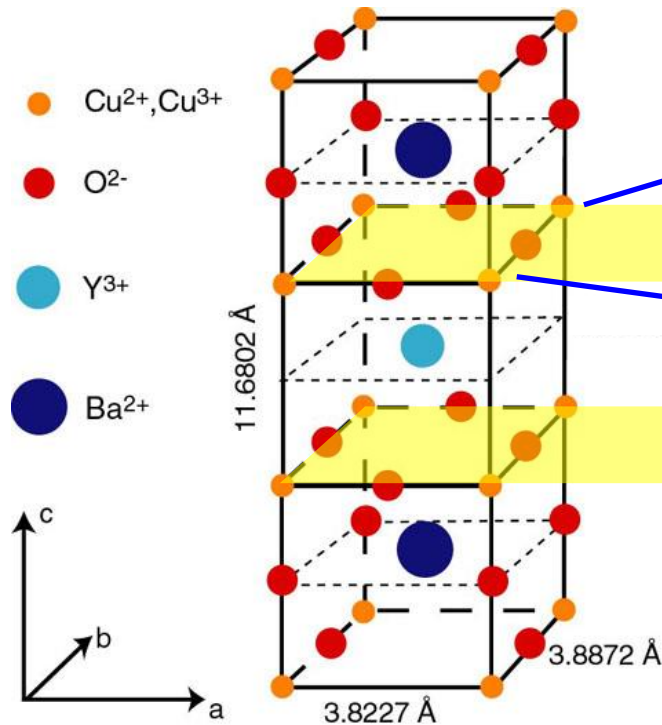


Graphene, Fe-based superconductors,  
**Quantum oscillations in cuprate superconductors,**  
Topological insulators, Molecular magnets,  
Model magnetic systems, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
Energy-related materials, Petroleum, Natural Products,  
Bio-macromolecular complexes and the Brain



# First Key Ingredient for ('Cuprate') High-Temperature Superconductors:

## the Copper – Oxygen Plane



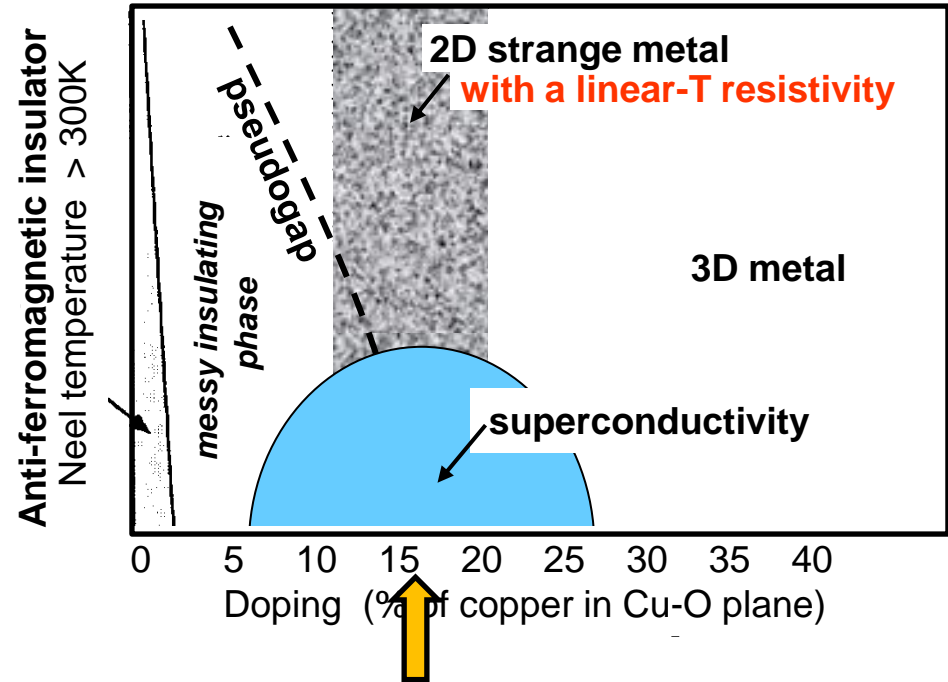
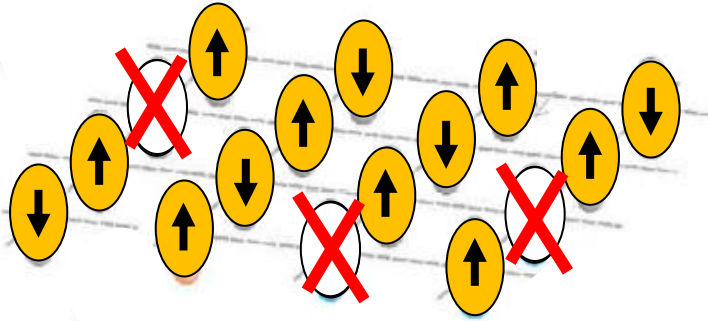
**The 2D Copper-Oxygen Plane...**  
*...the playground of high-temperature  
superconductivity*

**With one electron on each Copper atom,  
the electrons cannot move  
...and you have an insulator**



# Second Key Ingredient for ('Cuprate') High-Temperature Superconductors:

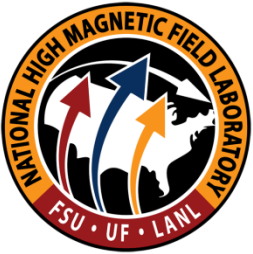
## Removing electrons from the Copper – Oxygen Plane



Remove ~5% to ~27% of the electrons...

...and you have a HIGH-TEMPERATURE SUPERCONDUCTOR

For more than a dozen different materials, the same 16% doping  
...optimizes superconductivity (highest transition temperature)



# Large Fermi Surface in Tl-2201 in the overdoped regime

Original measurement using Angle-Dependent Magneto-resistance Oscillations:

N.E. Hussey, M. Abdel-Jawad, A. Carrington, A.P. Mackenzie, L. Balicas,

“A coherent three-dimensional Fermi surface in a high-transition-temperature superconductor”

**Nature 425, 814 (2003)**

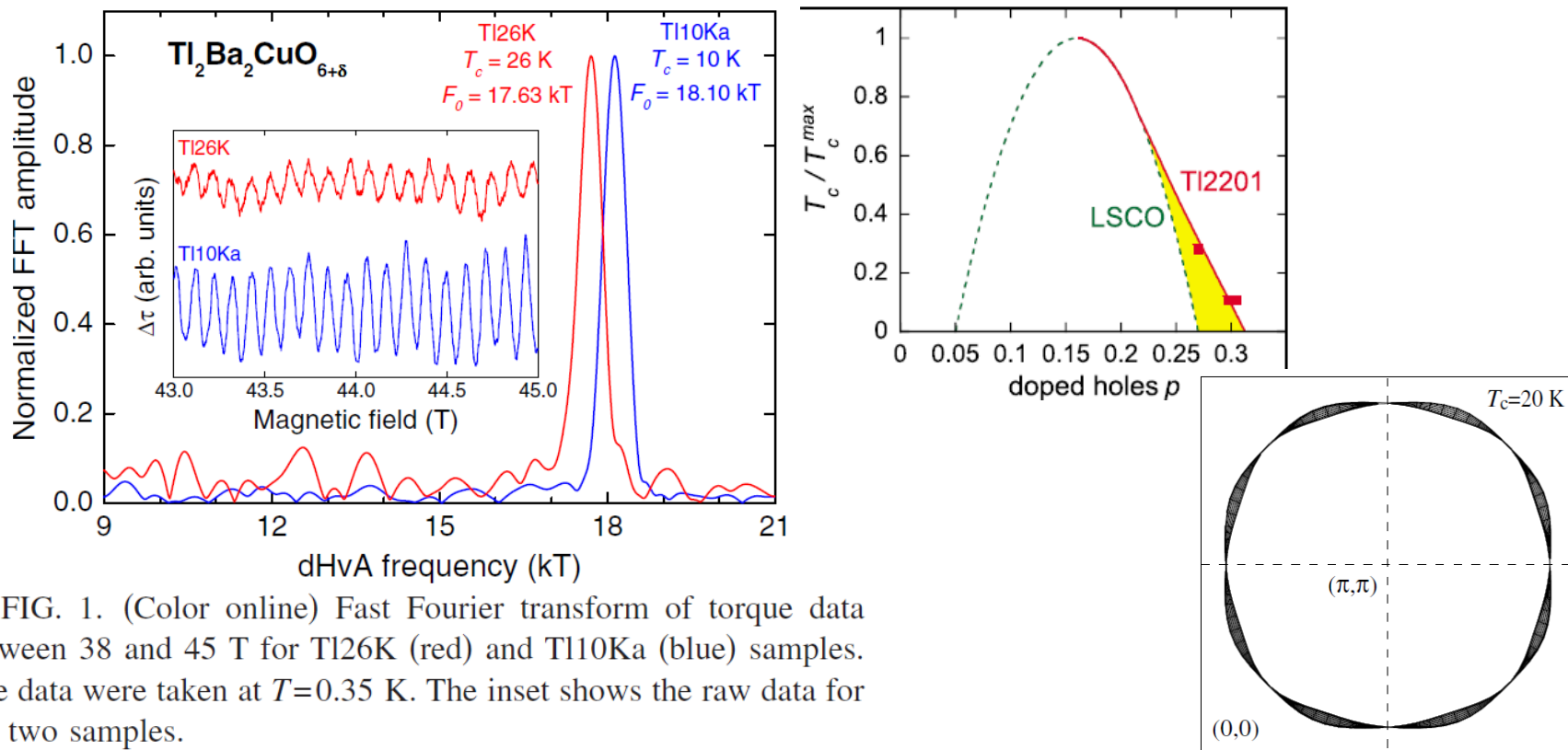
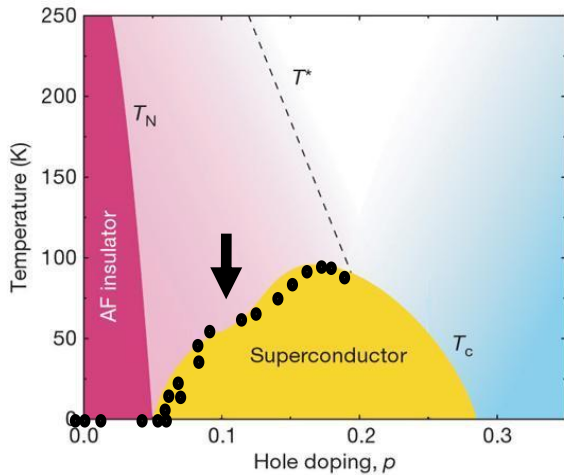


FIG. 1. (Color online) Fast Fourier transform of torque data between 38 and 45 T for Tl26K (red) and Tl10Ka (blue) samples. The data were taken at  $T=0.35$  K. The inset shows the raw data for the two samples.

A.F. Bangura, P.M.C. Rourke, T.M. Benseman, M. Matusiak, J.R. Cooper, N.E. Hussey, and A. Carrington  
*Fermiology and electronic homogeneity of the superconducting overdoped cuprate  $Tl_2Ba_2CuO_{6+\delta}$  revealed by quantum oscillations*  
**Phys. Rev. B 82, 140501(R) (2010)**



