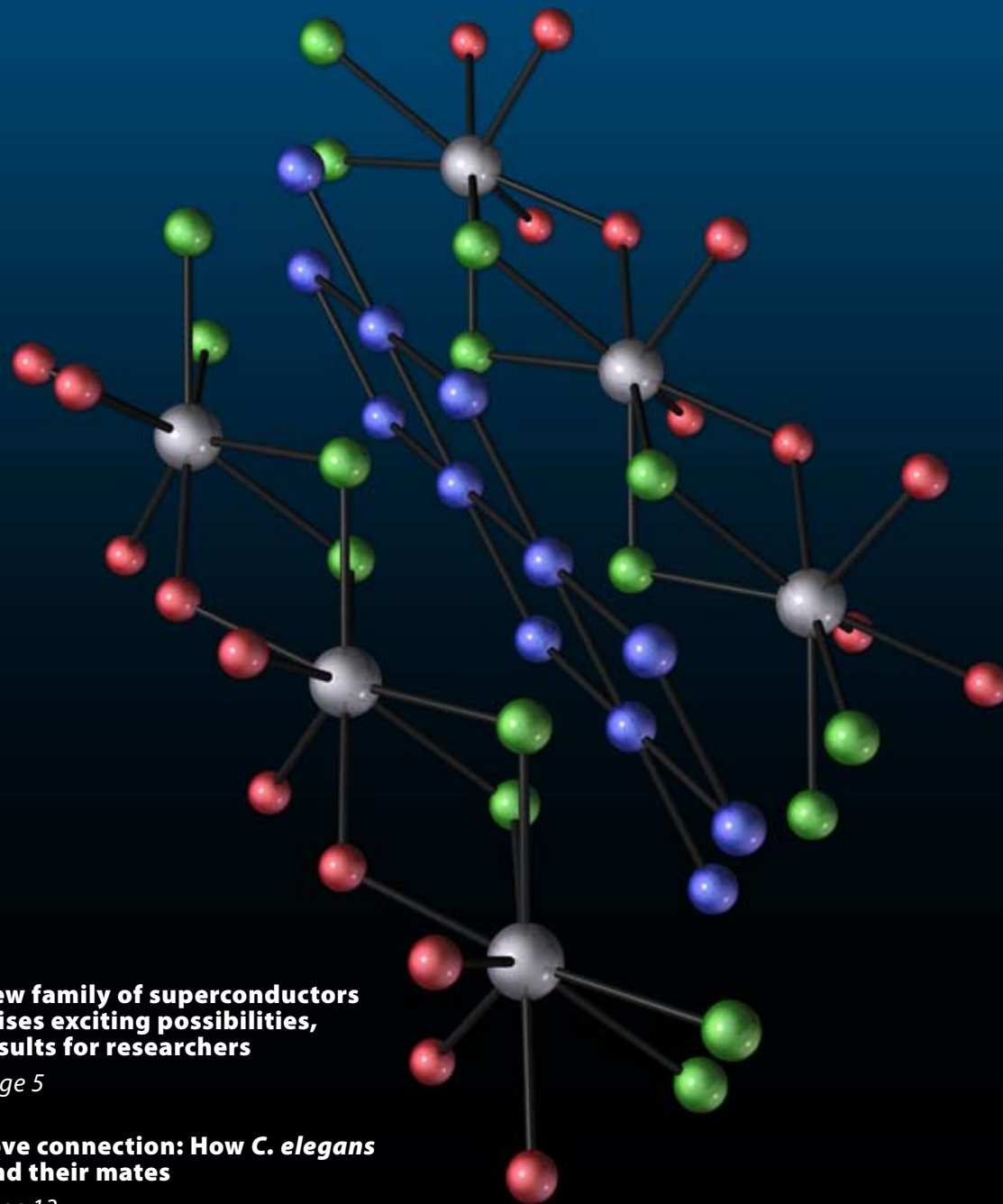


NATIONAL HIGH MAGNETIC FIELD LABORATORY

# MAG LAB REPORTS

FLORIDA STATE UNIVERSITY • UNIVERSITY OF FLORIDA • LOS ALAMOS LAB



- **New family of superconductors raises exciting possibilities, results for researchers**

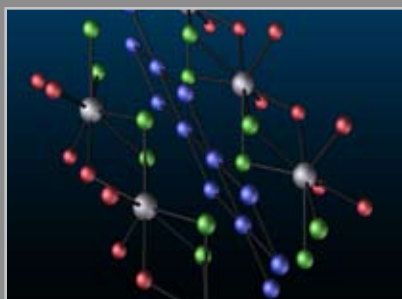
*Page 5*

- **Love connection: How *C. elegans* find their mates**

*Page 13*

- 3** *From the Director's Desk*
- 5** Research suggest novel superconductors are in a class all their own
- 8** Stanford, Mag Lab collaborate to glean data on magnetic order in  $\text{Ba}_3\text{Mn}_2\text{O}_8$
- 10** Examining quadrupolar nuclei with high magnetic fields
- 13** Mate or hibernate? How *C. elegans* answer that question
- 16** ICR looks ahead to next-generation FT-ICR mass spectrometer
- 18** Summer of science: multiple outreach initiatives close successfully
- 20** People in the news
- 22** Steve Hill selected as EMR director
- 23** Science Starts Here: Chris Ramsey

Trying to reduce your carbon footprint? Sign up for an online subscription at <http://www/mediacenter/publications/subscribe.aspx>



**On the cover:**

A new family of superconductors known as doped rare-earth iron oxyarsenides or oxypnictides has come under increasing focus from the research community. Learn more on page 5.

Published by:

**National High Magnetic Field Laboratory**

1800 East Paul Dirac Drive  
Tallahassee, Florida 32310-3706

Tel: 850 644-0311

Fax: 850 644-8350

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

Director: GREG BOEBINGER

Associate Director for Management  
and Administration: BRIAN FAIRHURST

Director, Public Affairs: SUSAN RAY

Editing and Writing: AMY MAST, SUSAN RAY

Art Direction and Production: RICHARD LUDLOW

This document is available in alternate formats upon request. If you would like to be added to our mailing list, please write Amy Mast at the address shown at left, call 850 644-1933, or e-mail [winters@magnet.fsu.edu](mailto:winters@magnet.fsu.edu).

## Thanks to you, we're open

The best news is the best possible news for a user facility: Because of cooperation with budget cuts across the lab, conservation efforts by our DC magnet users, and the recent assistance of the National Science Foundation and Florida State University in helping with our mounting power bills, our DC magnets will remain operating through the end of the year!

As such, there is DC magnet time newly made available in November and December. Interested users should contact Eric Palm to make requests for magnet time. Magnet time on an urgent basis can also occasionally be provided (so called "vulture time") if a scheduled experiment is not able to run and magnet time comes available at the last minute.

This news comes at the right time because demand for DC and pulsed magnet time has peaked dramatically this year due to the discovery of the pnictide superconductors (also called the iron arsenides), a completely new class of high-temperature superconductors.

Perhaps 2008 will become known for ushering in a new Iron Age.

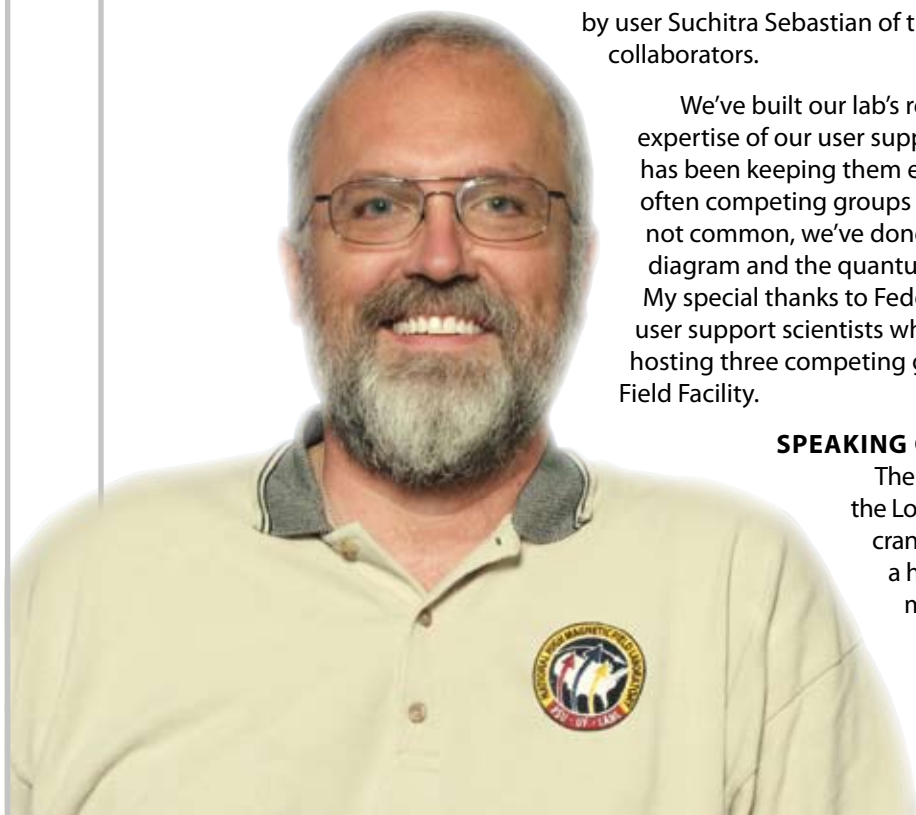
Experiments on the iron arsenides have launched a flurry of activity (indeed several flurries) at the National High Magnetic Field Laboratory. Because high magnetic fields kill superconductivity, and because superconductivity in these compounds is unusually resistant to magnetic fields, many collaborations among users and in-house scientists have developed virtually overnight. New users have come from Japan, China, Europe and the United States to study these promising materials.

One of the first examples of upper critical magnetic field measurements is featured on page 5 in this issue of *Mag Lab Reports*. Another highlight is the observation of quantum oscillations to determine the Fermi surface in one of the iron arsenides by user Suchitra Sebastian of the University of Cambridge and her collaborators.

We've built our lab's reputation in large part on the expertise of our user support scientists, and the pnictides buzz has been keeping them especially busy, hosting multiple and often competing groups of visiting scientists. Although it is not common, we've done it before – with the URu<sub>2</sub>Si<sub>2</sub> phase diagram and the quantum oscillations in YBCO for example. My special thanks to Fedor Balakirev and any others of our user support scientists who have had the honor (honor?) of hosting three competing groups simultaneously at the Pulsed Field Facility.

