Introduction to the Magnets and Probes for Solid-State NMR at NHMFL

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MagLab NMR Facility

https://nationalmaglab.org/user-facilities/nmr-mri

- The MagLab NMR facility provides users a variety of superconducting magnets with field strengths from 300 to 900 MHz, and also the 1.5 GHz Series-Connected Hybrid magnet, to address both biological and materials applications.

Superconducting NMR magnets:

- 900 MHz 105 mm NMR Magnet
- 830 MHz 31 mm NMR Magnet
- 800 MHz 63 mm NMR Magnet #1
- 800 MHz 63 mm NMR Magnet #2
- 800 MHz 63 mm NMR Magnet #3 (Gainesville)
- 750 MHz 89 mm NMR & MRI/S System (Gainesville)
- 600 MHz 89 mm NMR Magnet #1
- 600 MHz 89 mm NMR Magnet #2
- 600 MHz 89 mm MAS DNP System
- 600 MHz 89 mm Wide Bore Bruker Avance Neo (Gainesville)
- 600 MHz 51 mm NMR & MRI/S System (Gainesville)
- 500 MHz 89 mm NMR Magnet for Solid State
- 500 MHz 54 mm NMR System (Gainesville)
- 400 MHz 89 mm NMR Magnet
- 300 MHz 89 mm NMR Magnet

35.2 T / 1.5 GHz Series-Connected Hybrid magnet

Our capabilities:

Aligned membrane protein NMR
Biological MAS NMR
Ultrafast MAS
Ultra high field NMR
Quadrupolar and low-γ NMR
In-situ battery NMR/MRI
MAS DNP and Overhauser DNP

MagLab's Magnets are available to scientists around the world free of charge!

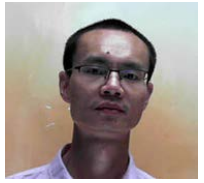
Request magnet time at:
https://nationalmaglab.org/user-resources/request-magnet-time

NMR Probe Development Program

- The RF group led by William Brey and Peter Gor'kov develops probe technology for high-field solid-state NMR.
  - Low-E coil significantly reduces 1H RF heating to lossy biological samples. We share our design with NMR community by licensing to Bruker which is known as Efree.
  - More sensitive and efficient RF circuits.
  - New probe frame design makes probe maintenance much easier.
  - Probes for unique magnets.