# 2007: Small Fermi Surface in the Underdoped YBCO – The Pseudogap State Looks like an Ordinary Fermi Liquid !

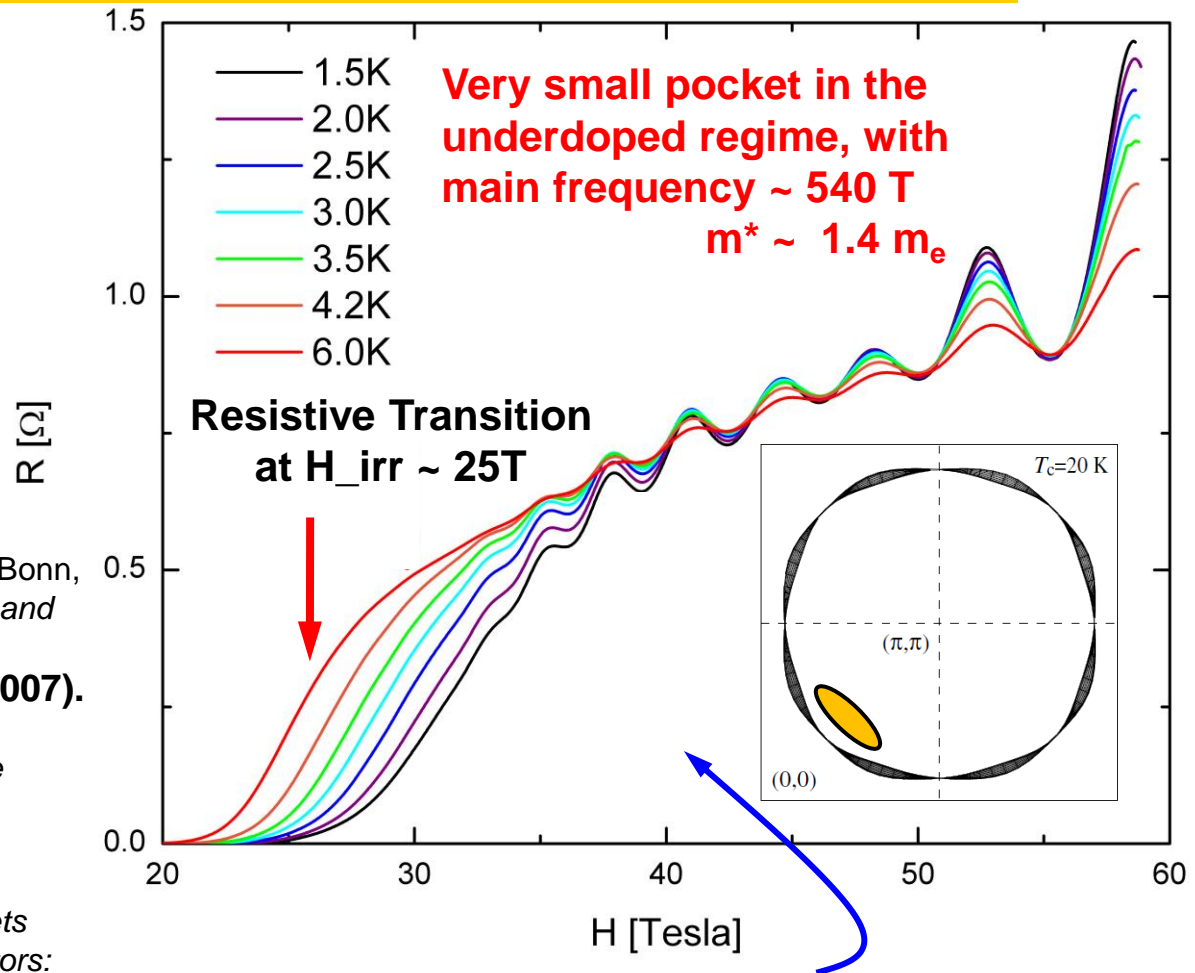


N. Doiron-Leyraud, C. Proust, D. LeBoeuf, J. Levallois, J-B Bonnemaïson, R. Liang, D.A. Bonn, W.N. Hardy, L. Taillefer, "Quantum oscillations and the Fermi surface in an underdoped high- $T_c$  superconductor." **Nature 447, 565-568 (2007).**

Yelland, E. A. *et al.* Quantum oscillations in the underdoped cuprate  $YBa_2Cu_4O_8$ . **Phys. Rev. Lett. 100, 047003 (2008).**

Bangura A. F. *et al.* Small Fermi surface pockets in underdoped high temperature superconductors: observation of Shubnikov-de Haas oscillations in  $YBa_2Cu_4O_8$ . **Phys. Rev. Lett. 100, 047004 (2008).**

Jaudet C. *et al.*, de Haas–van Alphen oscillations in the underdoped high-temperature superconductor  $YBa_2Cu_3O_{6.5}$ . **Phys. Rev. Lett. 100, 187005 (2008).**



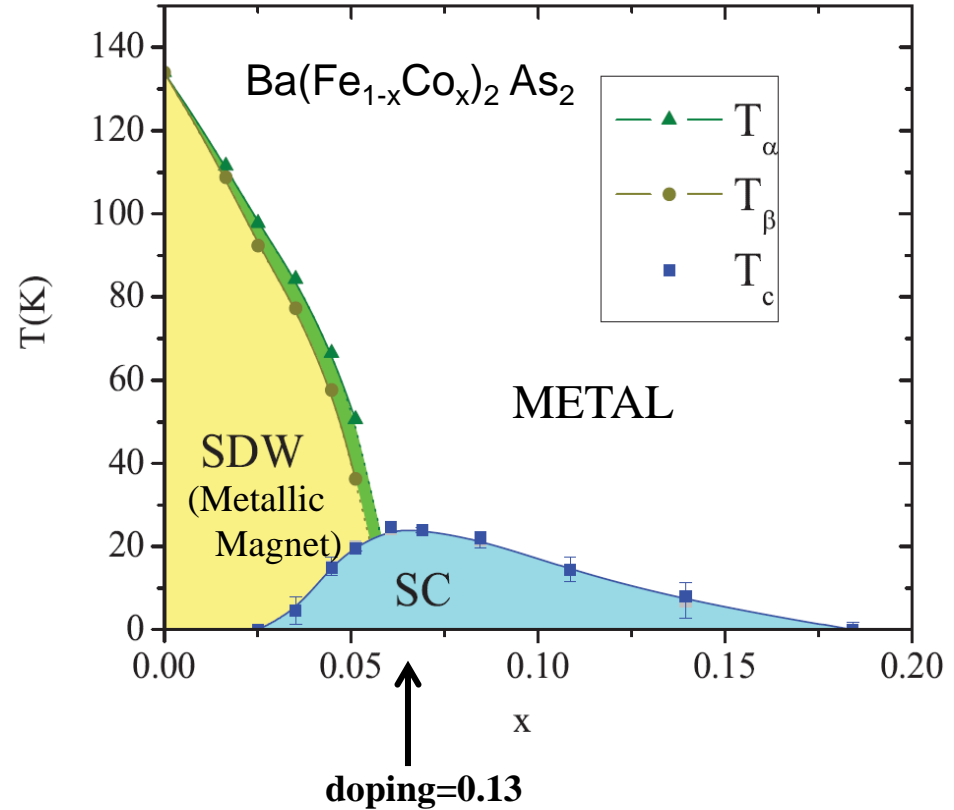
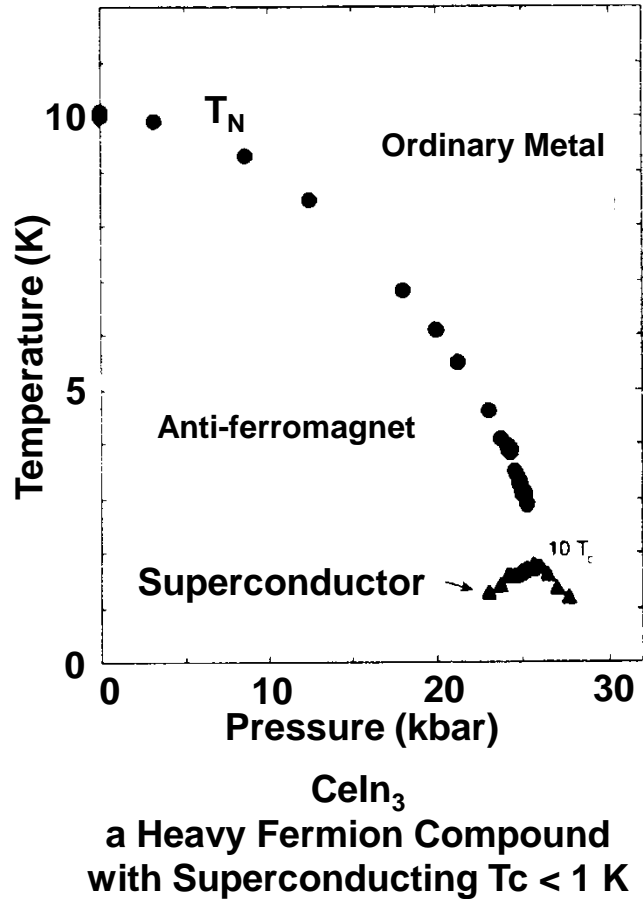
B.J.Ramshaw, B. Vignolle, J. Day, R. Liang, W.N. Hardy, C. Proust, D.A. Bonn, Angle dependence of quantum oscillations in  $YBa_2Cu_3O_{6.59}$  shows free spin behavior of quasiparticles **Nature Physics 7, 234 (2010)**

Suchitra E. Sebastian *et al.* A multi-component Fermi surface in the vortex state of an underdoped high- $T_c$  superconductor. **Nature 454 200 (2008)**



**Superconductivity is Stabilized  
Near Quantum Critical Points,  
*but no one knows why.***

N.D. Mathur et al., Nature **394**, 39 (1998)

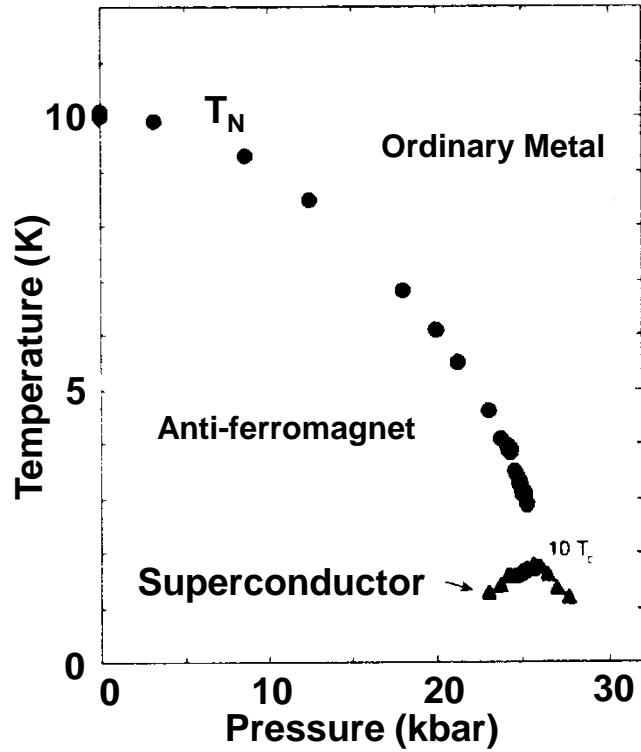


Jiun-Haw Chu, James G. Analytis, Chris Kucharczyk, Ian R. Fisher, Phys. Rev. **B 79**, 014506 (2009)  
*Determination of the phase diagram of the electron doped superconductor Ba(Fe<sub>1-x</sub>Co<sub>x</sub>)<sub>2</sub>As<sub>2</sub>*

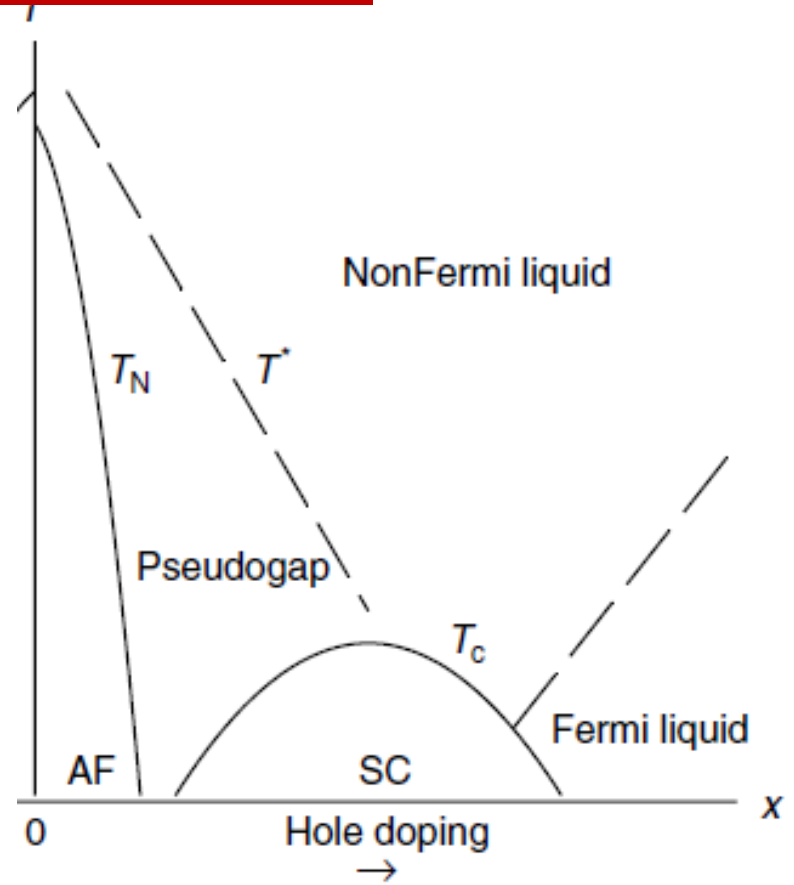


**Superconductivity is Stabilized  
Near Quantum Critical Points,  
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N.D. Mathur et al., Nature **394**, 39 (1998)