### SPEAKING OF HIGH IMPACT...

The 100-T Multi-shot Magnet Project at the Los Alamos branch of the MagLab is cranking out the science. This project is a hallmark of interagency funding for mid-scale projects and the scientific capabilities it enables. Sponsored by both the Department of Energy and the National Science Foundation, the one-of-a-kind magnet – having now achieved 89 T – offers non-destructive magnetic fields from



65 T to 85 T to an international user community.

Now in its first maintenance cycle to replace key components, its first nine months of providing pulses were marked by breadth of condensed matter research, variety of the user institutions involved and quality of publications. Have a look:

#### **SEMICONDUCTORS**

Tuning alloy disorder in diluted magnetic semiconductors in high fields to 89 T. S.A. Crooker, N. Samarth, **Applied Physics Letters**, vol. **90**, 102109 (5 March 2007). User from Penn State University.

#### **HEAVY FERMIONS**

Fermi Surface of CeIn<sub>3</sub> above the Neel Critical Field. N. Harrison, S.E. Sebastian, C.H. Mielke, A. Paris, M.J. Gordon, C.A. Swenson, D.G. Rickel, M.D. Pacheco, P.F. Ruminer, J.B. Schillig, J.R. Sims, A. H. Lacerda, M.T. Suzuki, H. Harima and T. Ebihara, **Physical Review Letters**, vol. **99**, 056401 (3 August 2007). Users from University of Cambridge, Kobe University, and Shizuoka University.

#### **HIGH-TEMPERATURE SUPERCONDUCTIVITY**

Quantum Oscillations in the Underdoped Cuprate YBa<sub>2</sub>Cu<sub>4</sub>O<sub>8</sub>, E. A. Yelland, J. Singleton, C.H. Mielke, N. Harrison, F.F. Balakirev, B. Dabrowski and J.R. Cooper, **Physical Review Letters**, vol. **100**, 047003 (1 February 2008). Users from Bristol University, Northern Illinois University, and University of Cambridge.

#### **FRUSTRATED MAGNETS**

Fractalization drives crystalline states in a frustrated spin system. Suchitra E. Sebastian, N. Harrison, P. Sengupta, C. D. Batista, S. Francoual, E. Palm, T. Murphy, N. Marcano, H. A. Dabkowska and B. D. Gaulin **Proceedings of the National Academy of Sciences** (in press, July 2008). Users from University of Cambridge and McMaster University.

And so the show continues ...

*Gregory S. Boebinger*

GREGORY S. BOEBINGER



# Two-band superconductivity in $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$ at very high magnetic fields

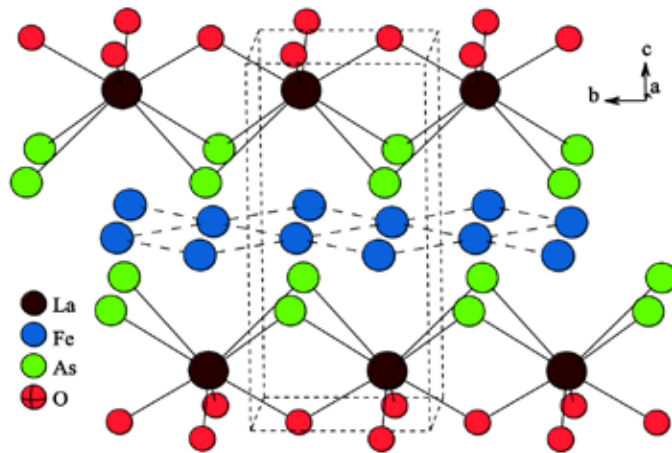
F. Hunte<sup>1</sup>, J. Jaroszynski<sup>1</sup>, A. Gurevich<sup>1</sup>, D.C. Larbalestier<sup>1</sup>, R. Jin<sup>2</sup>, A.S. Sefat<sup>2</sup>, M.A. McGuire<sup>2</sup>, B.C. Sales<sup>2</sup>, D. Christen<sup>2</sup>, D. Mandrus<sup>2</sup>

<sup>1</sup>National High Magnetic Field Laboratory, Florida State University

<sup>2</sup>Oak Ridge National Laboratory

A new family of superconductors referred to as doped rare-earth iron arsenides or pnictides comprised of alternating layers of  $\text{REO}_{1-x}\text{F}_x$  and FeAs has been the focus of research worldwide since early 2008. This follows the report of superconductivity in fluorine-doped lanthanum oxide iron arsenide at 26 K by the research group of Hideo Hosono<sup>1</sup> of the Tokyo Institute of Technology. Transition temperatures quickly rose to 40-43 K by replacing La with Ce and to 52-55 K by replacing La with Nd, Pr, and Sm<sup>2-6</sup>.  $\text{SmFeAsOF}$  holds the record 55 K transition temperature observed up to the time of this report. These first polycrystalline samples were prepared by solid state synthesis.

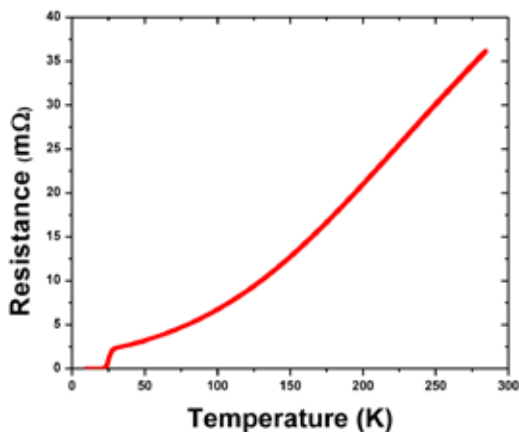
Band structure calculations indicate a departure from conventional superconductivity by phonon-mediated pairing. Several experiments also point to unconventional multiband superconductivity in the layers of paramagnetic Fe ions. Calculations further suggest that superconductivity originates from the d-orbitals of Fe ions which would normally be expected to destroy superconductivity by pair-breaking in the traditional mechanism of s-wave Cooper pairing<sup>7,8</sup>. This suggests that new non-phonon pairing mechanisms are responsible for the high  $T_c$  superconducting state.



**Figure 1: Crystal structure of LaFeAsOF**

Layers of La and O are separated by sheets of Fe and As. Each atom in a La layer forms pyramids above and below the layer with four atoms of O and four atoms of As such that the As atoms are adjacent to the Fe atoms. The tetragonal unit cell is shown in dotted lines.

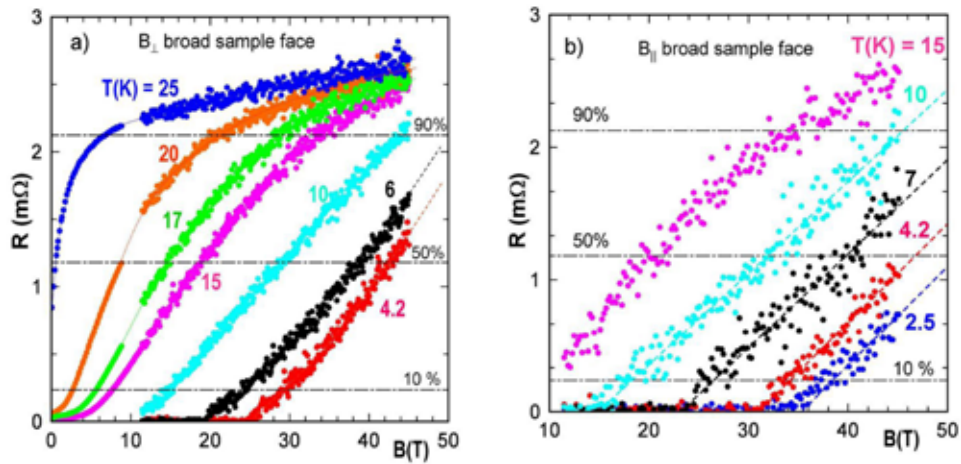
F-doped  $\text{-LaFeAsO}$  is a semimetal exhibiting strong antiferromagnetic fluctuations in addition to a possible spin density wave instability around 150 K in the parent undoped  $\text{LaFeAsO}$ .<sup>2,9-12</sup> Several disconnected pieces of the Fermi surface may contribute to superconductivity thus exhibiting the multi-gap pairing, which has recently attracted so much attention in  $\text{MgB}_2$ .<sup>7,8,14,15</sup>



**Figure 2: Temperature dependence of resistance**

Resistance shows a  $T_c$  onset at 30 K and  $RRR \sim 15$ , with a nominal resistivity of  $\sim 0.15 \text{ m}\Omega\text{cm}$  at  $T_c$ , suggestive of a clean-limit material.

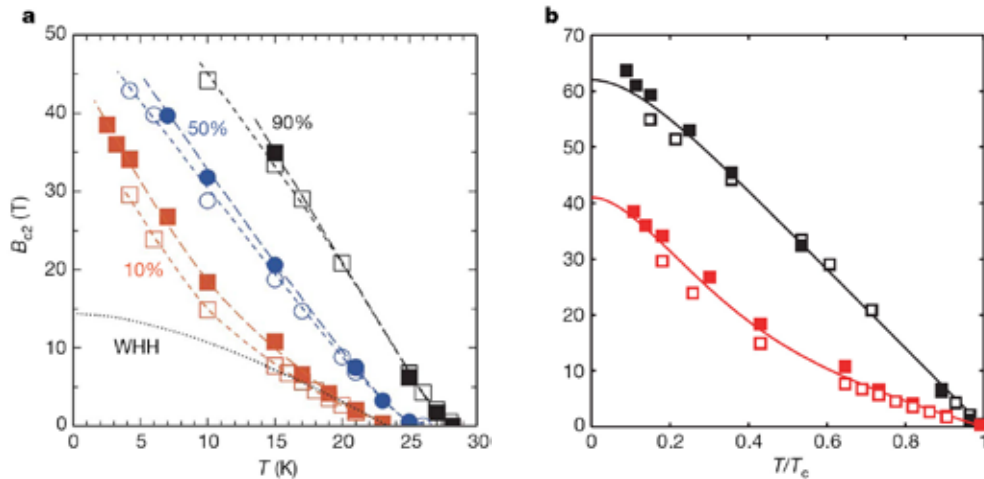




**Figure 3: Magnetoresistance up to 45T**

$R(B)$  clearly delineates zero resistance in this polycrystal well above 35T at low temperatures. Some small texture is deduced from the angular sensitivity of the transitions.

Our recent study of  $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$  synthesized by David Mandrus' research group<sup>13</sup> at Oak Ridge National Laboratory showed remarkable enhancement of the upper critical fields  $B_{c2}$ , particularly at low temperatures as compared to those expected from the already high slopes of  $dB_{c2}/dT \approx 2 \text{ T/K}$  near  $T_c$ . The deduced  $B_{c2}(0) \approx 63\text{--}65 \text{ T}$  exceeds the paramagnetic limit, consistent with strong coupling and important two-band effects<sup>19</sup>.