William Brey

Peter Gor'kov



Wenping Mao

Jason Kitchen

Steven Ranner

Faith Scott
DNP

Joe Collins
Machinist

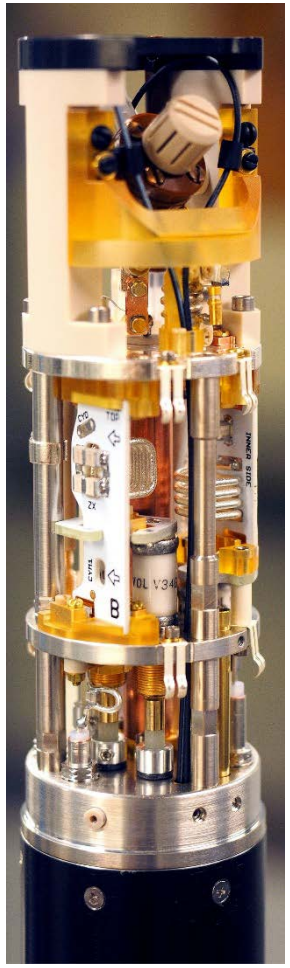
830 MHz
1HX 3.2 mm MAS

1500 MHz
1HX 3.2 mm MAS

In-House Built Solid-State NMR Probes

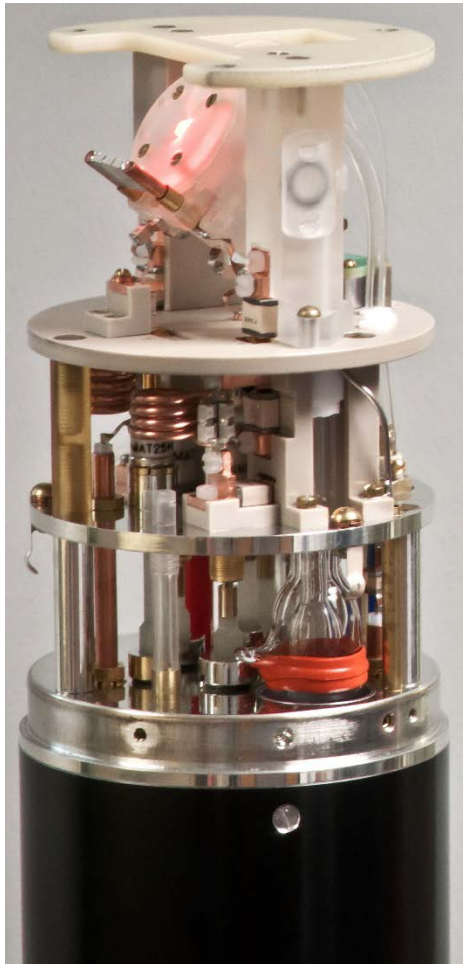
Magnet	Coil		Sample volume	Max spinning speed	RF channels	Note
14.1 T / 600 MHz	Static cross-coil	Φ 5.0 mm	110 µL		^{1}H-X	Biological oriented sample Wideline NMR
		Rectangular 4.0x6.0 mm	240 µL			
	MAS cross-coil	Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X-Y	
	MAS single-coil	Φ 3.2 mm	30 µL	24 kHz	^{1}H-X-Y	MAS DNP, in construction
18.8 T / 800 MHz	Static cross-coil	Φ 5.0 mm	110 µL		^{1}H-X	Biological oriented sample Wideline NMR
		Rectangular 4.0x6.0 mm	240 µL			
	MAS cross-coil	Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X-Y	
		Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X-Y-^{2}H	
	MAS single-coil	Φ 1.3 mm	2.5 µL	65 kHz	^{1}H-X-Y	^{1}H detection
		Φ 0.75 mm	0.29 µL	110 kHz	^{1}H-X-Y	^{1}H detection
19.5 T / 830 MHz	MAS cross-coil	Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X-Y	
21.1 T / 900 MHz	Static cross-coil	Φ 5.0 mm	110 µL		^{1}H-X	Biological oriented sample Wideline NMR
		Rectangular 4.0x6.0 mm	240 µL			
	MAS cross-coil	Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X	Extended VT range
		Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X-Y	
35.2 T / 1500 MHz	Static cross-coil	Φ 3.0, 4.0, 5.0 mm	26, 58, 110 µL		^{1}H-X	Biological oriented sample Wideline NMR
		Rectangular 4.0x4.0 mm	101 µL			
	MAS cross-coil	Φ 3.2 mm	22, 36 µL	24, 20 kHz	^{1}H-X	X: ^{103}Rh ~ ^{11}B
		Φ 2.0 mm	11 µL	38 kHz	^{1}H-X-Y	
	MAS single-coil	Φ 1.3 mm	2.5 µL	65 kHz	^{1}H-X-Y	^{1}H detection, in construction