**CeIn<sub>3</sub>**  
a Heavy Fermion Compound  
with Superconducting  $T_c < 1$  K



**Hole-doped High-Temperature  
Superconducting Cuprate**  
Maximum  $T_c \sim 40-150$ K

# National High Magnetic Field Laboratory



1.4 GW Generator

Los Alamos National Laboratory



101T Pulse Magnet  
10mm bore



Graphene, Fe-based superconductors,  
Quantum oscillations in cuprate superconductors,  
Topological insulators, Molecular magnets,  
**Model magnetic systems**, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
Energy-related materials, Petroleum, Natural Products,  
Bio-macromolecular complexes and the Brain



# Materials Research on Chinese Terracotta Warriors (479-221 BC)

## Saving Lives for more than 2000 Years



Terracotta Army to protect the emperor in the afterlife...instead of the real army



Calcite -  $\text{CaCO}_3$   
Bone White -  $\text{Ca}_5(\text{CO}_3)_2(\text{OH})_2$   
White Lead -  $2\text{Pb}(\text{CO}_3)_2 \cdot \text{Pb}(\text{OH})_2$

Soot - carbon black

**Han Purple\*\*\* -  $\text{BaCuSi}_2\text{O}_6$**

Cinnabar -  $\text{HgS}$   
Hematite -  $\text{Fe}_2\text{O}_3$   
Red Lead -  $\text{Pb}_3\text{O}_4$

Malachite -  $\text{Cu}_2\text{CO}_3(\text{OH})_2$

**Han Blue\*\*\* -  $\text{BaCuSi}_4\text{O}_{10}$**

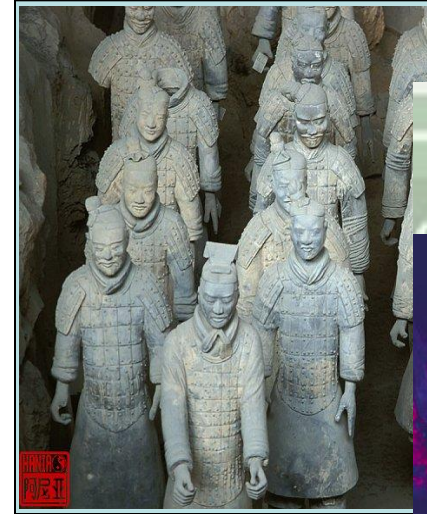
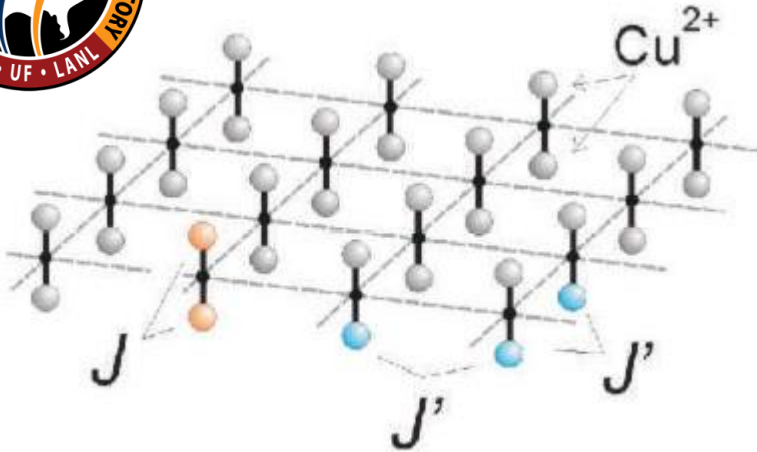
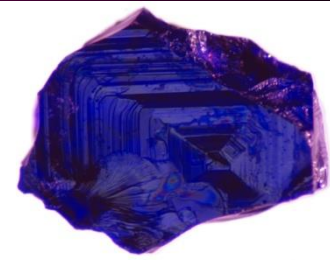
\*\*\* man-made pigments

J. Zuo et al., *J. Raman Spectrosc.* **34**, 121 (2003)

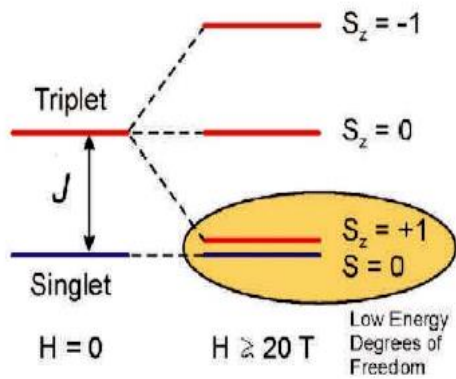
41 H. Langhals & D. Bathelt, *Angew. Chem. Int. Ed.* **42**, 5676 (2003)



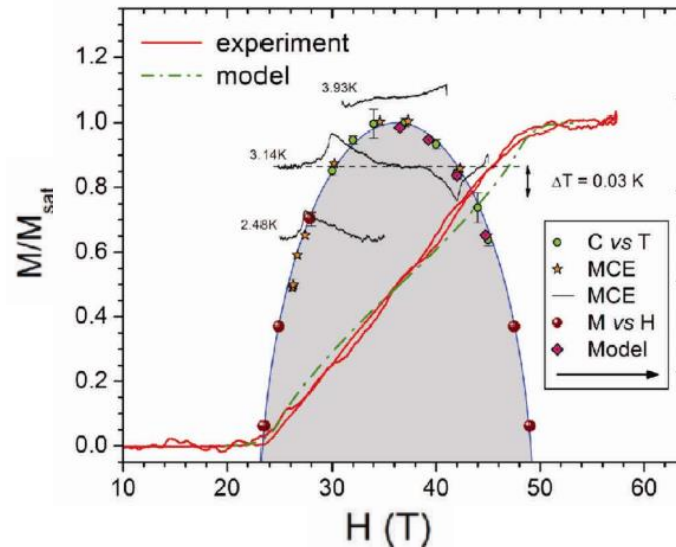
# 2500 Years of Materials Research on $\text{BaCuSi}_2\text{O}_6$



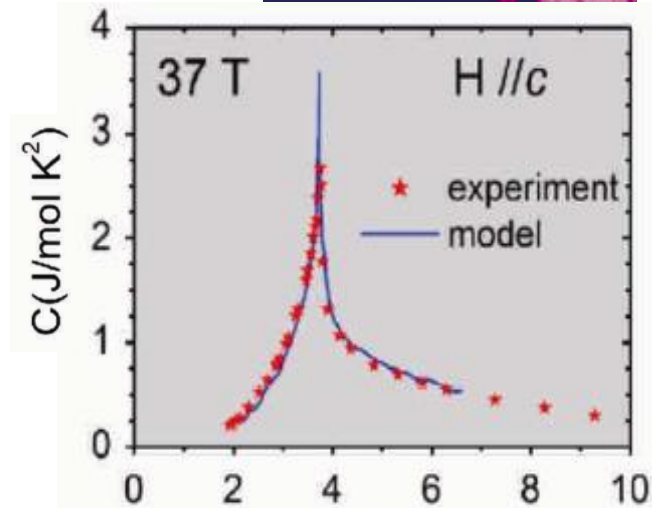
$\text{BaCuSi}_2\text{O}_6$ : A quasi-2D magnetic insulator  
with a gapped spin dimer ground state



Magnetic fields create a gas of bosonic spin triplet excitations, called triplons



Slow increase in **MAGNETIZATION** is evidence of electron spin correlations.



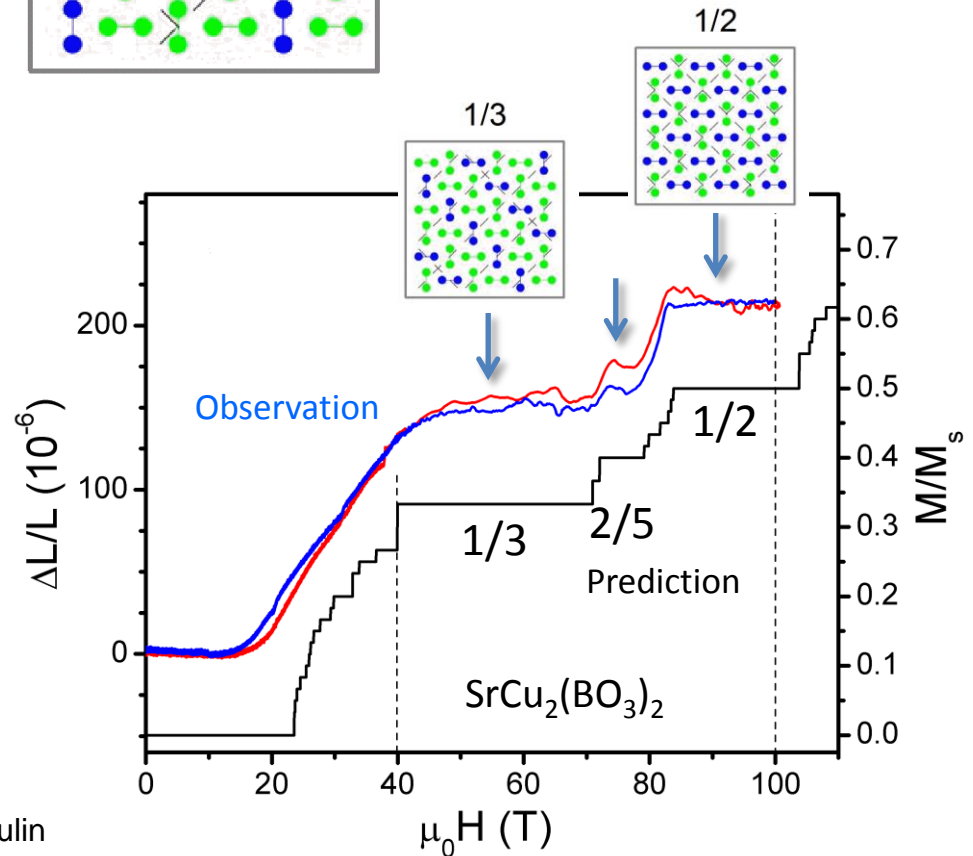
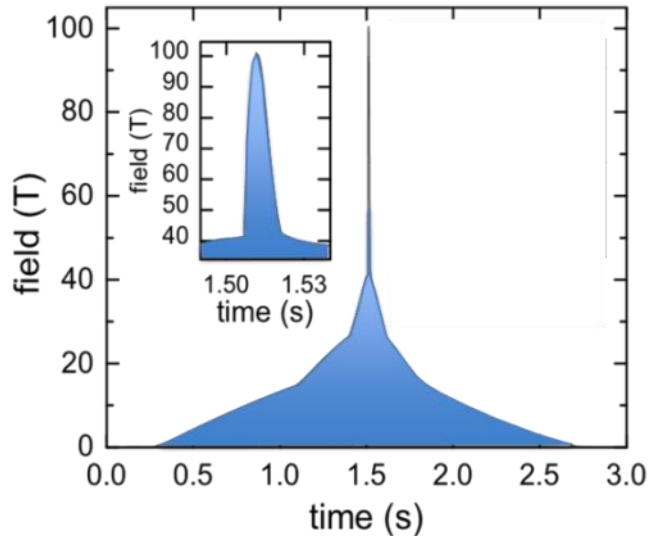
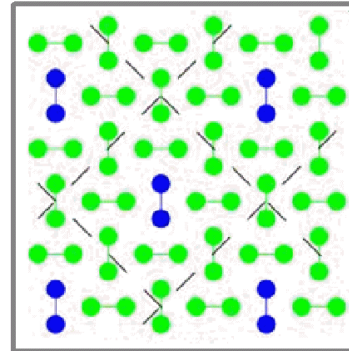
Lambda transition in **SPECIFIC HEAT** due to Bose condensation of triplons



# Crystalline spin transitions at 75T and 82T: New Magnetic Spin Textures revealed at ultrahigh magnetic fields

MPI-CPfS, Dresden, Univ. of Wyoming, LANL, McMaster University, NHMFL

- $\text{SrCu}_2(\text{BO}_3)_2$  realizes the “Shastry-Sutherland Model”: *Orthogonal spin dimers on square lattice*
- Dimers are *coupled*; magnetization increases in a complex series of plateaus as *stable magnetic textures* are formed



Marcelo Jaime, Ramzy Daou, Scott A. Crooker,  
Franziska Weickert, Atsuko Uchida, Adrian E. Feiguin,  
Cristian D. Batista, Hanna A. Dabkowska, and Bruce D. Gaulin  
*PNAS*, (July 2012)