**Figure 4: Two-band superconductivity in  $\text{LaFeAsO}_{0.89}\text{F}_{0.11}$**

Full and open symbols correspond to parallel and perpendicular field orientations of the slightly textured sample. Because of the almost reversible magnetization of the sample, we associate the bottom of the transition with the lower  $B_{c2}$  and the top with the higher, which we are assume to be with  $B$  perpendicular and parallel to the planes respectively.

The dashed line at left in Figure 4 is the Werthamer-Helfand-Hohenberg (WHH)<sup>17</sup> curve defined by the slope of  $B_{\min}(T)$  at  $T_c$ . At right,  $B_{\max}(T)$  (black) and  $B_{\min}(T)$  (red) are plotted as functions of the reduced temperature  $T/T_c$ . At right, the lines are fits to the Gurevich 2-gap model<sup>18</sup> of  $B_{c2}$ . They are consistent with  $B_{c2}$  being determined by heavy, 3D-like carriers at low temperatures and lighter 2D carriers at higher  $T$ . Our data provide strong experimental support for recent models that deduce this family to be one in which two-band superconductivity plays a major role as with  $\text{MgB}_2$ .<sup>16</sup>

The proliferation of research on the oxypnictides has seen the rapid evolution of the new family of superconductors from the first bulk polycrystalline materials to the growth of single crystals. These higher quality samples will allow for the characterization of the arsenides while fully revealing the novel physics of competing superconducting and magnetic orders. The importance of the manifestations of superconductivity in the oxypnictides is evident in the fact that critical temperatures and critical fields have surpassed those of  $\text{Nb}_3\text{Sn}$ , the Chevrel phases and  $\text{MgB}_2$ . With the observation of very high upper critical fields comparable to the high- $T_c$  cuprates, these materials might ultimately become a viable option for high magnetic field applications.

## ACKNOWLEDGEMENTS

Work at the Magnet Lab was supported by IHRP under the NSF Division of Materials Research through DMR-0654118, the U.S. Department of Energy and the State of Florida, by the NSF Focused Research Group on Magnesium Diboride (FRG), and by AFOSR. Work at ORNL was supported by the Division of Materials Science and Engineering, Office of Basic Energy Sciences. We are grateful for discussions with G. Boebinger, E. Hellstrom, P. Lee, J. Jiang, and C. Tarantini at the Magnet Lab.

## REFERENCES

1. Y. Kamihara, *et al.*, *J. Am. Chem. Soc.* **130**, 3296-3297 (2008).
2. G.F. Chen, *et al.*, *Phys. Rev. Lett.* **100**, 247002 (2008).
3. X.H. Chen, *et al.*, Preprint at (<http://arxiv.org/abs/0803.3603v1>) (2008).
4. Z-A. Ren, *et al.*, *Europhysics Letters* **82**, 57002 (2008).
5. Z-A. Ren, *et al.*, Preprint at (<http://arxiv.org/abs/0803.4283>) (2008).
6. Z-A Ren, *et al.*, *Chin. Phys. Lett.* **25**, 2215 (2008).
7. D.J. Singh and M.H. Du, *Phys. Rev. Lett.* **100**, 237003 (2008).
8. I.I. Mazin, *et al.*, submitted to *Phys. Rev. Lett.* Preprint at (<http://arxiv.org/abs/0803.2740v1>) (2008).
9. C. Cao, P.J. Hirschfeld & H-P. Cheng, *Phys. Rev. B* **77**, 220506 (2008).
10. J. Dong, *et al.*, *Europhysics Letters* **83**, 27006 (2008).
11. F. Ma and Z-Y. Lu Preprint at (<http://arxiv.org/abs/0803.3286v1>) (2008).
12. M.A. McGuire, *et al.*, Preprint at (<http://arxiv.org/abs/0804.0796>) (2008).
13. A.S. Sefat, *et al.*, *Phys. Rev. B* **77**, (2008).
14. K. Kuroki, *et al.*, Preprint at (<http://arxiv.org/abs/0803.3325v1>) (2008).
15. S. Lebegue, *Phys. Rev. B* **75**, 035110 (2007).
16. J. Nagamatsu, *et al.*, *Nature* **410**, 63-64 (2001).
17. N.R. Werthamer, E. Helfand and P. C. Hohenberg, *Phys. Rev.* **147**, 295-302 (1966).
18. A. Gurevich, *Physica C* **456**, 160-169 (2007); *Phys. Rev. B* **67**, 184515 (2003).
19. F. Hunte, *et al.*, *Nature* **453**, 903-905 (12 June 2008).



# Magnetic order in the frustrated spin dimer compound $\text{Ba}_3\text{Mn}_2\text{O}_8$

E. C. Samulon<sup>2</sup>, I. R. Fisher<sup>2</sup>, Y.-J. Jo<sup>1</sup>, L. Balicas<sup>1</sup>, Y. Kohama<sup>3</sup>, P. Sengupta<sup>3</sup>, C. D. Batista<sup>3</sup>, M. Jaime<sup>3</sup>

<sup>1</sup> National High Magnetic Field Lab, Florida State University

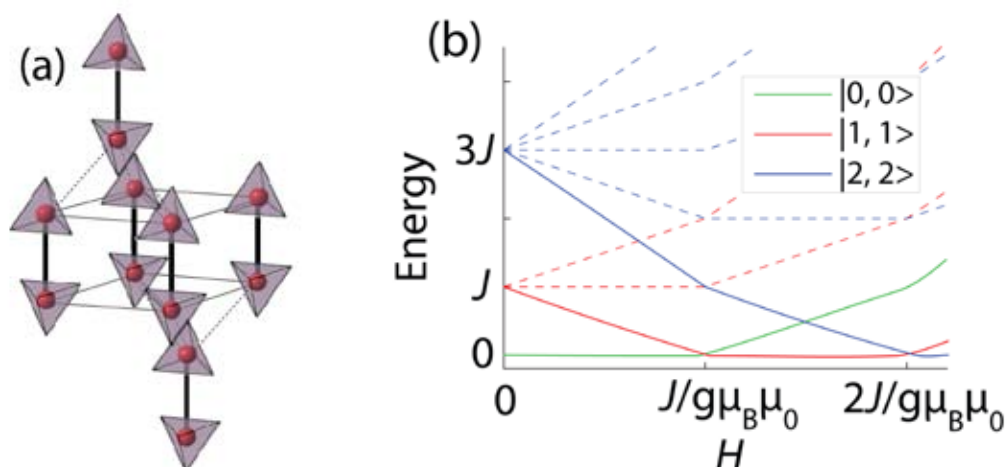
<sup>2</sup> Stanford University

<sup>3</sup> Los Alamos National Laboratory

Antiferromagnetic exchange on a triangular lattice leads to geometric frustration - the system cannot satisfy all of the pairwise interactions simultaneously, such that the minimum energy of the system does not correspond to the minimum energy of all local interactions. The classical solution to the Heisenberg antiferromagnet on a triangular lattice with only nearest neighbor interactions is the well known  $120^\circ$  structure. In this case, the main effect of the frustration is simply to produce a non-collinear structure. As a new twist on an old story, we experimentally examined the slightly more complex case of a triangular lattice decorated by vertical magnetic (spin) dimers, realized by the compound  $\text{Ba}_3\text{Mn}_2\text{O}_8$ <sup>1</sup>.

Spin dimer compounds comprise pairs of strongly coupled magnetic ions. Antiferromagnetic intradimer exchange leads to a ground state that is a product of singlets, but an applied magnetic field can be used to close the spin gap to excited triplet states, resulting at low temperatures in a state characterized by long range magnetic order. Close to the critical field, the effective Hamiltonian that describes the low-energy degrees of freedom of such a system can be expressed in terms of an effective spin- $\frac{1}{2}$  model, or equivalently a lattice gas model of hard-core bosons<sup>2</sup>. Under favorable conditions a variety of interesting magnetic states can be realized, including a Bose-Einstein condensate<sup>3</sup> and possibly even a spin supersolid<sup>4</sup>.

This class of material offers several specific advantages over simple (non-dimerized) magnetic lattices. First, variation of an external magnetic field can be used to tune the triplet density, providing easy access to more of the quantum phase diagram including the quantum critical point (QCP). Second, one can, at least in principle, "engineer" effective Hamiltonians that would be unphysical for simple spin systems<sup>4</sup>. An additional novelty specific to  $\text{Ba}_3\text{Mn}_2\text{O}_8$  is the magnitude of the spin on each ion. Although most other well studied dimer compounds comprise  $S = \frac{1}{2}$  moments, the  $\text{Mn}^{5+}$  valence in  $\text{Ba}_3\text{Mn}_2\text{O}_8$  corresponds to an electron configuration  $3d^2$  and hence  $S = 1$ . This material therefore allows a detailed exploration of the interplay between single ion anisotropy, which favors uniaxial structures, and frustration, which favors non-collinear structures.



**Figure 1:**

(a) Crystal structure of  $\text{Ba}_3\text{Mn}_2\text{O}_8$  showing vertical dimers comprising two  $\text{MnO}_4$  tetrahedra, arranged on a triangular lattice. (b) Energy spectrum relative to the ground state as a function of magnetic field for an isolated dimer consisting of two  $S = 1$  moments with antiferromagnetic exchange  $J$ . Singlet ground state and excited triplet and quintuplet states are shown in green, red and black, respectively.