In-House Built Solid-State NMR Probes

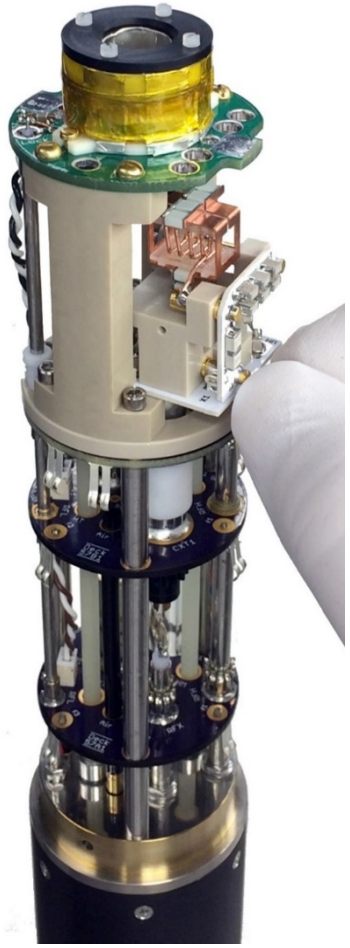


800 MHz
^{1}HXY 0.75 mm MAS
1H Detection

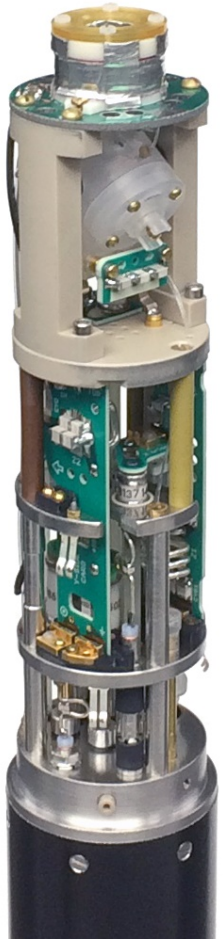
800 MHz
1HXY 1.3 mm MAS
1H Detection



900 MHz
1HXY 3.2 mm MAS



1500 MHz
1HX Static



1500 MHz
1HXY 2.0 mm MAS

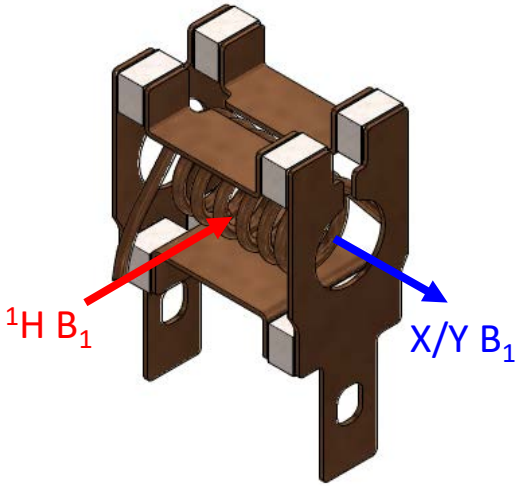
1500 MHz
1HX 3.2 mm MAS
X 2

Single Coil vs Cross Coil

Strip-shield solenoid

Scroll

Solenoid

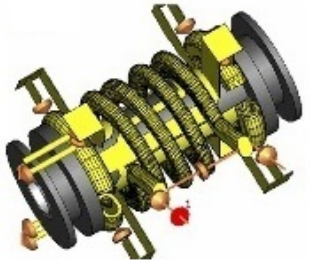


Low-E cross-coil

- Outer LGR tuned to ^{1}H
- Inner solenoid tuned to X/Y
- B_1 field generated by two coils are perpendicular