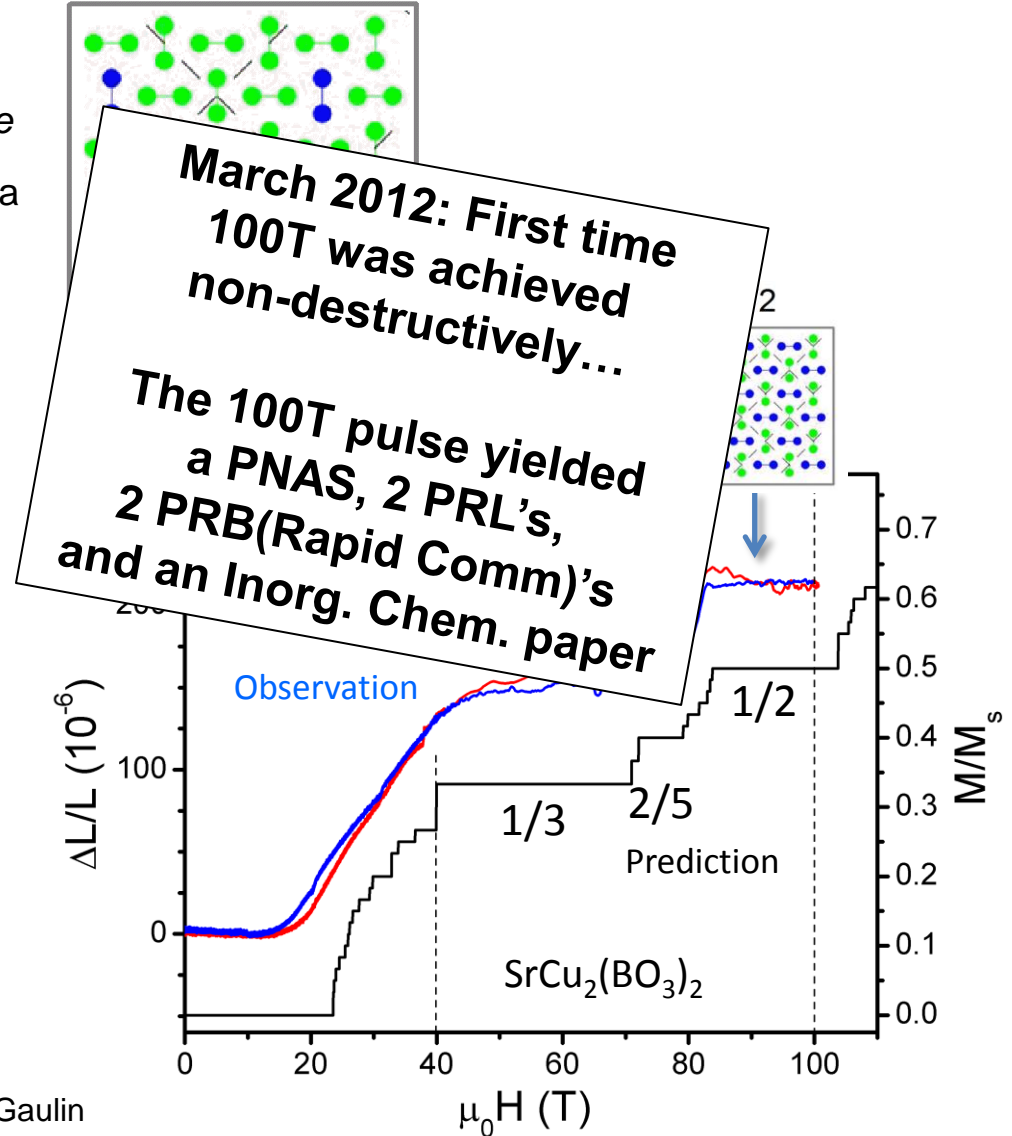
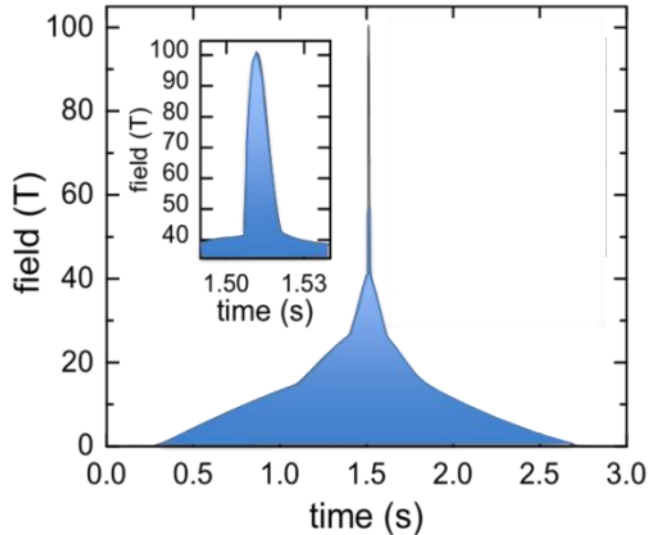


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**PNAS, (July 2012)**





## High Magnetic Fields and Energy

# National High Magnetic Field Laboratory



Florida State University

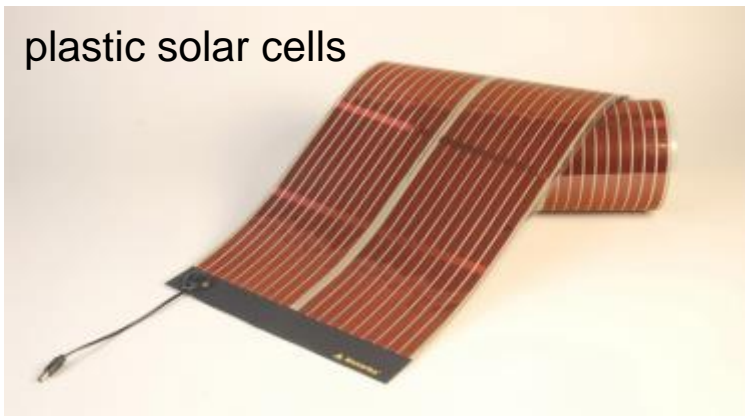


Graphene, Fe-based superconductors,  
Quantum oscillations in cuprate superconductors,  
Topological insulators, Molecular magnets,  
Model magnetic systems, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
**Energy-related materials**, Petroleum, Natural Products,  
Bio-macromolecular complexes and the Brain

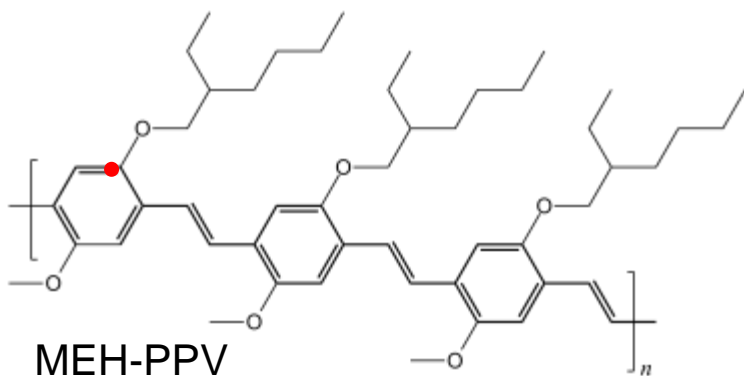


# High-field EPR probes charge carriers in plastic solar cells

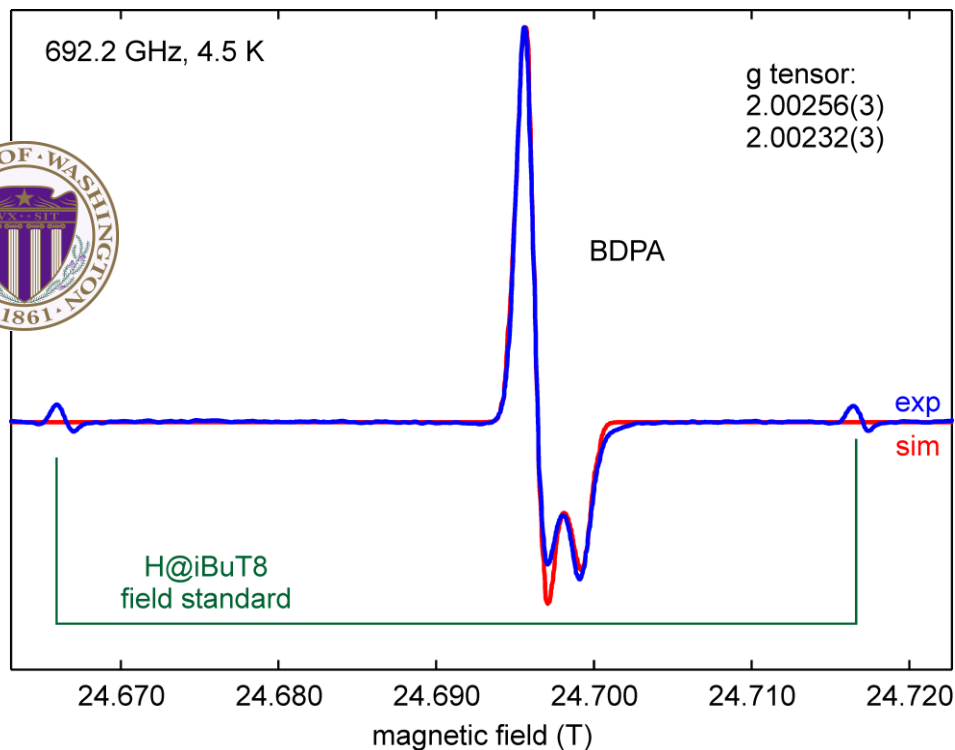
plastic solar cells



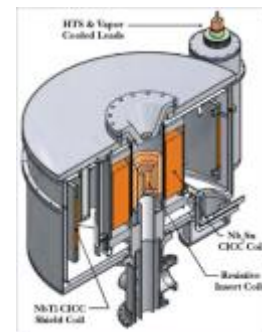
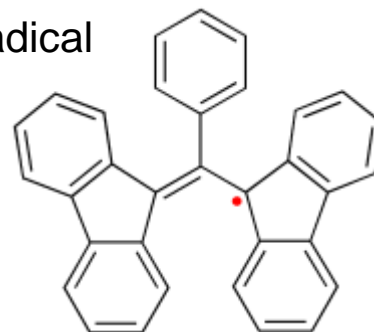
If the unpaired electron is delocalized over a large volume, its g factor is nearly that of a free electron (2.0023 and isotropic). As such, high magnetic fields are required to measure the g-tensor in carbon-centered radicals in organic photovoltaics.



MEH-PPV  
carbon-centered radical



BDPA  
model radical



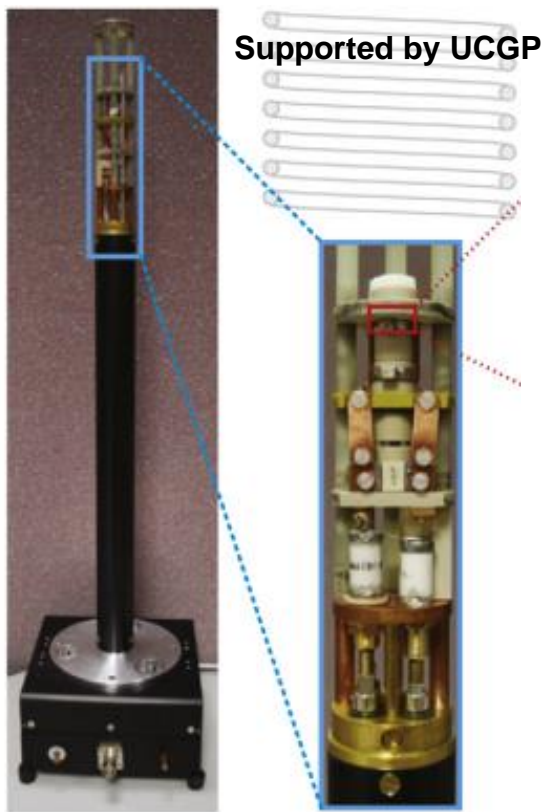
SCH will provide even greater g resolution