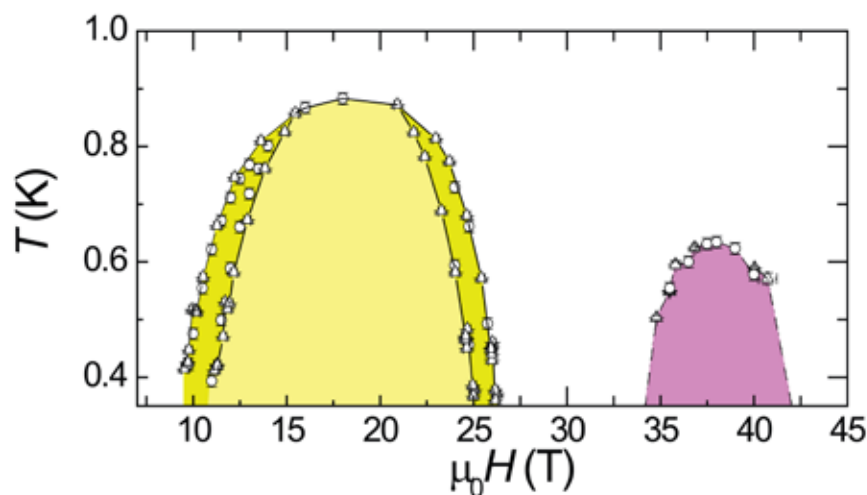
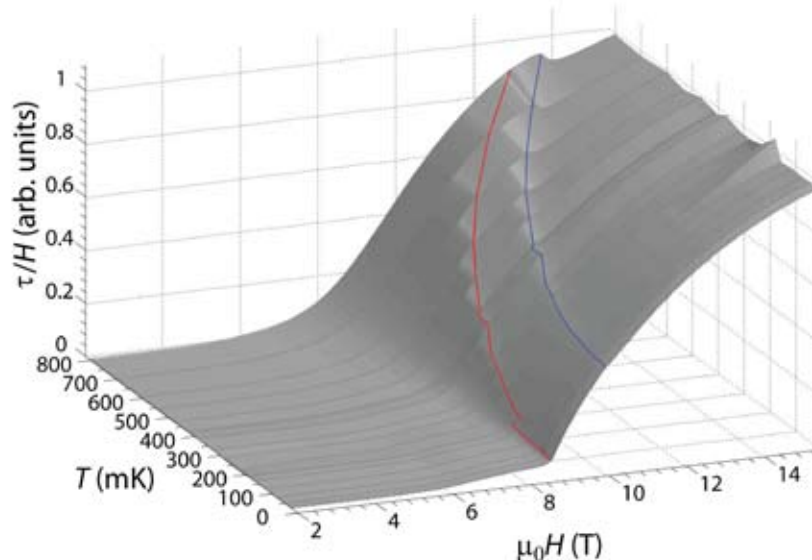
Via a series of torque (Figure 2), heat capacity and magnetocaloric effect measurements performed at the NHMFL, we have established the magnetic phase diagram of  $\text{Ba}_3\text{Mn}_2\text{O}_8$  for fields oriented both parallel and perpendicular to the dimer axis (Figure 3). These measurements reveal a remarkable sequence of



ordered states associated with the  $S_z = 1$  triplet (yellow) and  $S_z = 2$  quintuplet (purple) states. Analysis of the spin Hamiltonian reveals candidates for these phases, which for fields oriented perpendicular to the dimer axis correspond to complex modulated structures characterized by multiple order parameters and stabilized by the competition between geometric frustration and single ion anisotropy<sup>1</sup>.

**Figure 2:**

Field and temperature dependence of the magnetic torque (scaled by the field strength) for fields applied close to perpendicular to the dimer axis. A linear interpolation scheme between field sweeps (dark lines) has been used to generate the 3D surface. Red and blue lines indicate phase transitions.



**Figure 3:**

Phase diagram obtained from heat capacity (circles) and MCE (triangles) measurements for fields perpendicular to the dimer axis. Yellow and purple regions correspond to singlet/triplet and triplet/quintuplet ordered states, respectively.

The authors thank S. E. Brown, S. Hill, M. D. Lumsden and M. B. Stone for useful discussions. Work at Stanford University is supported by the National Science Foundation, Division of Materials Research under grant DMR-0705087. Crystal growth equipment purchased with support from the Department of Energy, Office of Basic Energy Sciences, under contract DE-AC02-76SF00515. A portion of this work was performed at the National High Magnetic Field Laboratory, which is supported by NSF Cooperative Agreement No. DMR-0084173, by the State of Florida, and by the DOE.

#### REFERENCES

1. E. C. Samulon, *et al.*, *Phys. Rev. B* **77**, 214441 (2008).
2. T. M. Rice, *Science* **298**, 760 (2002).
3. S. E. Sebastian, *et al.*, *Nature* **441**, 617 (2006).
4. P. Sengupta and C. D. Batista, *Phys. Rev. Lett.* **98**, 227201 (2007).

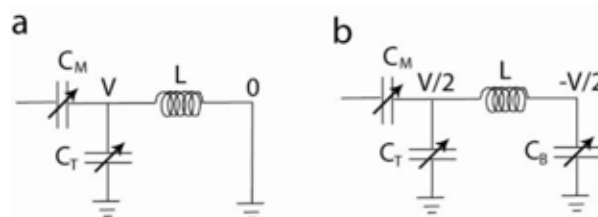
# Solid State NMR of Low- $\gamma$ Quadrupolar Nuclei using High $B_0$ and $B_1$ Magnetic Fields.

Zhehong Gan<sup>1</sup>, Peter Gor'kov<sup>1</sup>, William Brey<sup>1</sup>, Paul J. Sideris<sup>2</sup>, Ulla Gro Nielsen<sup>2</sup>, Clare P. Grey<sup>2</sup>

<sup>1</sup> National High Magnetic Field Lab, Florida State University

<sup>2</sup> SUNY-StonyBrooks

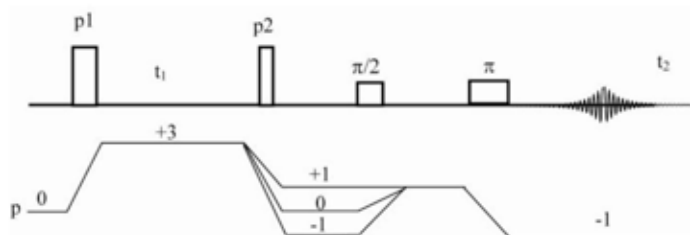
Many of magnetically active nuclei in the Periodic Table are quadrupolar nuclei with spins  $S > 1/2$  and low gyro-magnetic ratio  $\gamma$ . The list includes  $^{25}\text{Mg}$ ,  $^{39}\text{K}$ ,  $^{43}\text{Ca}$ ,  $^{45,47}\text{Ti}$ ,  $^{67}\text{Zn}$ ,  $^{73}\text{Ge}$ ,  $^{95,97}\text{Mo}$  and  $^{99,101}\text{Ru}$ ; all are commonly found in many solid materials such as glasses, minerals, catalysts, ceramics and semiconductors. Solid state NMR of these nuclei has become a powerful tool to probe structure at atomic level with the capability of resolving individual chemical sites. However, the spectral sensitivity and resolution for the low- $\gamma$  quadrupolar nuclei are often prohibitively low. The NMR signal intensity is proportional to  $\gamma^{5/2}$  while the second-order quadrupolar broadening is proportional to  $\gamma^{-1}$  to the central transition that gives rise to the high resolution spectra. Some of nuclei even have low natural abundance. High magnetic fields play an important role to overcome these difficulties of low- $\gamma$  quadrupolar nuclei. We have demonstrated in the past that the spectral resolution and sensitivity of quadrupolar nuclei can be dramatically enhanced by high static magnetic fields  $B_0$  up to 40 T using the Magnet Lab's hybrid magnet.<sup>1</sup> In this report, we present recent development on sensitivity enhancement by high radio-frequency (*rf*) magnetic field  $B_1$ . Using a so-called balanced probe circuit, higher *rf* field can be generated to enhance the efficiency of some widely used experiments for quadrupolar nuclei such as the Multiple-Quantum Magic-Angle Spinning (MQMAS)<sup>2</sup> and the Satellite-Transition Magic-Angle Spinning (STMAS)<sup>3</sup>. High  $B_0$  and  $B_1$  magnetic fields make an optimal set up at the Magnet Lab for solid state NMR spectroscopy of insensitive low- $\gamma$  quadrupolar nuclei. We also present in this report some recent collaboration with Professor Clare Grey's group (Chemistry/SUNY-StonyBrooks) using this unique capability at the Magnet Lab on their discovery of Mg/Al ordering in layered double hydroxides (LDHs) published in the latest issue of journal *Science*<sup>4</sup>.



**Figure 1:**

(a) conventional and (b) balanced LC resonant circuits. The balanced circuit reduces the peak *rf* voltage from  $V$  to  $V/2$ .

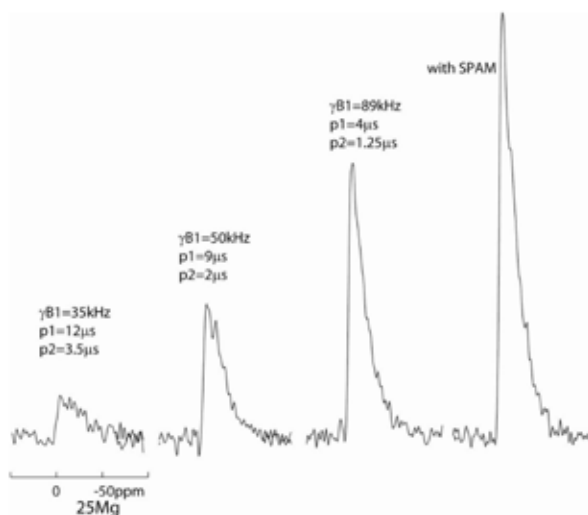
The strength of *rf* field  $B_1$  is an important parameter for many NMR experiments. The field depends not only the geometry of the sample coil, the quality factor  $Q$  of resonance circuit but also the input *rf* power to the probe. High  $B_1$  field can be generated by increasing the power to the point before probe arcing. Figure 1 describes the basic concept of a balanced resonant circuit to reduce the high *rf* voltage in the probe circuit. Conventional  $LC$  resonant loop consists of one tuning capacitor  $C$  and sample coil  $L$ . One end of the coil is at ground and the other end has the highest voltage  $V$  in the circuit. The balanced circuit has two tuning capacitors, one on each side of the coil. The tuning capacitances are arranged in a way that the voltages at the two ends are  $V/2$  and  $-V/2$ , respectively. The middle point of the coil is at virtual ground. This simple modification effectively reduces the voltage by factor of 2 and enables the doubling of *rf* field provided the availability of a strong-enough *rf* amplifier.



**Figure 2:**

SPAM shifted-echo MQMAS pulse sequence. The  $\pi/2$  pulse (same phase as  $p_2$ ) adds the signals from three coherence transfer pathways.