^{1}H detection
Fast MAS

Higher ^{1}H sensitivity



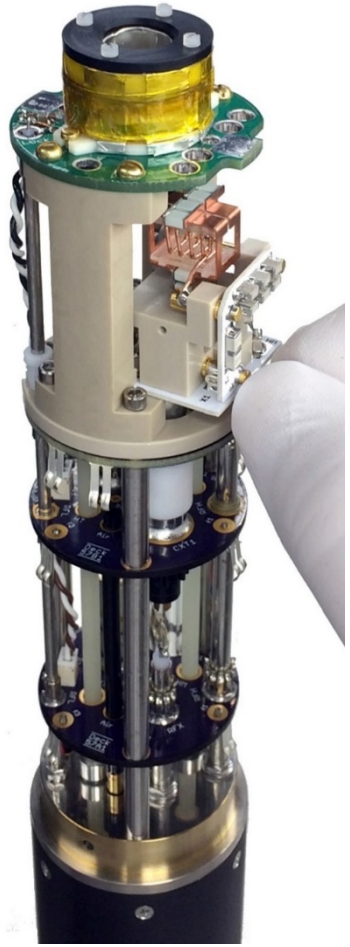
DOTY XC

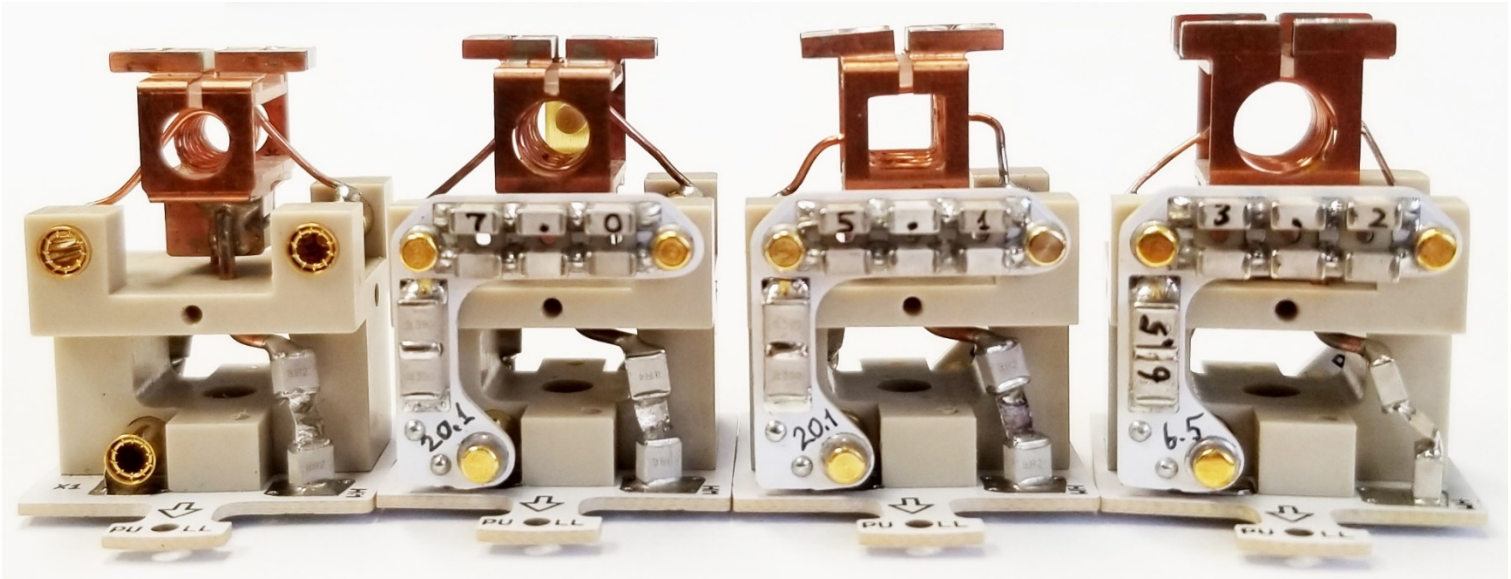
X detection

Low ^{1}H RF heating for lossy sample
High ^{1}H B1 homogeneity
High X/Y sensitivity
High isolation between ^{1}H and X/Y

MAGC

Various RF Coils for Different Sample Shapes and Dimensions (Static Probe)