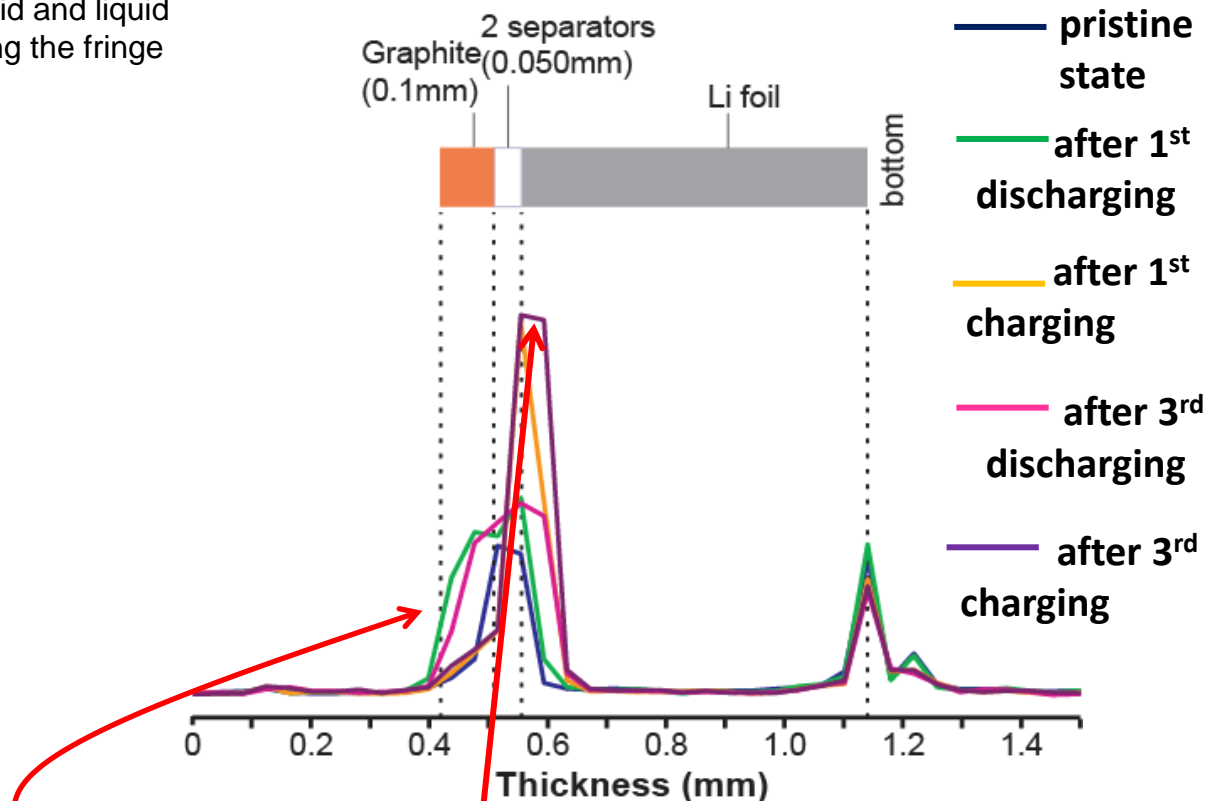
# *In Situ* $^7\text{Li}$ NMR Stray Field Imaging (STRAFI) in a Half-Cell Battery

Yong Yang at Xiamen University, Jim Zheng at FSU, Riqiang Fu at NHMFL

A STRAFI probe was designed to image solid and liquid materials containing quadrupolar nuclei using the fringe field of a superconducting magnet.



## Imaging $\text{Li}^+$ ion transfer between electrodes



Reveals formation and changes of irreversible microstructures of the Li components in the interface between electrolyte and electrodes  
Reveals a non-uniform Li-ion distribution in the graphite for the first time

Facilities: NMR/MRI Facility (19.6 Tesla Magnet)

Citation: ***Non-Destructive Monitoring of Charge-Discharge Cycles on Lithium Ion Batteries Using  $^7\text{Li}$  Stray-Field Imaging***, Joel A. Tang, Sneha Dugar, Guiming Zhong, Naresh S. Dalal, Jim P. Zheng, Yong Yang, & Riqiang Fu, **Scientific Reports** 3:2596, 1-6 (2013);

***Solid-State STRAFI NMR Probe for Material Imaging of Quadrupolar Nuclei***, Joel A. Tang, Guiming Zhong, Sneha Dugar, Jason Kitchen, Yong Yang, & Riqiang Fu, **J. Magn. Reson.** 225:93-101 (2012).

# National High Magnetic Field Laboratory



Florida State University



Graphene, Fe-based superconductors,  
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Topological insulators, Molecular magnets,  
Model magnetic systems, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
Energy-related materials, **Petroleum**, Natural Products,  
Bio-macromolecular complexes and the Brain



# Ion Cyclotron Resonance: Mass Spectroscopy

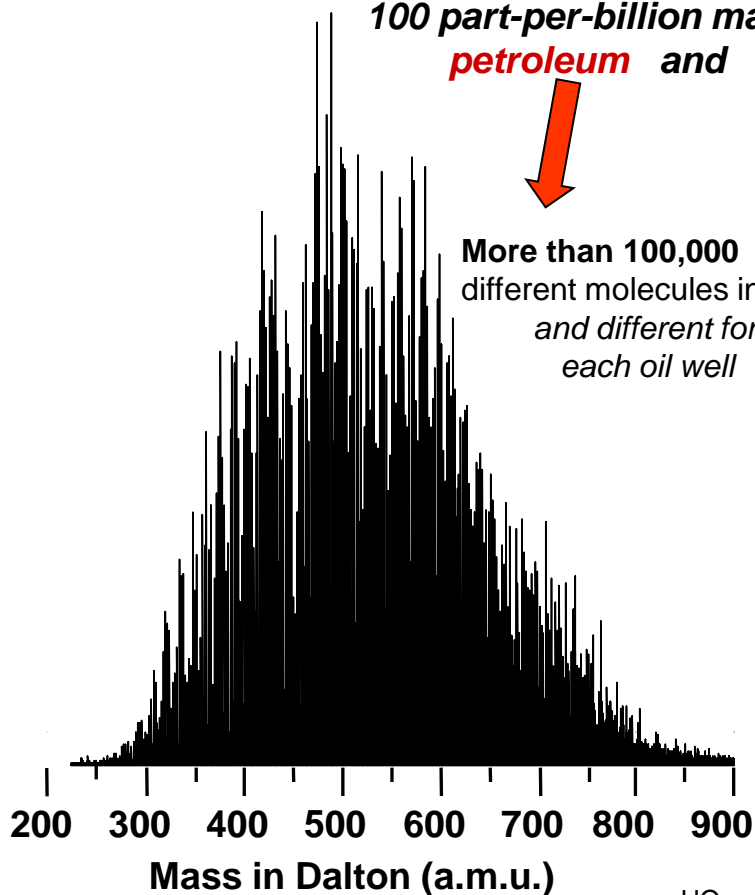
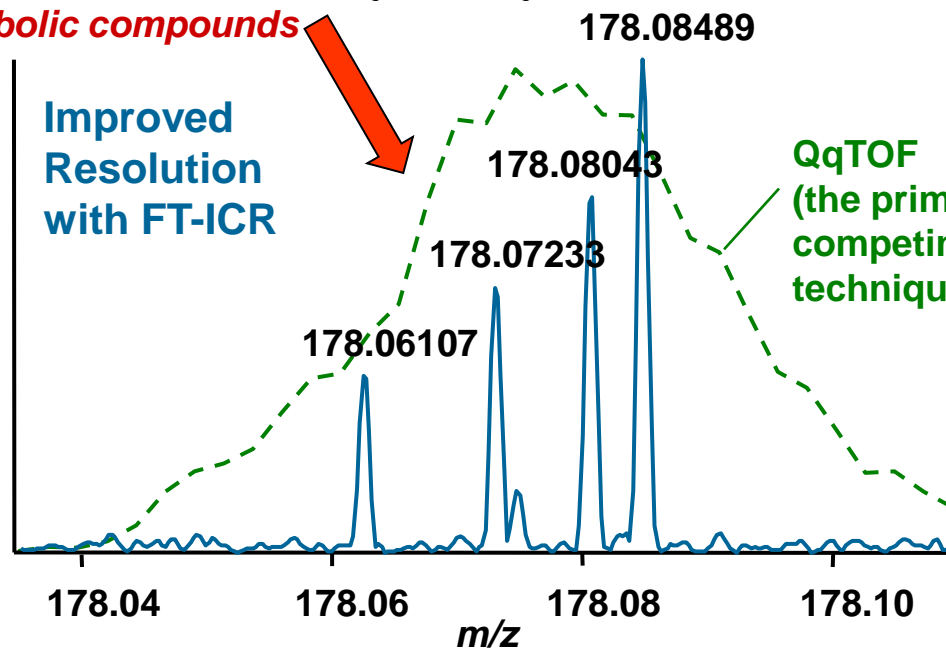
With a 14 T high-homogeneity wide-bore magnet,  
100 part-per-billion mass resolution and accuracy to analyze

**petroleum** and **metabolic compounds**

More than 100,000  
different molecules in oil  
and different for  
each oil well

Improved  
Resolution  
with FT-ICR

QqTOF  
(the primary  
competing  
technique)

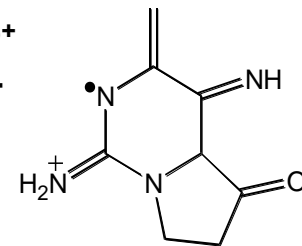
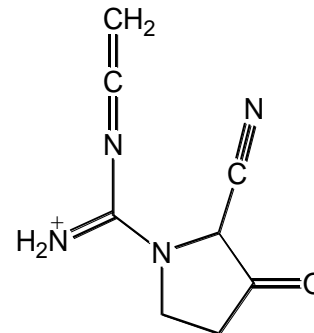
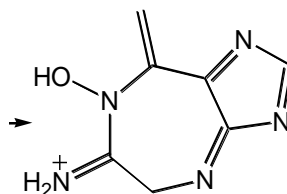
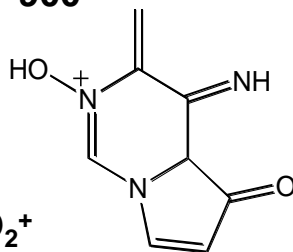


$C_7H_8N_5O^+$   
 $m/z$  178.07234

$^{12}C_7^{13}C_1H_9N_4O^+$   
 $m/z$  178.08044

$C_8H_8N_3O_2^+$   
 $m/z$  178.06110

$C_8H_{10}N_4O^+$   
 $m/z$  178.08491





# Petroleum Analysis with Ion Cyclotron Resonance

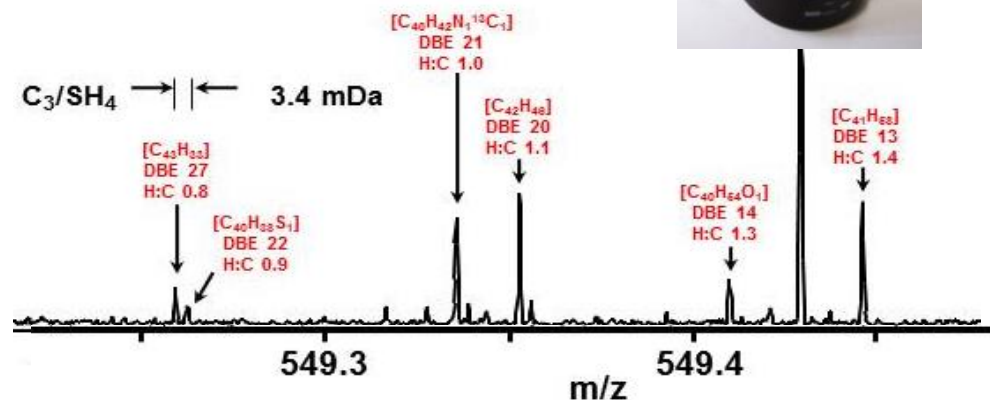
Woods Hole Oceanographic Institute and National High Magnetic Field Laboratory



Ion Cyclotron Resonance (ICR) can develop a “fingerprint” of the Deepwater Horizon oil by identifying 10,000’s of compounds in each sample.