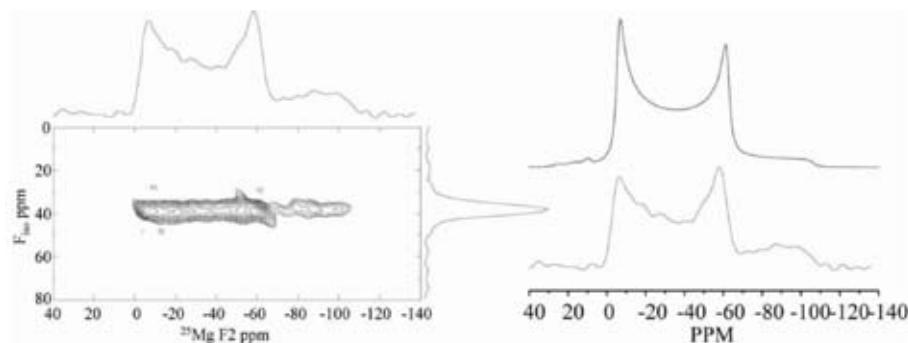
One experiment that can benefit greatly from the high  $rf$  field is the MQMAS experiment. The ingenious experiment was invented by Lucio Frydman in 1995<sup>2</sup> and has since become widely used for solid state NMR of quadrupolar nuclei. The experiment correlates the  $3/2 \leftrightarrow -3/2$  multiple-quantum transition with the  $1/2 \leftrightarrow -1/2$  central transition under magic-angle spinning. In the form of a two dimensional experiment, the correlation refocuses the anisotropic second-order quadrupolar broadening achieving the so-called isotropic spectral resolution capable to resolving sites separated by just a few  $ppm$  in chemical shift. However, the efficiency for the multiple quantum excitation and conversion is low, typically  $\sim 10\%$ , and it depends on the nutation frequency  $\gamma B_1$  of the applied  $rf$  field. The order of magnitude reduction in signal intensity makes the application of MQMAS particularly challenging to low- $\gamma$  quadrupolar nuclei because in addition to the intrinsic low sensitivity low- $\gamma$  also contributes to low nutation frequency  $\gamma B_1$ .



**Figure 3:**

First  $t_1$ -slice of 2D shifted-echo MQMAS experiment of  $^{25}\text{Mg}$ -enriched Mg/Al-33 with various  $\gamma B_1$ , pulse length and pulse scheme.

The MQMAS efficiency can also be improved by optimizing the multiple-quantum excitation and conversion such as RIACT<sup>5</sup>, DFS<sup>6</sup>, FAM<sup>7</sup>, and SPAM<sup>8</sup> for. Figure 2 shows the shifted-echo MQMAS pulse sequence<sup>9</sup> incorporated with the SPAM scheme (soft-pulse-added mixing). The shifted-echo sequence is generally more efficient over the Z-filtered sequence<sup>10</sup> for samples with large quadrupolar broadening and long  $T_2$ . By simply adding a central-transition selective  $\pi/2$  pulse (the third pulse in Figure 2), the SPAM mixing combines constructively the signals from three coherence transfer pathways resulting an overall efficiency enhancement by about 50%<sup>8</sup>.



**Figure 4:**

$^{25}\text{Mg}$  MQMAS spectrum of Mg/Al-33 Layered Double Hydroxide ( $\text{Mg}^{2+}_{1-x}\text{Al}^{3+}_x\text{OH}_2(\text{Anion}^{n-})_x\text{H}_2\text{O}$ ,  $x = 0.33$ ) acquired at 19.6T. The line shape fitting yields  $C_q = 4.58\text{MHz}$  and  $\eta = 0$ . [*Science*, 321 (2008) 113]

Figure 3 demonstrates the enhancement of  $^{25}\text{Mg}$  MQMAS by high  $B_1$  field and SPAM. The results show that the MQMAS signal intensity increases more than linearly with the  $rf$  field and the SPAM sequence adds approximately another 50%. The highest  $\gamma B_1 \sim 89\text{kHz}$  is achieved with balanced probe circuit, being only limited by the maximum output of the 1kW  $rf$  amplifier. For the conventional unbalanced circuit, the peak  $rf$  field is no more than  $\gamma B_1 \sim 50\text{kHz}$  before the probe starts arching. For some applications with low- $\gamma$  nuclei, the enhancement by high  $rf$  field can become critical whether MQMAS is feasible. Figure 4 shows the  $^{25}\text{Mg}$  MQMAS spectrum of  $^{25}\text{Mg}$ -enriched Mg/Al layered double hydroxide (LDH). The spectrum clearly shows only one resonance, providing strong evidence of only one Mg local environment in this material. The quadrupolar coupling constant  $C_q = 4.58\text{MHz}$  and the

C3 symmetry  $\eta=0$  of the Mg atom confirm the  $\text{Mg}(\text{OMg})_3(\text{OAl})_3$  environment found in a so-called “honeycomb” ordering of Mg and Al.<sup>4</sup> The enhanced sensitivity by high  $B_0$  and  $B_1$  and optimized pulse sequence allow us now to acquire MQMAS spectra of natural abundant samples without the need of isotope enrichment.

In summary, high magnetic fields, both  $B_0$  and  $B_1$ , and pulse sequence development greatly enhance NMR sensitivity of quadrupolar nuclei, particularly for the MQMAS experiment. The progresses at the NHMFL have established a unique capability for solid state NMR for insensitive low- $\gamma$  quadrupolar nuclei and made it available for users.

#### REFERENCES

1. Z.H. Gan, *et al.*, *J. Am. Chem. Soc.* **124**, 5634 (2002).
2. L. Frydman and J. S. Harwood, *J. Am. Chem. Soc.* **117**, 5367 (1995).
3. Z. Gan, *J. Am. Chem. Soc.* **122**, 3242 (2000).
4. P. Sideris, U. Nielsen, Z. Gan and C. Grey, *Science* **321**, 113 (2008).
5. G. Wu, D. Rovnyak, P. C. Huang and R. G. Griffin, *Chem. Phys. Lett.* **277**, 79 (1997).
6. A. P. M. Kentgens and R. Verhagen, *Chem. Phys. Lett.* **300**, 435 (1999).
7. P. K. Madhu, A. Goldbourt, L. Frydman and S. Vega, *Chem. Phys. Lett.* **307**, 41-47 (1999).
8. Z.H. Gan and H.T. Kwak, *J. Magn. Reson.* **168**, 346 (2004).
9. D. Massiot, B. Touzo, D. Trumeau, J. P. Coutures, J. Virlet, P. Florian and P. J. Grandinetti, *Solid State Nucl. Mag.* **6**, 73 (1996).
10. J. P. Amoureux, C. Fernandez and S. Steuernagel, *J. Magn. Reson. Ser. A* **123**, 116 (1996).



# Worm Sex 101: How *Caenorhabditis elegans* males find their mates

Written by Arthur S. Edison on behalf of the *C. elegans* mating team:

**Fatma Kaplan<sup>1</sup>, Ramadan Ajredini<sup>1</sup>, Cherian Zachariah<sup>1</sup>, Arthur S. Edison<sup>1</sup>, Jagan Srinivasan<sup>2</sup>, Paul Sternberg<sup>2</sup>, Rabia U. Malik<sup>3</sup>, Frank Schroeder<sup>3</sup>, Hans Alborn<sup>4</sup>, Peter Teal<sup>4</sup>,**

<sup>1</sup> National High Magnetic Field Lab, University of Florida

<sup>2</sup> Caltech and Howard Hughes Medical Institute

<sup>3</sup> Cornell University

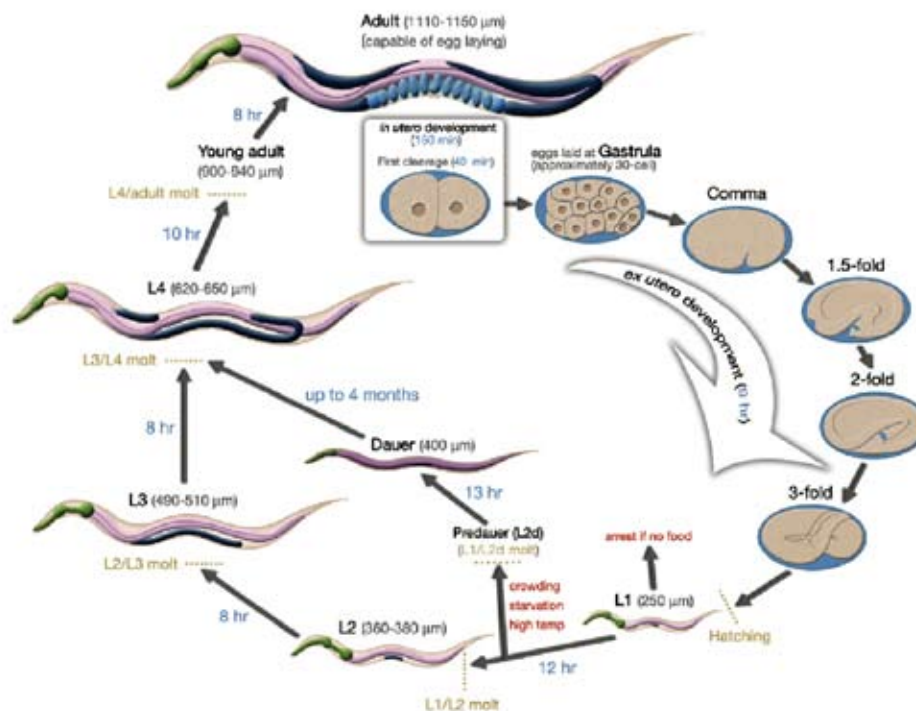
<sup>4</sup> USDA Laboratory

## SUMMARY

This story describes the identification of a chemical mating signal produced by a small worm that was facilitated by the new technology of the Magnet Lab 1-mm HTS probe. The probe allowed us to collect much smaller samples than would be required with conventional technology. As a result, we were able to efficiently examine the composition and activity of the material as a function of development (e.g. time) of the organism and discover new biology.

## BACKGROUND

*Caenorhabditis elegans* is a nematode that reaches about 1-mm in length as an adult. This small worm is one of the best-studied laboratory animals in the world. The adult worms have fewer than 1000 cells, and the fate of every cell division has been mapped from a single fertilized egg to adult. The nervous system of this animal is very simple with just about 300 neurons. The worm's entire anatomy has been studied by thin-section electron microscopy. And, it is very easy to grow and manipulate in the lab using molecular genetic techniques. Many major biological discoveries have been made using *C. elegans* including apoptosis (programmed cell death) and RNA interference, both of which resulted in Nobel Prizes. Despite all of this research, very little has been known about the chemistry that *C. elegans* uses to communicate with its environment.