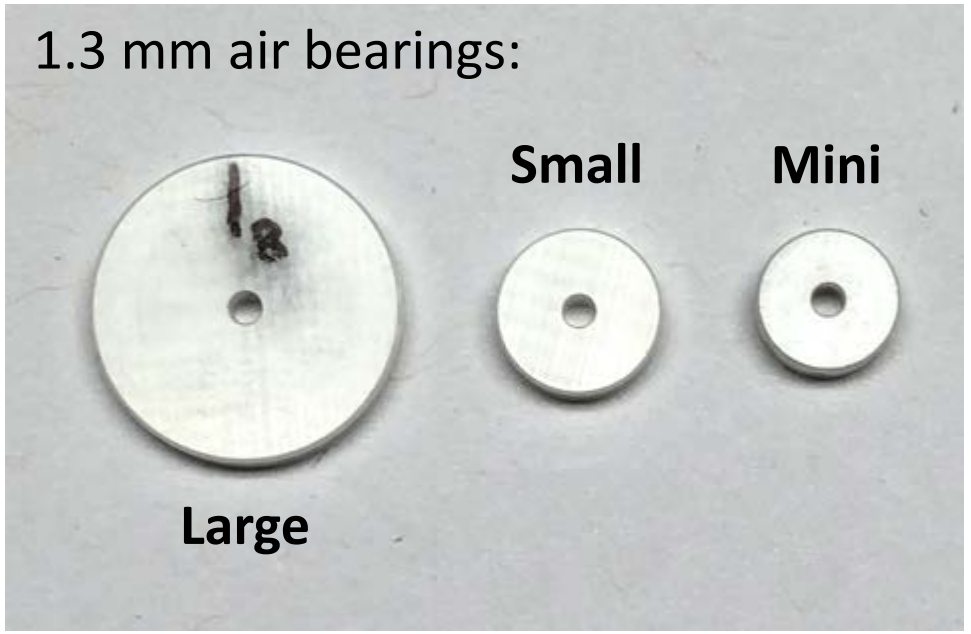


Φ3 mm Φ4 mm 4x4 mm Φ5 mm

Magic Angle Spinner

3.2 mm
Pencil rotor

1.3 mm
Bruker rotor

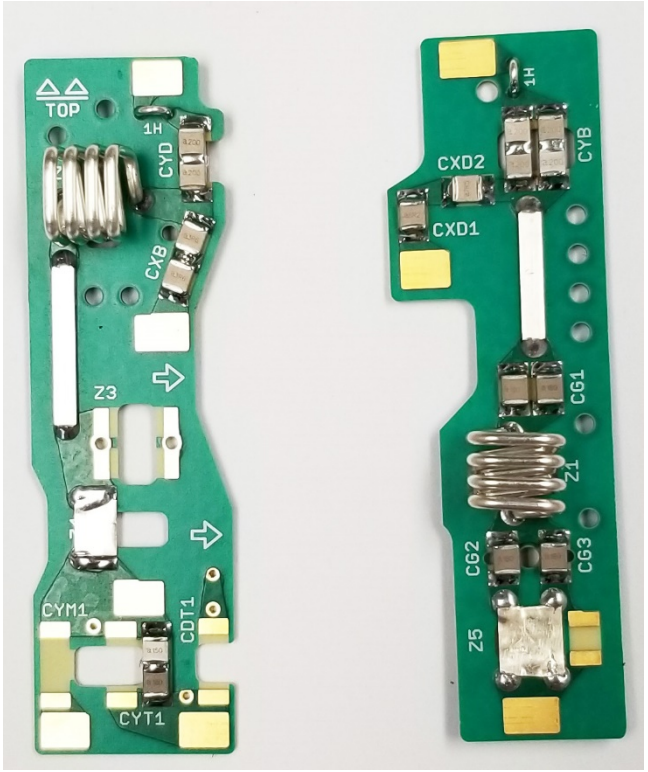


3.2 mm
Bruker rotor

1.3 mm (compact)
Bruker rotor

Reconfigurable Resonant Mode Using Tuning Cards

Probe No. 54				LE 3.2 MAS 800 HXYD			
Mode				f_x (MHz)	f_y (MHz)	C_x value	Tune cards label
H	X	Y	D				
^{1}H	^{13}C	^{15}N	^{2}H	201.185	81.105	2.1	H C N D
^{1}H	^{13}C	^{15}N	-	201.185	81.105	2.1	H C N
^{1}H	^{13}C	^{17}O	-	201.185	108.465	2.1	H C O _
^{1}H	^{11}B	^{17}O	-	256.704	108.465	0.3	H B O _
^{1}H	-	^{25}Mg	-	-	48.979	58.2	H - Mg -
^{1}H	-	^{67}Zn	-	-	50.061	58.2	H - Mg -
^{1}H	-	^{91}Zr	-	-	74.380	26.0	H - Cl -
^{1}H	-	^{35}Cl	-	-	78.393	22.4	H - Cl -
^{1}H	-	^{15}N	-	-	81.105	20.2	H - Cl -
^{1}H	^{17}O	-	-	108.465	-	12.1	H O - -
^{1}H	^{77}Se	-	-	152.591	-	4.9	H Se
^{1}H	^{207}Pb	-	-	167.386	-	2.1	207 Pb
^{1}H	^{13}C	-	-	201.185	-	2.1	H C to Na
^{1}H	^{27}Al	-	-	208.481	-	1.7	H C to Na
^{1}H	^{23}Na	-	-	211.642	-	1.4	H C to Na



Tuning cards can be made per user's request.

Thank You!