The MagLab’s 9.4T ICR magnet can resolve 0.003 mDa and therefore can distinguish  $C_3$  from  $SH_4$  (greater than one part in 100,000 resolution) to allow for sulfur differentiation from pure hydrocarbons....the ability that launches “PETROLEOMICS”

## Deepwater Horizon Petroleum



**Facilities:** NHMFL Ion Cyclotron Resonance Facility

**Citation:** *Expansion of the Analytical Window for Oil Spill Characterization by Ultrahigh Resolution Mass Spectrometry: Beyond Gas Chromatography*; McKenna, A.M.; Nelson, R.K.; Reddy, C.M.; Savory, J.J.; Kaiser, N.K.; Fitzsimmons, J.E.; Marshall, A.G. and Rodgers, R.P.;

**Environmental Science & Technology**, 47, 7530-7539 (2013)



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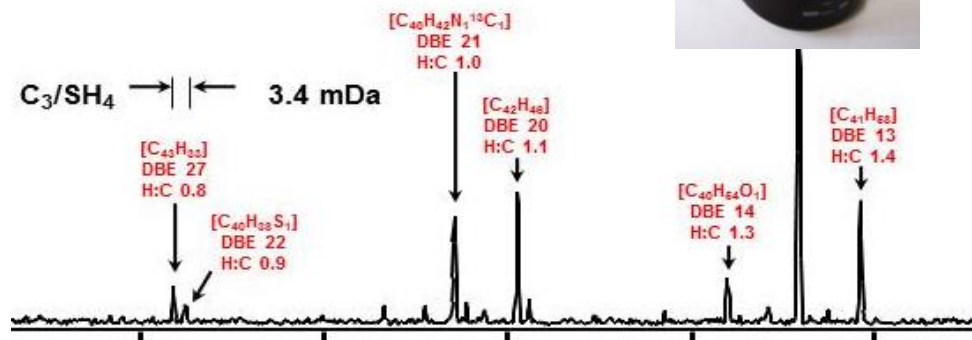
Woods Hole Oceanographic Institute and National High Magnetic Field Laboratory



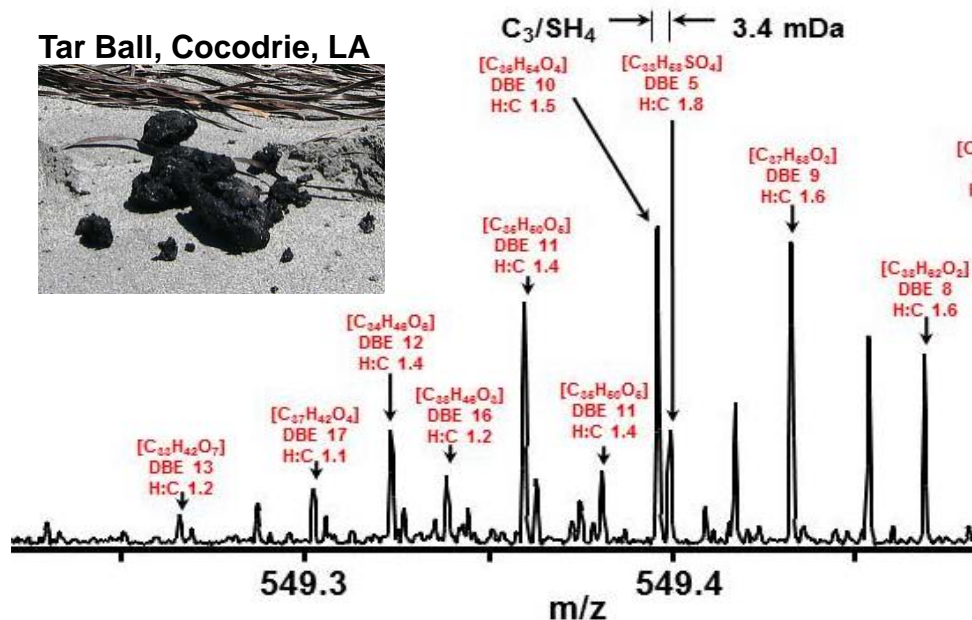
## Deepwater Horizon Petroleum

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## Tar Ball, Cocodrie, LA



One might have expected to see fewer compounds in a weathered tar ball, because all volatile compounds would have evaporated.

Instead there are three times as many compounds, because bacteria and sunlight have led to the oxidation of many compounds.

High magnetic fields provide unique opportunities to probe the environmental fate of spilled oil, toxicology, and molecular modeling of biotic/abiotic weathering.

**Facilities:** NHMFL Ion Cyclotron Resonance Facility

**Citation:** *Expansion of the Analytical Window for Oil Spill Characterization by Ultrahigh Resolution Mass Spectrometry: Beyond Gas Chromatography*; McKenna, A.M.; Nelson, R.K.; Reddy, C.M.; Savory, J.J.; Kaiser, N.K.; Fitzsimmons, J.E.; Marshall, A.G. and Rodgers, R.P.;

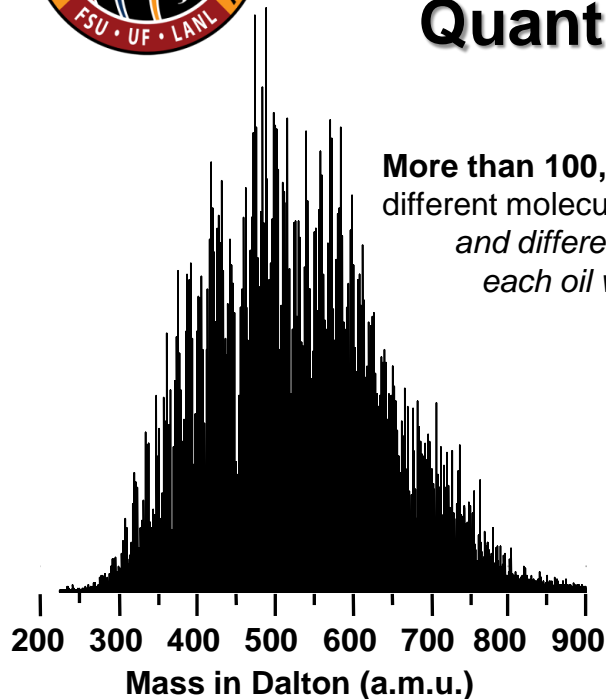
**Environmental Science & Technology**, 47, 7530-7539 (2013)





# Inventing 'Petroleomics': Quantitative Analysis of Petroleum

More than 100,000  
different molecules in oil  
*and different for  
each oil well*



...what is in the crud  
that clogs the oil pipelines ?  
(costing \$10,000,000 a day)

**NOT** polymerization...  
rather a physical entanglement  
of relatively small molecules



...how do we make useful  
fuel from this low grade crude?  
(we have enough of this stuff  
to achieve energy independence)

...what cyclic compounds are in this "residue"?  
...and sulfur ligands / acids / <insert word here>  
(individualize refinement and mitigate pollution)





## High Magnetic Fields and Life

# National High Magnetic Field Laboratory

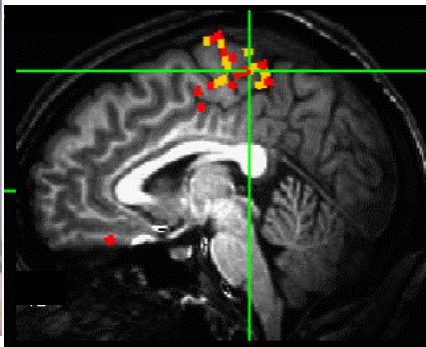


University of Florida

11.4T MRI Magnet  
400mm warm bore



Advanced Magnetic  
Resonance Imaging  
and Spectroscopy Facility



Graphene, Fe-based superconductors,  
Quantum oscillations in cuprate superconductors,  
Topological insulators, Molecular magnets,  
Model magnetic systems, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
Energy-related materials, Petroleum, **Natural Products**,  
Bio-macromolecular complexes and the Brain

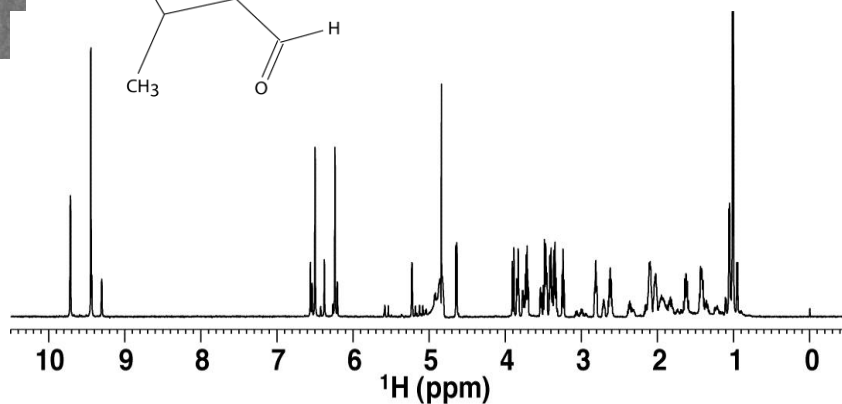
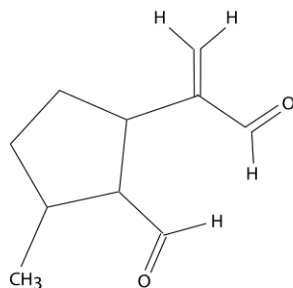


# Chemical Warfare in the Natural World: Solving Molecular Structures of Ultra-Small Samples

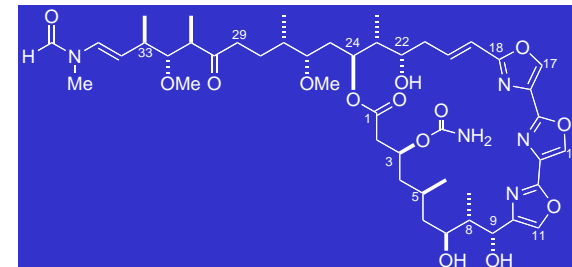
- High Quality NMR Spectrum from a single milking of a single walking stick... no purification... 10nL sample (0.1mm)<sup>3</sup>



Anisomorphal



and from an unusual shell-less mollusk on the coral reef...



YBCO  
rf coil

# National High Magnetic Field Laboratory



Florida State University

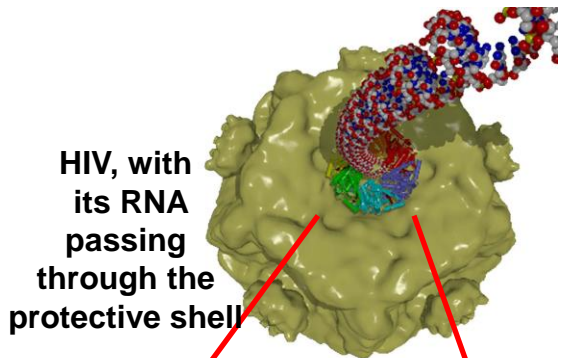


Graphene, Fe-based superconductors,  
Quantum oscillations in cuprate superconductors,  
Topological insulators, Molecular magnets,  
Model magnetic systems, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
Energy-related materials, Petroleum, Natural Products,  
**Bio-macromolecular complexes** and the Brain



# Fighting Viruses: Plugging the RNA Channels

Structure of Macro-bio-assemblies: too big for X-rays alone to solve



*Ion Cyclotron Resonance weighs the pieces of the RNA channel to detect how much deuterium (heavy hydrogen) has exchanged with the hydrogen*

Hydrogen/Deuterium Exchange Rate reveals which side of the RNA channel is on the virus exterior

**> 100 h<sup>-1</sup> FAST**

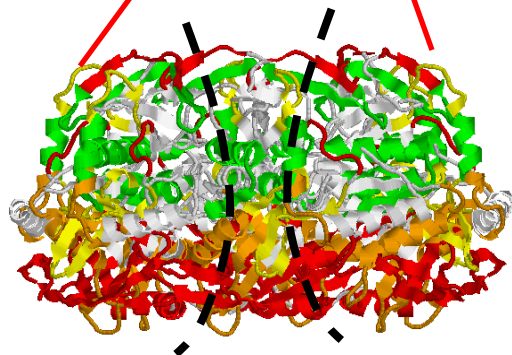
10 h<sup>-1</sup> - 100 h<sup>-1</sup>

1 h<sup>-1</sup> - 10 h<sup>-1</sup>

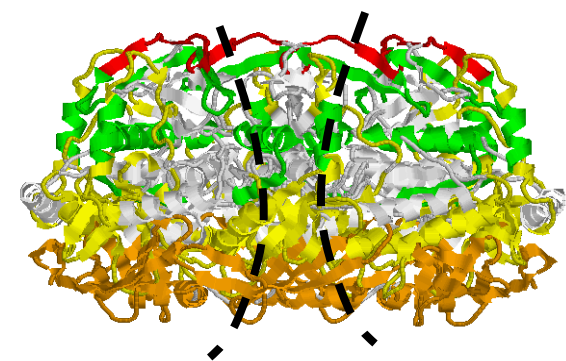
0.1 h<sup>-1</sup> - 1 h<sup>-1</sup>

**< 0.1 h<sup>-1</sup> SLOW**

*This is the EXTERIOR...  
...design a drug to attack HERE*



RNA Channel (side view)  
mass increase rates when fully exposed to deuterium

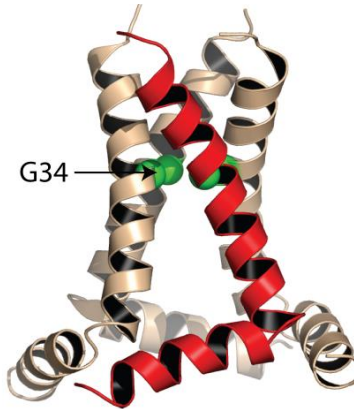
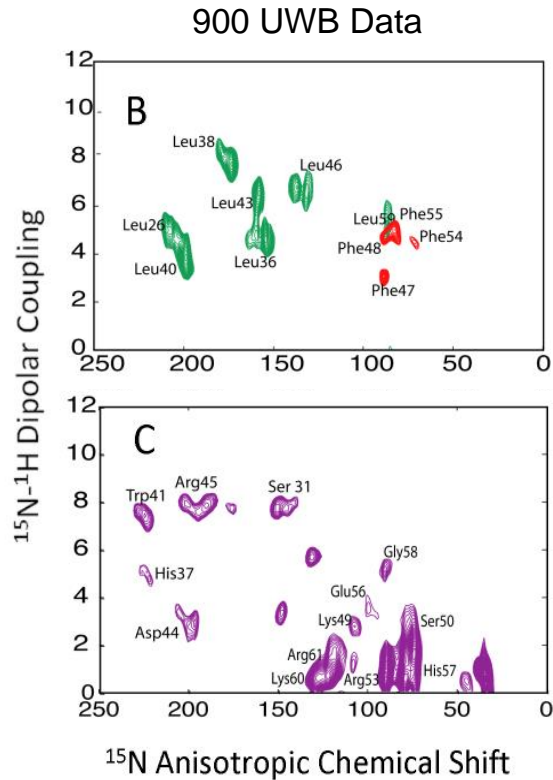