**Figure 1:** Developmental life stages of *C. elegans*. Figure from <http://www.wormatlas.org/>

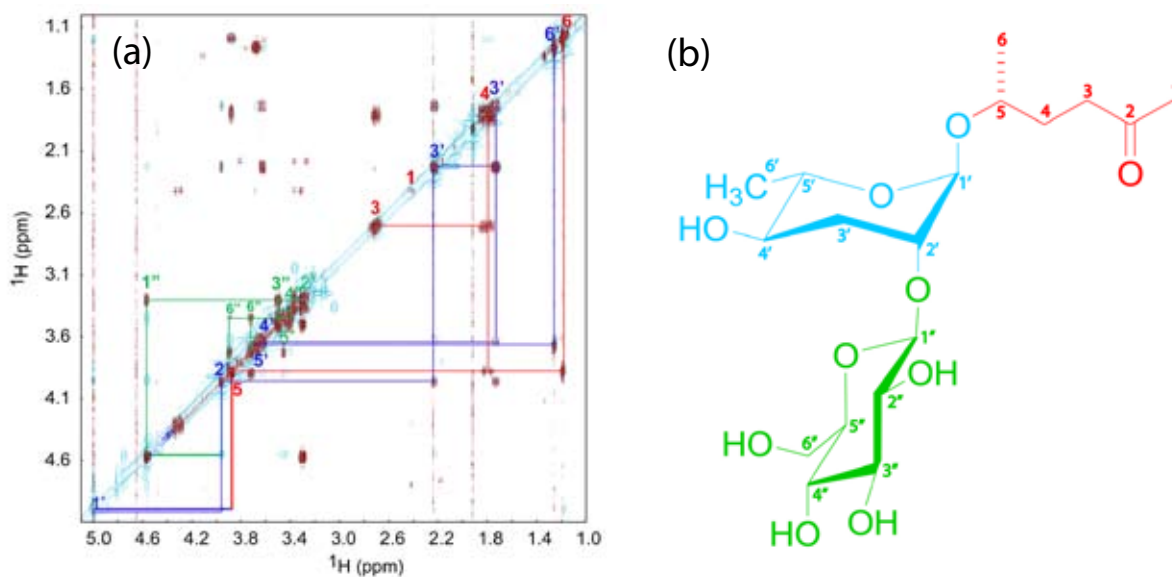
*C. elegans* grow in just 3.5 days from a fertilized egg to a sexually mature adult by going through four larval stages (L1-L4). The worms come in two sexes: male and hermaphrodite. Hermaphrodites make both eggs and sperm and can self-fertilize. Hermaphrodites can mate with males to produce over 1000 progeny

with an increase of genetic diversity. In contrast, if males are scarce, hermaphrodites will self fertilize, but the number of progeny is limited to a few hundred by the amount of sperm. Under conditions of low food and high worm density, *C. elegans* enter an alternate developmental stage called dauer (Figure 1). For several decades, researchers have known that worms secrete a dauer pheromone to sense their population density<sup>1</sup>, and the chemical identities of 3 different dauer pheromones were recently published<sup>2,3</sup>.

In 2002 Paul Sternberg's group at Caltech and HHMI also showed that hermaphrodites produce a chemical signal that attracts males<sup>4</sup>, and the goal of our study was to discover the *C. elegans* mating pheromone. The complete scientific story of this work has been recently published<sup>5</sup> and are just summarized below.

## RESULTS/DISCUSSION

*C. elegans* eats bacteria (*Escherichia coli*), and large amounts of *C. elegans* can be grown in liquid culture by adding both worms and *E. coli*. Furthermore, starting the culture with fertilized eggs can synchronize the worms' growth cycle. Because we wanted to isolate a chemical that was secreted by worms, we began our study by growing standard liquid cultures of worms and bacteria and analyzing the liquid supernatant. This preparation was difficult to use, because the bacteria produce many small molecules, making the "haystack" too big to find the "needle". Therefore, we developed a way to separate worms from bacteria and to incubate the hermaphrodites in water to isolate their released chemicals. This "worm water" was collected at each of the defined developmental stages (Figure 1) and tested for its ability to attract males. In collaboration with Jagan Srinivasan in the Sternberg laboratory, we found that worm water from sexually mature young adult and adult hermaphrodites attracted males, but at earlier developmental stages there was no response.



**Figure 2:**

The NHMFL 1-mm HTS probe was important for this study. We used about 0.4 L of culture to obtain the material for the COSY and NOESY spectra (A) that led to the identification of one of the mating pheromones, ascr#4 (B). Previous studies utilized over 300 L to identify the first dauer pheromone.

Using young adult worm water, Fatman Kaplan and Ramadan Ajredini in the Edison lab then conducted a series of chemical fractionations, followed by bioassays. Male *C. elegans* were essentially the "detector" in this purification. At one stage in the purification, we lost all the activity but could regain it by adding all the fractions together. This showed that there was more than one chemical involved in attracting males.

The Mag Lab 1-mm HTS probe<sup>6</sup> was very important for this project, because we did not need to produce large amounts of sample. Previous studies to identify the first dauer pheromone required several 300 L liquid cultures<sup>2</sup>. Because of the extremely high sensitivity of the 1-mm HTS probe, we were able to start with just 0.4 L of liquid culture. We analyzed chemical fraction "A" that that was necessary but not sufficient for activity; if we took fraction "A" away, all activity was lost, but it alone was not active.

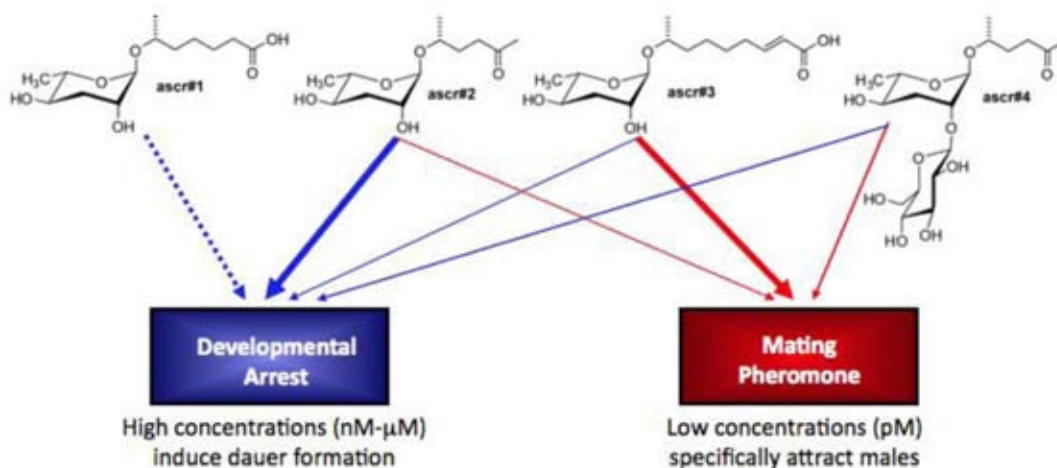
Figure 2A shows an expansion and overlay of 2D NOESY and COSY NMR data of fraction "A" from the 1-mm HTS probe. The structure of the major chemical in this fraction is shown in Figure 2B and is called ascr#4. The "ascr" stands for an ascaroside sugar (the cyclic part of the structure), and the "#4" indicates that it is the



fourth new chemical discovered in this group; the preceding three are the known dauer pheromones. Just when the Fatma and Cherian in the Edison laboratory had collected the NMR data from fraction "A", Frank Schroeder (Cornell University) came to give a seminar at UF. Frank was part of the team that identified two of the *C. elegans* dauer pheromones called ascr#2 and ascr#3<sup>3</sup>, and we realized at that point that the mating pheromone we were finding was very similar to the dauer pheromones.

The Schroeder lab synthesized all of the different known ascarosides, and Jagan in the Sternberg lab tested them for male specific attraction. We were surprised to find that the known dauer pheromones, ascr#2 and ascr#3, were both active in attracting males. Ascr#3, in particular, is active at about 1 pM concentrations, so it is very potent. Both of these compounds attract males with a bell-shaped curve response: at low or high concentrations the effect is gone. We also tested for and found synergy, because of the observation that more than two fractions in our purification were required for activity.

We then tested for all the known ascarosides by using liquid chromatography-mass spectrometry with Peter Teal and Hans Alborn in the USDA laboratory in Gainesville. Hans found that all known ascarosides were present in very low concentrations in many of the fractions from worm water. When we combined synthetic compounds in the approximate ratios found by mass spec, we were able to reproduce the male mating response with natural material.



**Figure 3:**

*C. elegans* ascarosides have dual roles in male mating response and dauer formation.

This study was the first to link—via small molecules—two major behavioral traits in *C. elegans*: dauer formation and mating. At very low concentrations (picomolar), ascarosides tell males that there are hermaphrodites nearby and that they are ready to mate. Incidentally, hermaphrodites are not attracted to the signal at these low concentrations. At higher concentrations, hermaphrodites are repelled (but males are indifferent). At the highest concentrations (high nanomolar to low micromolar), the worms enter dauer, because the signal indicates that there are too many worms for the available resources (Figure 3).

This study also nicely demonstrates the synergy that is possible when new technology (e.g. HTS NMR probes) is coupled with important biological problems.

## REFERENCES

1. J.W. Golden and D.L. Riddle, *Science* **218**, 578-580 (1982).
2. P.Y. Jeong, *et al.*, *Nature* **433**, 541-5 (2005).
3. R.A. Butcher, *et al.*, *Nat. Chem. Biol.* **3**, 420-2 (2007).
4. J.M. Simon and P.W. Sternberg, *Proceedings of the National Academy of Sciences of the United States of America* **99**, 1598-1603 (2002).
5. J. Srinivasan, *et al.*, "A blend of small molecules regulates both mating and development in *Caenorhabditis elegans*," *Nature* In Press (2008).
6. W.W. Brey, *et al.*, *J. Magn. Reson.* **179**, 290-3 (2006).

## Next-Generation Fourier Transform Ion Cyclotron Resonance Mass Spectrometer: Report from a joint NSF/DOE Workshop

During January 2008, the National High Magnetic Field Laboratory (National Science Foundation) and the Environmental Molecular Sciences Laboratory (Department of Energy) staged a workshop, "Science Challenges and Design Concepts for the Next-Generation High-Performance FT-ICR Mass Spectrometer" at the Magnet Lab in Tallahassee, FL. Organized by Jean Futrell (EMSL) and Alan Marshall, the workshop was attended by 32 participants from the United States, Germany, Korea, Russia, Sweden, and The Netherlands. The program began with formal presentations including overviews (Futrell and Marshall), "Ion Simulations as a Guide to FT-ICR Performance" (Eugene Nikolaev, Russian Academy of Sciences), "High-Field ICR Magnet Design/Performance" (Gerhard Roth, Bruker), "Novel FT-ICR Instrumentation" (Ron Herren, FOM/AMOLF, The Netherlands), and "FT-ICR for Proteomics" (Ljiljana Pasa-Tolic, EMSL). The presentations were followed by discussion groups on magnet design, chaired by Tom Painter, instrumentation, chaired by Chris Hendrickson, and applications, chaired by Ljiljana Pasa-Tolic.



### SCIENCE DRIVERS

The workshop consensus is that a concerted effort to design, build, and test a new, high-field 21 T FT-ICR MS system is fully justified to advance the characterization and understanding of complex biological, chemical, and materials systems. Because many mass spectrometry applications are limited by discontinuous "steps" in resolving power, a 21 T instrument enables improvements that are transformative rather than incremental. For example, it becomes possible to distinguish between N-terminal and C-terminal peptide fragments in MS/MS experiments, to narrow the possible proteins to a single unique identification. Similarly, higher magnetic field will provide definitive resolution, identification, and quantitation of up to thousands of organic constituents of mixtures as complex as petroleum or biological fluids.

### ENGINEERING FEASIBILITY

Current superconducting persistent magnet technology makes it possible to develop and deploy a 21 T system in a 3- to 5-year time frame. A full systems design approach is essential to achieve optimum performance: e.g., high-level modeling is required to define plasma effects in ion motion and perturbation of ion motion by ion-ion interaction and ion-conductor interactions in all trapping, ion preparation and storage components, including the ICR cell itself. The latest generation of massively parallel supercomputers is now capable of carrying out the extensive modeling calculations in ICR cells of arbitrary geometry, ion source design, intermediate ion processing steps, and intermediate accumulation and storage stages.

The successful design and development of an integrated 21 T High-Field FT-ICR MS system is eminently feasible. However, to do so requires solutions to several major technical challenges. In particular, improvements

in ion formation and transfer efficiencies, effective ion injection into intense magnetic fields (the magnetic mirror problem), advances in understanding ion motion, control of ion motion and trajectories, high-sensitivity detection, and high-precision digitization and processing of signals are all required. All of these challenges can be solved but will require coordinated efforts and teaming by an international ensemble of expert modelers and experimentalists.

### SITING

The third charge to the workshop was to recommend where such instrument(s) should be placed to optimize successful implementation and usage. Workshop participants unanimously supported the development of such systems at national user facility laboratories (specifically, at the Mag Lab and EMSL) available to the broader scientific community for the following reasons:

*Expertise.* Most important, the Mag Lab and EMSL together offer unparalleled technical expertise in design, development, and operation of new FT-ICR instrumentation. Users of those facilities are attracted as much for the in-house expertise as for the instrumental capabilities.

*Cost.* Because much of the spectrometer (other than magnet) is custom-built in-house, the capital cost is lower by a factor of ~3. In addition, there is a major savings in the cost of service contracts with the use of national user facilities. Because most of the spectrometer is custom-built, troubleshooting, maintenance, and repair are inherently available in-house, representing major savings relative to a typical spectrometer service contract of 10% of the purchase price per year.

*Continuous upgrading.* Most mass spectrometry user facilities are predicated on purchase of major new equipment in the first year, and then not again until the project is renewed (i.e., every 5 years, if successful). In contrast, the Mag Lab and EMSL provide continuous upgrading of their instruments so that performance remains at the leading edge.

*Exceeding commercial instrument performance.* Commercial instruments are limited to techniques for which they hold patents, whereas national user facilities can implement the best practices developed by their staff and collaborating scientists, including vendors. In addition, whether new developments are first conceived in-house or externally, EMSL and the Mag Lab can implement them immediately, whereas others must wait (typically a couple of years) until a vendor brings out a new model that includes such improvements. Thus, EMSL and the Mag Lab typically provide lead instrumental capabilities not available elsewhere for 1-3 years.

*User program infrastructure.* Both the Mag Lab and EMSL are configured as external user facilities, with computerized logging of user proposals, on-site accommodation, and staff assigned to help users.

*Range of experiments.* Because 21 T FT-ICR instrumentation is a major capital investment, its capabilities should span the full range of important applications. No individual investigator program can cover that range. Because FT-ICR programs at EMSL and Mag Lab are highly complementary, the combination of the two facilities covers the entire range of applications projected by the Workshop.

*Cyber-connectivity.* Both EMSL and the Mag Lab provide for extensive capability for remote data reduction (and even instrument operation—one of Mag Lab's FT-ICR instruments has been operated from Birmingham, England).

*Outreach.* A major impact of the FT-ICR MS programs at the Mag Lab and EMSL is that they are providing pilot data for new entrants into the field. Those groups often go on to acquire their own instruments. Thus, unlike some other major user facilities (e.g., synchrotrons), which tend to attract mainly the same users from year to year, the cumulative number of FT-ICR MS external users increases steadily with time. Thus, national FT-ICR MS facilities not only serve the user base but also expand it. Such facilities also serve the broader educational outreach mission of supporting institutions. For example, the Mag Lab hosts an annual one-day Open House (4,600 attendees in 2008) as well as tours and classroom visits (e.g., ~10,000 middle school students per year) to increase its public outreach.

Copies of the full workshop proceedings and summary are available on request. Proposals for development of 21 T FT-ICR mass spectrometers for EMSL and the Mag Lab are being prepared for submission to multiple funding agencies later this year.

## Research shows programs for teachers make a difference



Over the past few years, the Center for Integrating Research & Learning has expanded its mission to include research on the effectiveness of its research experiences programs.

Research on 1999-2006 research experience for teachers participants has been completed, and preliminary data indicate that RET programs provide strategies and content that enable teachers to make changes in how they teach science. The data also indicate that such changes occur over the long term.

CIRL's research agenda will be expanded this summer to include investigating how girls make decisions regarding pursuing science as a career

path and decisions about high level science classes in high school. Two articles are being submitted to educational research journals and papers will be presented at three major educational research conferences.

### WORKSHOPS, CAMPS AND MORE

Summer for the Center for Integrating Research & Learning includes workshops, the research experiences programs for teachers and undergraduates, Girls in Science camps, and other activities that serve teachers and students.

A full schedule of workshops for elementary through high school teachers provided an opportunity for teachers to visit area laboratories and to translate the experiences into hands-on inquiry activities; QuarkNet/SuperNet provided advanced content and physics inquiry activities, with a focus on creating a community of physics educators across the country; and two sets of workshops for the Panhandle Area Educational Consortium expanded professional development opportunities for rural schools while enhancing teachers' knowledge of physics.

Thirty-three students participated in SciGirls I and II camps for middle school and high school girls, and Operation Filmmaker Goes Science for middle school students produced documentary films with a science focus.

Nineteen undergraduate students participated in the Summer REU program, working in labs at FSU, UF, and LANL.

Seventeen teachers participated in the RET program and worked on real-world research, expanding their understanding of the nature and processes of science. The experience changes how teachers think about science and about how science is presented in the classroom.

### MENTORSHIP IS ENDURING

In the spring, the lab hosted 14 middle-school students who worked with mentors to conduct research. The skills that students hone are ones that serve them well as they move through middle school to high school and college. While the program only lasts one semester, the results are long lasting.

One former middle school participant, Sharmini Pitter, says, "I can never say enough about how much the mentorship program meant to me. I am planning on going into graduate school in geochemistry, which was my subject in the mentorship program."

T. H. Dohrman reported that he is a successful businessman who started an Undergraduate Research Board at the University of South Florida. Of this he says, "Although I did not pursue a career in the





sciences, this experience helped me understand the importance of research in the modern world. Without this experience, I may not have worked so hard to get other undergraduates involved in research.”

Many scientists at the Magnet Lab spend countless hours working with students and teachers. The effects of experiences provided by committed scientists at the lab are incalculable.

As the academic year came to a close, Outreach Coordinator Carlos Villa reported that he reached more than 8000 K-12 students in and around the Tallahassee area. Villa is planning for “virtual classroom outreach” to Florida and other states to expand CIRL’s programming and provide outreach to remote locations. A pilot outreach with the Ohio Virtual High School is planned to determine how to best provide high-school students with a taste of the excitement of real-world science. Plans are being made to expand outreach to community groups in surrounding counties, such as Boys’ and Girls’ Clubs.

Recently, 14 students from a local middle school exhibited their research projects at the Magnet Lab with many scientists and staff asking questions and providing feedback. Part of a pilot science research class, the students worked with CIRL staff and scientists from the lab to learn more about data collection, display of data, and communicating results. This is the only science research class in this area, and students with an interest in science and technology and their parents have ensured the continuation of the class next year. CIRL expects to provide continued support for this program, which was developed by a former RET participant, David Rodriguez of Swift Creek Middle School. Rodriguez gives credit to the lab and to the program for providing a glimpse of how science is conducted in the real world. He translates this to his students through the elective class.

CIRL continues to look for ways to expand and enhance programming from establishing new programs and nurturing partnerships to finding ways to correlate outreach activities with new science standards. We continue to grow and find creative ways to support formal and informal science education.



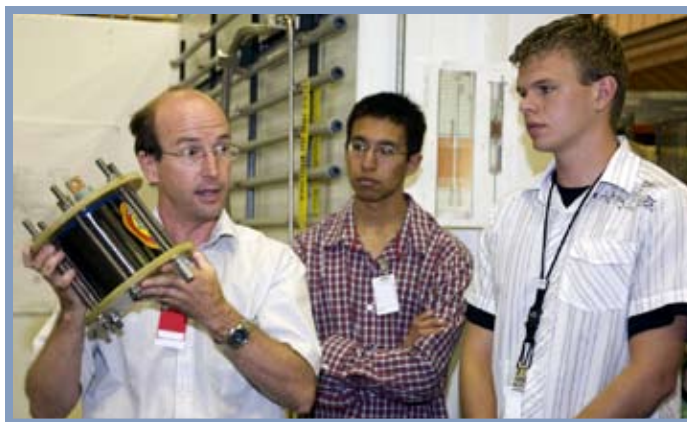
## Students enjoy summertime LANL tour

By Tatjana K. Rosev, LANL

Students touring the MST-NHMFL learned about magnetic fields, inertial storage motor-generators for high field pulsed magnets, and capacitor-driven pulsed magnets. The tour was part of the Summer Lecture Series sponsored by the LANL Institutes, Materials Physics Applications Division, and the Students’ Association.

The lectures are designed to present the innovative science at the lab to students, postdoctoral researchers, and staff. In the course of 18 talks and several site visits, participants had a unique opportunity to tour facilities and learn about the lab directly from top scientists.

Photo Credit: Sandra Valdez, Records Management, Media Services, and Operations



Marcelo Jaime shows students a pulsed electromagnet during the magnet lab tour. A new generation of this type of magnets is locally designed and assembled by a team led by the Mag Lab’s Chuck Swenson. The Los Alamos-born magnets, when driven by a 1.6 megajoule capacitor bank, deliver 25 millisecond-long pulses of up to 65 tesla.

## People



Collaborative groups based at the Tallahassee and Los Alamos branches of the Magnet Lab authored two of the year's most influential physics papers, according to the editors of the *Journal of Physics: Condensed Matter*. Each year, the journal selects a small group of its most groundbreaking and popular published papers, highlighting physics advancements and trends.

Magnet Lab Seaborg Postdoctoral Associate **Susan Cox**, based at the Pulsed Field Facility in Los Alamos, is first author on "Evidence for the charge-density-wave nature of the stripe phase in manganites," in which heat capacity measurements of manganite compounds were analyzed. Cox, LANL Fellow **John Singleton** and **Peter Littlewood**, who holds positions at Cambridge University and the Magnet Lab, collaborated with a group from Edinburgh, Scotland.