RNA Channel mass increase rates when attached to Procapsid

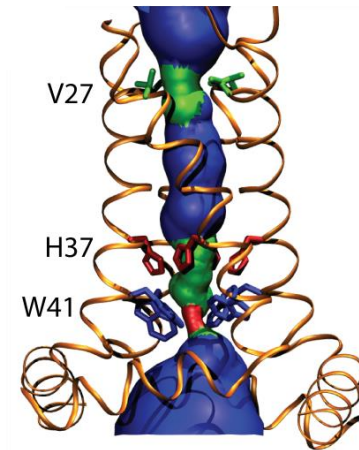
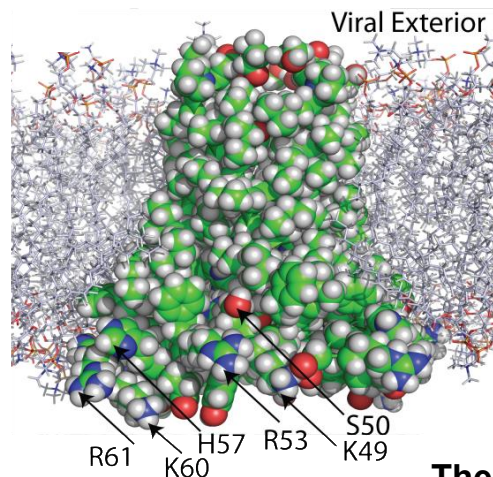
**WHICH surface is the EXTERIOR of the virus ?**



# First Fully Functional Membrane Protein Structure Measured in a Native-Like Membrane Environment



- M2 Protein (22-62) from Influenza A
- Structure determined in uniformly aligned liquid-crystalline lipid bilayers



The largest structure solved by ssNMR (20 kDa)

**A collaboration:**

D. Busath, Dept. of Physiology and Developmental Biology, BYU;  
H.-X. Zhou, Dept. of Physics, FSU

Sharma et al., 2010 Science



# Quadrupolar Nuclei: the REST of the Periodic Table

## Quadrupolar Nuclei: the REST of the Periodic Table

**Elements with:**

- Only  $I=1/2$  nuclear spins
- Quadrupolar nuclei (i.e.  $I > 1/2$ )

H 2																	He
Li 6,7	Be 9											B 10,11	C 12	N 14	O 17	F 19	Ne 21
Na 23	Mg 25											Al 27	Si 28	P 31	S 33	Cl 35,37	Ar
K 39,41	Ca 43	Sc 45	Ti 47,49	V 50,51	Cr 53	Mn 55	Fe 56	Co 59	Ni 61	Cu 63,65	Zn 67	Ga 69,71	Ge 73	As 75	Se 78	Br 79,81	Kr 83
Rb 85,87	Sr 87	Y 89	Zr 91	Nb 93	Mo 97	Tc 99	Ru 99,101	Rh 103	Pd 105	Ag 107	Cd 112	In 113,115	Sn 117	Sb 121,123	Te 127	I 127,131	Xe 129,131
Cs 133	Ba 135,137	La 138,139	Hf 177,179	Ta 181	W 183	Re 185,187	Os 187,189	Ir 191,193	Pt 195	Au 197	Hg 201	Tl 203,205	Pb 207,209	Bi 209	Po	At	Rn
Fr	Ra	Ac															

Ce	Pr 141	Nd 143,145	Pm	Sm 147,149	Eu 151,153	Gd 155,157	Tb 159	Dy 161,163	Ho 165	Er 167	Tm	Yb 173	Lu 175,176
Th	Pa	U 235,238	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

## NMR of New Materials in DC Powered Magnets

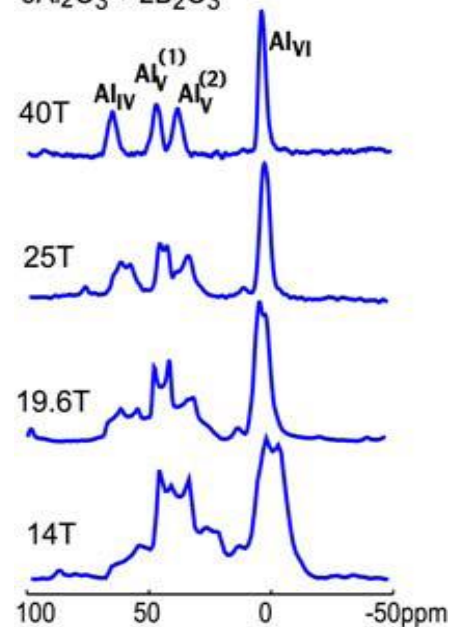
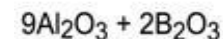
$I = 1$   $^2\text{H}$ ,  $^6\text{Li}$ ,  $^{14}\text{N}$

$I = 3/2$   $^7\text{Li}$ ,  $^{11}\text{B}$ ,  $^{23}\text{Na}$ ,  
 $^{69,71}\text{Ga}$ ,  $^{87}\text{Rb}$ ...

$I = 5/2$   $^{17}\text{O}$ ,  $^{25}\text{Mg}$ ,  $^{27}\text{Al}$ ,  
 $^{47}\text{Ti}$ ,  $^{67}\text{Zn}$ ...

- ❖ Catalysts:  
    surface chemistry
- ❖ Porous materials:  
    clays and zeolites
- ❖ Batteries and fuel cells:  
    ion transport

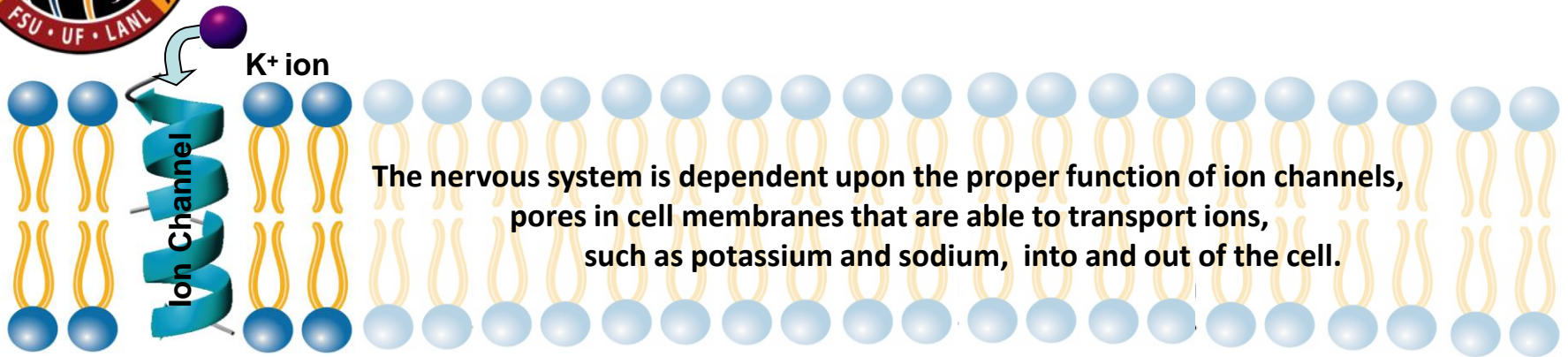
High Field MAS



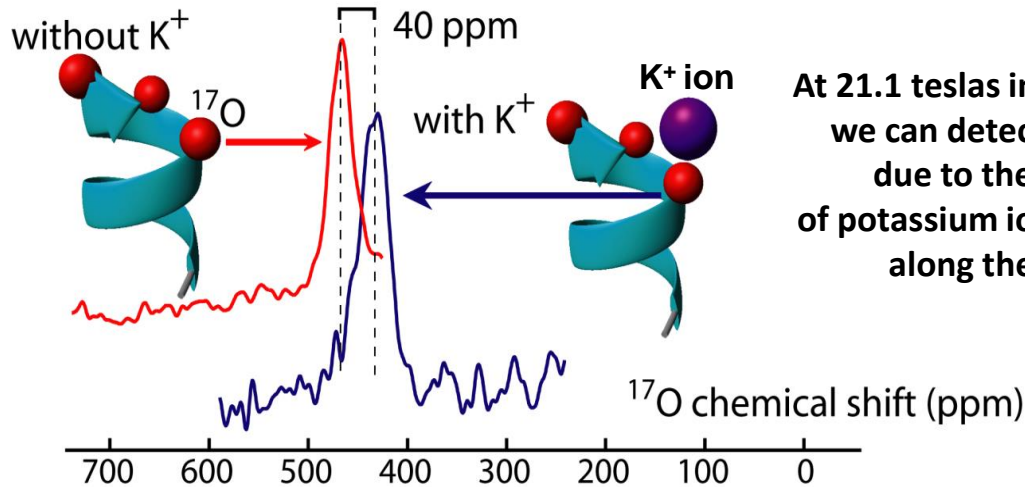




# Quadrupolar NMR: Oxygen-17 NMR Spectroscopy



Because  $^{17}\text{O}$  is a quadrupolar nucleus, it is a very sensitive indicator of the electric fields of nearby ions.



At 21.1 teslas in the 900MHz magnet we can detect NMR line shifts due to the electric fields of potassium ions at particular sites along the ion channel

The shift in the  $^{17}\text{O}$  NMR signal upon detecting the electric field from a nearby potassium ion ( $\text{K}^+$ ).



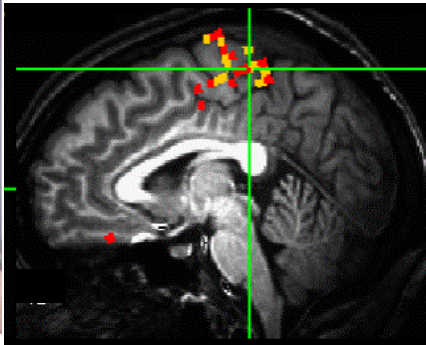
# National High Magnetic Field Laboratory



University of Florida

11.4T MRI Magnet  
400mm warm bore

Advanced Magnetic  
Resonance Imaging  
and Spectroscopy Facility



Graphene, Fe-based superconductors,  
Quantum oscillations in cuprate superconductors,  
Topological insulators, Molecular magnets,  
Model magnetic systems, Frustrated magnets,  
Magnetic Bose-Einstein Condensates, Qubits,  
Energy-related materials, Petroleum, Natural Products,  
Bio-macromolecular complexes and **the Brain**



# MRI goes High-Definition



1mm dia

10 $\mu$ m dia

Imaging has improved  
from frog ovum to  
rat neuron in 20 years  
(10<sup>6</sup> : 1 volume ratio)

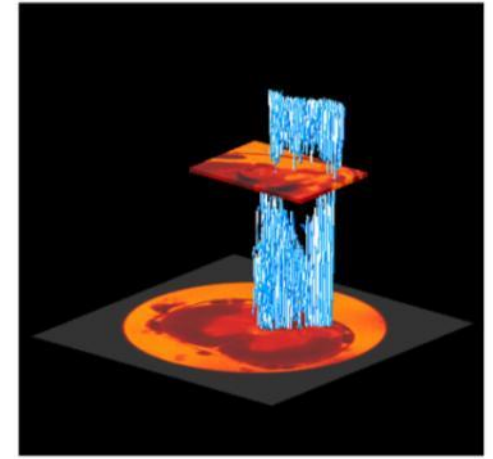
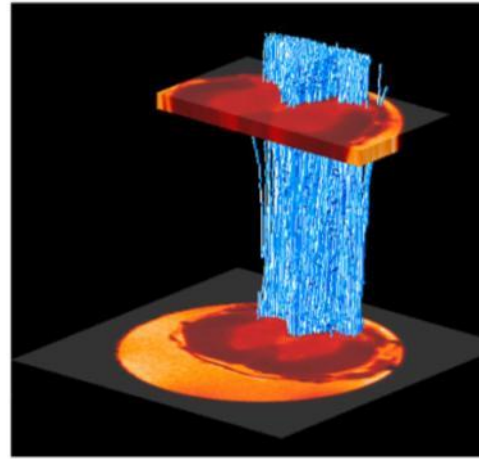
...and now sub-cellular structures:  
the cell's nucleus...and starting to resolve  
the 10,000 nucleoli *inside* the cell's nucleus



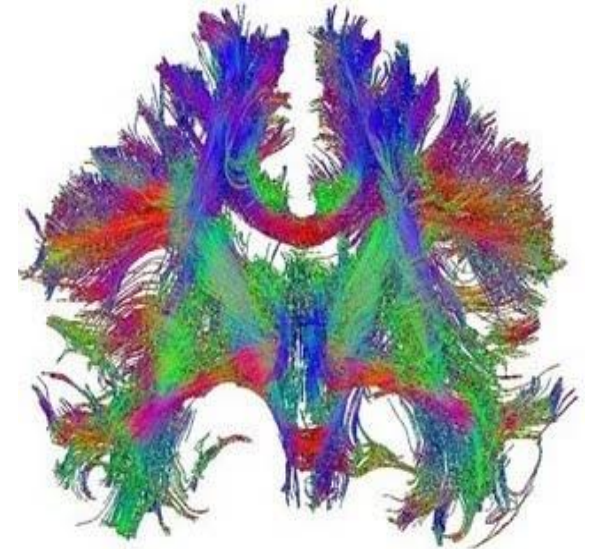
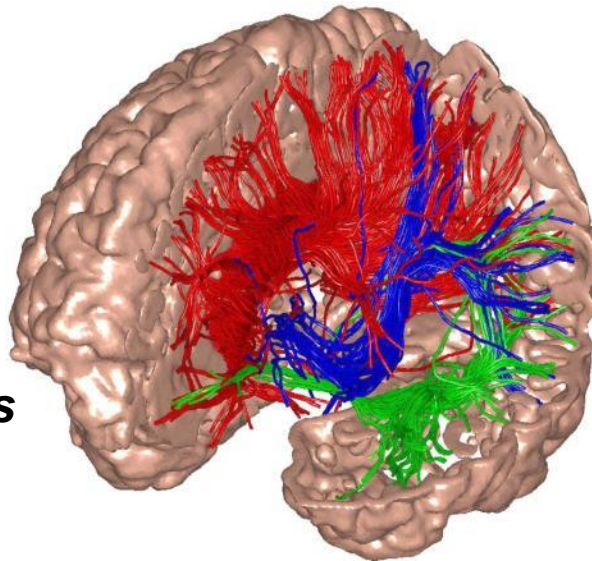
# Tracking Water Pathways in the Spinal Cord and Brain: Mapping the Water Diffusion Tensor from MRI

*Water diffusion is easy  
along nerves, difficult  
between nerves.*

*Healthy (left) and  
Damaged (right)  
MOUSE SPINAL CORDS*



*Water pathways  
in the HUMAN BRAIN  
can now resolve bundles  
as small as 100 axons*





# Quadrupolar Nuclei Revisited for MRI

$I = 1$   $^2\text{H}$ ,  $^{14}\text{N}$ ...  
 $I = 3/2$   $^{11}\text{B}$ ,  $^{23}\text{Na}$ ...  
 $I = 5/2$   $^{17}\text{O}$ ...

H 2																	He
Li 6,7	Be 9											B 10, 11	C	N 14	O 17	F	Ne 21
Na 23	Mg 25											Al 27	Si	P	S 33	Cl 35, 37	Ar
K 39, 41	Ca 43	Sc 45	Ti 47, 49	V 50, 51	Cr 53	Mn 55	Fe	Co 59	Ni 61	Cu 63, 65	Zn 67	Ga 69, 71	Ge 73	As 75	Se	Br 79, 81	Kr 83
Rb 85, 87	Sr 87	Y	Zr 91	Nb 93	Mo 97	Tc	Ru 99, 101	Rh	Pd 105	Ag	Cd	In 113 -5	Sn	Sb 121 -3	Te	I 127	Xe 129 -31
Cs 133	Ba 135 -7	La 138 -9	Hf 177 -9	Ta 181	W	Re 185 -7	Os 187 -9	Ir 191 -3	Pt	Au 197	Hg 201	Tl	Pb	Bi	Po	At	Rn
Fr	Ra	Ac															

Elements with:  
 Only  $I = 1/2$  nuclear spins  
 Quadrupolar nuclei  
 (i.e.  $I > 1/2$ )

Ce	Pr 141	Nd 143 -5	Pm	Sm 147 -9	Eu 151 -3	Gd 155 -7	Tb 159	Dy 161 -3	Ho 165	Er 167	Tm	Yb 173	Lu 175 -6
Th	Pa	U 235	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

**Second Generation MRI:**  
*because you're not just water and fat*





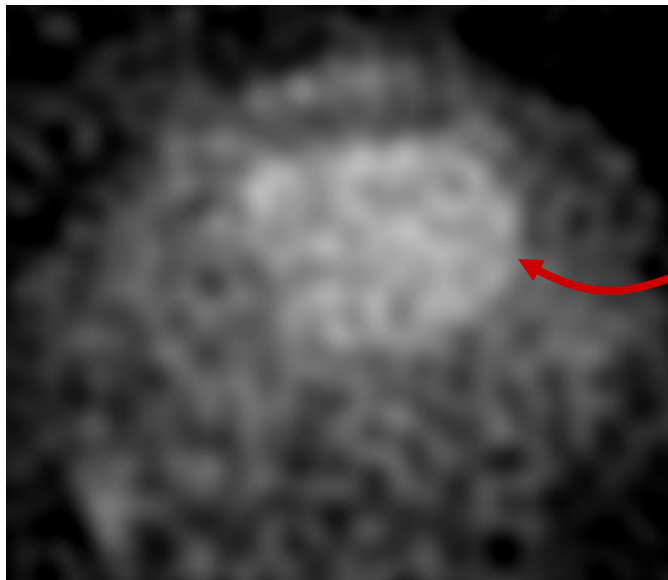
## Rapid Assessment of Chemotherapy using Sodium MRI

*In vivo*  $^{23}\text{Na}$  Images of mouse brain

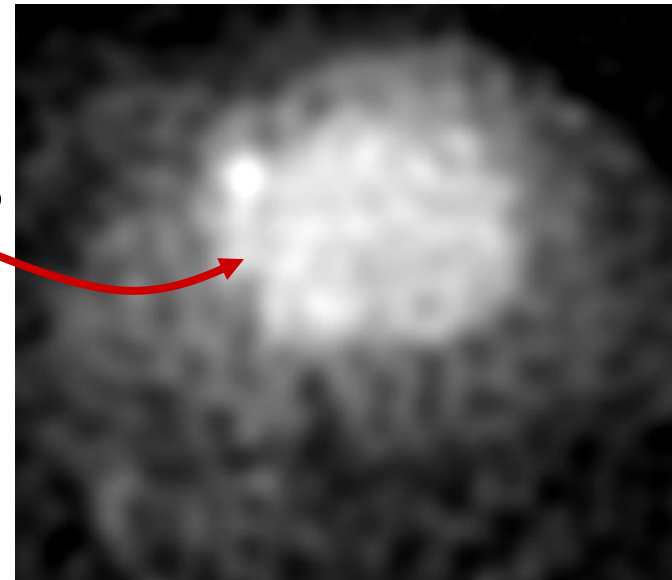
Sodium MRI is *thousands of times more difficult* than ordinary Hydrogen MRI

Sodium ( $^{23}\text{Na}$ ) inside the cells is a biomarker for imminent cell death.

*Before Therapy*



*4 Days after Therapy*



**TUMOR**

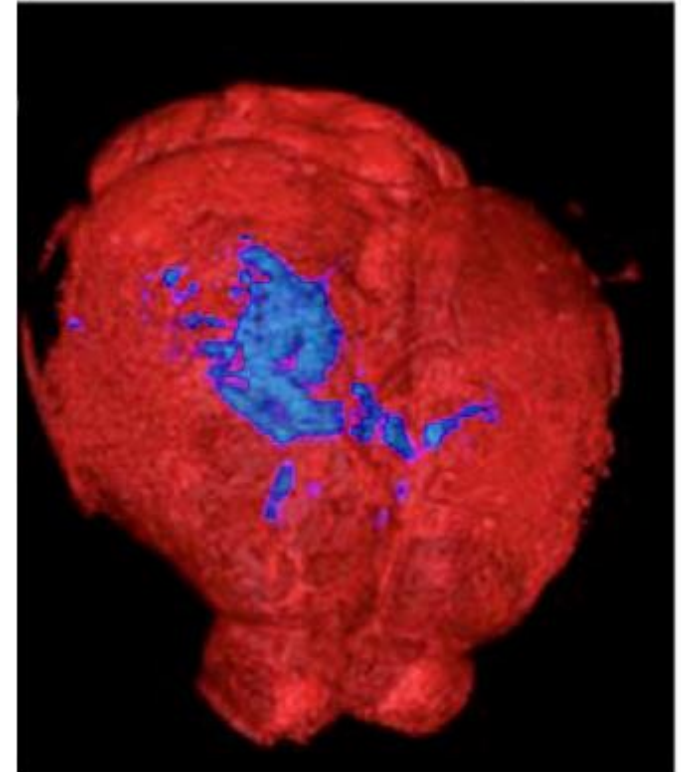
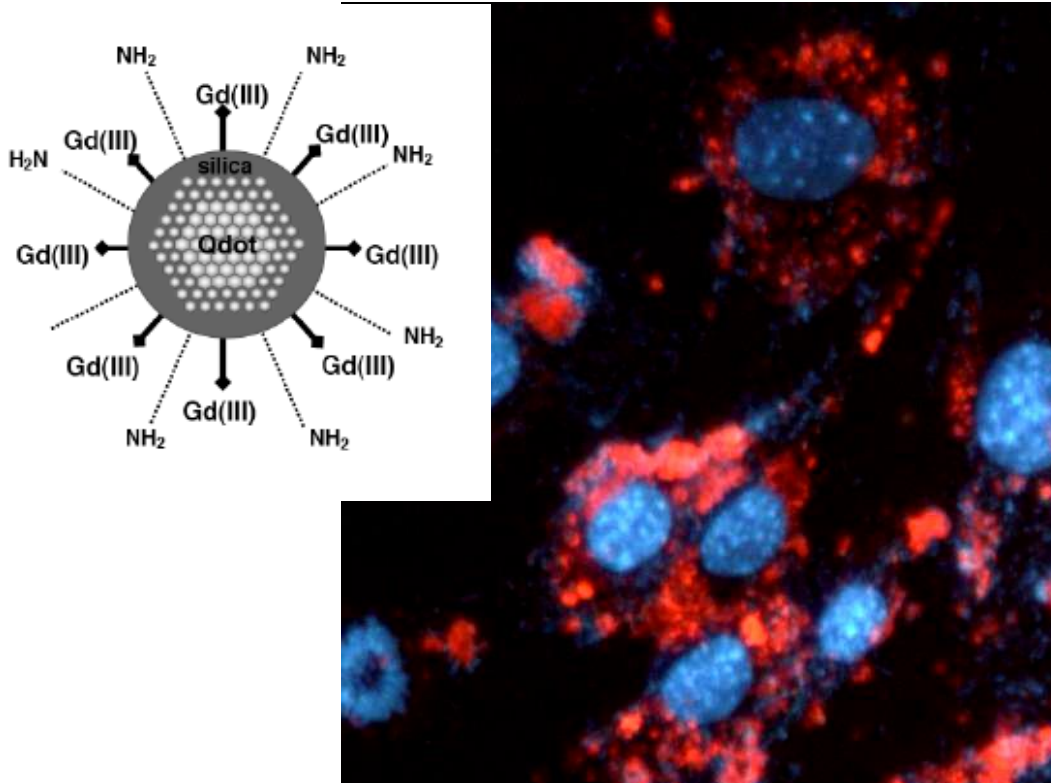
We learn that the chemotherapy is working  
even **BEFORE** the tumor cells die.



# Magnetic Quantum Dots for Live Stem Cell Tracking

Living stem cells, labeled with bio-compatible Gadolinium nanoparticles...

tracked *in vivo* using Magnetic Resonance Imaging in a mouse brain as they respond to brain damage resulting from hypoxia.





[www.magnet.fsu.edu](http://www.magnet.fsu.edu)