Magnet Lab Postdoctoral Associate **Haidong Zhou** is first author on "The origin of persistent spin dynamics and residual entropy in the stuffed spin ice  $\text{Ho}_{2.3}\text{Ti}_{1.7}\text{O}_{(7-\delta)}$ ," in which he showed that stuffing spin ices with extra spins appears to lead to new magnetic phases. In addition to its designation as a Top Paper, the work was presented as an invited talk at the International Conference on Crystal Growth held in Utah last year. Assistant Professor **Chris Wiebe**, Postdoctoral Associate **Youn-jung Jo**, Associate Scholar/Scientist **Luis Balicas**, Graduate Research Assistant **Jing Jing Qiu**, National Institute for Science and Technology (NIST) staff **Yiming Qiu**, **John Copley**, and **Jason Gardner**, **Peter Fouquet** at the Institut Laue-Langevin, and **Georg Ehlers** at the Spallation Neutron Source all collaborated on the project.

Aaron Dossey, Mag Lab external users **Spencer Walse** (USDA Laboratory) and **Oskar Conle** (Bolsterlang, Germany), and **Art Edison** won the 2007 Jack L. Beal Award for their paper on the identification of parectadial using the 1-mm HTS probe. The American Chemical Society and the Foundation Board of the American Society of Pharmacognosy give this annually for one of the outstanding papers of the year in the *Journal of Natural Products*. The paper is titled "Parectadial: A Novel Monoterpenoid from the Defensive Spray of *Parectatosoma mocquerysi*." Find it in the *Journal of Natural Products* *J Nat Prod.* **70**, 1335-8. (2007).



**Huan He**, a Ph.D. candidate in the Analytical Division of FSU's Department of Chemistry and Biochemistry and a member of the lab's Ion Cyclotron Resonance group, received a 2007-2008 FSU Graduate Student Research and Creativity Award. The award is based on "outstanding scholarly/creative productivity and national visibility as a graduate student at FSU." Only one candidate may be nominated from each academic department. He was recognized at the Spring Celebration of Excellence Ceremony and at the annual Research Recognition Dinner in April.

University of Florida physics professor **Mark Meisel** was named a 2008 American Physical Society Outstanding Referee. This highly selective award recognizes scientists who have been exceptionally helpful in assessing manuscripts for publication in the APS journals. The program will annually recognize ~130 of the 42,000 currently active referees, but in the inaugural year (2008) a larger group of 534 referees has been selected for Outstanding Referee designation.



Graduate Research Assistant **Myunggi Yi** (currently Postdoctoral Associate) of the lab's Nuclear Magnetic Resonance program is the 2008 recipient of the Dirac-Hellman Award for significantly advancing our understanding of biological systems through molecular dynamics simulations.



## People



**Alan G. Marshall**, the Robert O. Lawton Professor of Chemistry and Biochemistry at FSU and director of the Ion Cyclotron Program at the Magnet Lab, has been selected to receive the 2008 Ralph and Helen Oesper Award from the Cincinnati Section of the American Chemical Society. Eight of the past 26 awardees of the prestigious Oesper Award went on to win the Nobel Prize.

"Alan's receipt of the Oesper Award places him in an elite group of the world's best chemists," said Joseph Travis, dean of the FSU College of Arts & Sciences. "This recognition adds to Alan's enormous scientific reputation and reminds all of us how fortunate we are to count him a colleague at Florida State University."

The Oesper Award, which will be presented at a symposium at the University of Cincinnati in October, caps Marshall's prior national and international recognitions, including three American Chemical Society national awards, Spectroscopy Society of Pittsburgh Maurice F. Hasler Award, Pittsburgh Spectroscopy Award, American Society for Mass Spectrometry Distinguished Contribution Award, and the Thomson Medal of the International Society for Mass Spectrometry.

**Pinaki Sengupta**, a joint postdoc between the Magnet Lab Pulsed Field facility at LANL, the Condensed Matter and Statistical Physics group (T-11) and the Center for Non Linear Sciences (CNLS), has won two LANL awards. Sengupta won the LANL Postdoctoral Distinguished Performance Award for his body of work since arriving at LANL, and he won an honorable mention in the Leon Heller Postdoctoral Publication Prize in Theoretical Physics for his paper "Field-induced supersolid phase in spin-one Heisenberg models" by Sengupta and Batista, *Phys. Rev. Lett.* 98, 227201 (2007)



This spring and summer, EMR program Scholar/Scientist **Jurek Krzystek** spent three and a half months as an Invited Scholar/Researcher (Investigador Invitado) at the Institute of Molecular Science, University of Valencia, Spain, working with Prof. Miguel Julve in the area of coordination chemistry and magnetism of rhenium and other transition metals.

Through its nonprofit foundation, PBS&J donated \$15,000 to SciGirls, the two-week, hands-on summer camp run by the Mag Lab in partnership with WFSU-TV. SciGirls is designed to inspire girls ages 10-16 to pursue careers in science.

The **PBS&J** Foundation, Inc.

"Helping young girls experience the amazing world of science benefits the future of all science disciplines," said Charles Redding III, senior vice president of PBS&J. "More importantly, the lives of the girls who participate in these camps will be enriched, and Tallahassee's major universities and exceptional community college offer the perfect opportunity for them to further their knowledge," said Redding.

SciGirls started in 2006 for rising 6th, 7th and 8th grade- girls, and was expanded in 2007 to include SciGirls II for returning campers and rising 9th and 10th graders. The Magnet Lab covers the costs of SciGirls I campers, but SciGirls II costs \$300 per participant.

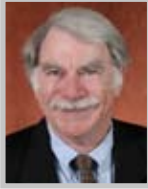
PBS&J ([www.pbsj.com](http://www.pbsj.com)) is an employee-owned firm that provides infrastructure planning, engineering, construction management, architecture, and program management services to public and private clients. The firm established the nonprofit PBS&J Foundation to provide the corporation's subsidiaries the tools and ability to promote and support education and other community-building endeavors.



# WHO RUNS WHAT: MAGNET LAB USER PROGRAM DIRECTORS



**Tim Cross:**  
NMR User  
Program  
Director



**Alan Marshall:**  
ICR program  
Director 1993-  
present



**Scott Hannahs:**  
DC Facilities and  
Instrumentation  
Director



**Eric Palm:**  
DC User  
Program  
Director



**Art Edison:**  
Director  
of AMRIS,  
University of  
Florida



**Chuck Mielce:**  
Head of Pulsed  
Field Facility  
User Program



**Marcelo Jaime:**  
Interim Center  
Leader, LANL,  
Pulsed Field  
Facility



**Neil Sullivan:**  
High B/T  
User Program  
Director

## Hill tapped to direct EMR program

Longtime Magnet Lab collaborator Stephen Hill has accepted a position as director of the Electron Magnetic Resonance (EMR) user program and as an FSU physics professor, cementing a relationship that has been building since Hill's postdoctoral work with the lab nearly 14 years ago. He began work on August 8.

Hill comes to the lab from the University of Florida, where he was an associate professor of physics and a Magnet Lab affiliate. He said he's looking forward to strengthening the connection between his own considerable international base of collaborators and the Magnet Lab's established user community.

"My first stop in the U.S. after my Ph.D. was Tallahassee, when I spent two years working with Jim Brooks. I've been coming back ever since," said Hill, who received his doctorate from the University of Oxford. "I look forward to both helping to integrate those communities more fully and to conducting my own research, which fits in very well with what's going on at the lab," said Hill.

A search committee led by outgoing Interim EMR Director Peter Fajer tapped Hill for the leadership position. Magnet Lab Director Gregory Boebinger said he's grateful for Fajer's leadership over the past two years.

"I give my heartfelt thanks to Peter for his service as interim director when we needed him most, during which time he and his colleagues returned the Mag Lab's EMR program to prominence and great promise," said Boebinger.



**Stephen Hill:**  
EMR User  
Program Director

## Merry Ann Johnson Retires

Merry Ann Johnson, long the Instrumentation and Operations and User Program coordinator working with former DC Field Facility Director Bruce Brandt and an integral part of the Magnet Lab experience for many users, was one of the Magnet Lab's earliest and longest-serving employees. She retired earlier this spring, leaving behind a network of users long familiar with her ready helpfulness and endless supply of peanut M&M's.



Merry Ann has always been as passionate about her loyalty to the Magnet Lab and its users as about her enthusiasm for FSU football and other Tallahassee institutions. She's persistent too; she started in the early 1990s trying to get road signs directing motorists to the Magnet Lab on streets ranging from Interstate 10 to Roberts Road. And I think the last ones that weren't finally refused were installed in 2005 or so.

Merry Ann and I began working together when one entered the Magnet Lab by a long wooden walkway that passed what is now the computer support offices and electronics shop to a stairwell emergency exit. Exterior door keys were made of metal and worked by turning a lock mechanism. I am grateful for her contributions to the Magnet Lab as a whole, the Instrumentation and Operations Group, the Users Program, and to me. I wish her well as retirement gives her much more time to spend with her grandchildren and many craft projects."

## Comments by Bruce Brandt

"Merry Ann came to the Magnet Lab in the early days, when everyone had a rather broad job description. She not only kept the I&O Group organized, she also organized the User Group (anyone who might be interested in being a Mag Lab user) meetings and the Users Committee meetings. She had experience organizing conferences and knew how to get support from the City of Tallahassee to pay for shuttle buses, worked with hotels to get special rates for visitors and conferees, made sure that the meals and refreshments were high quality and reasonable cost, greeted participants warmly, and often helped clean up afterwards.

## Science Starts Here

### Chris Ramsey

**POSITION:**

Postdoctoral Research Associate  
Department of Physics,  
University of Central Florida

**TIME AND ROLE AT THE MAGNET LAB:**

Graduate student under Naresh Dalal,  
2000-2004

**CURRENT WORK:**

"I study molecular magnets, primarily single-molecule magnets, which are about a billion times smaller than a basketball. My goal is to understand how quantum mechanics affects the magnetic properties of these molecules."

"My most recent work was performed with two long-time Mag Lab users: Enrique del Barco, my postdoc advisor at the University of Central Florida, and David Hendrickson (UC San Diego); and Mag Lab faculty member Steve Hill. In our paper titled "Quantum interference of tunnel trajectories between states of different spin length in a dimeric molecular nanomagnet," we studied a wheel-shaped molecule that behaves like two interacting single molecule magnets. We showed that the two halves of the molecule can simultaneously reverse their poles under special conditions. In the future we hope to exploit this phenomenon to perform computer operations on a single molecule."

"Enrique and I were very happy to form a University of Central Florida/University of Florida connection through this work. It seems like the Mag Lab has made Florida the place to be for research in magnetism."

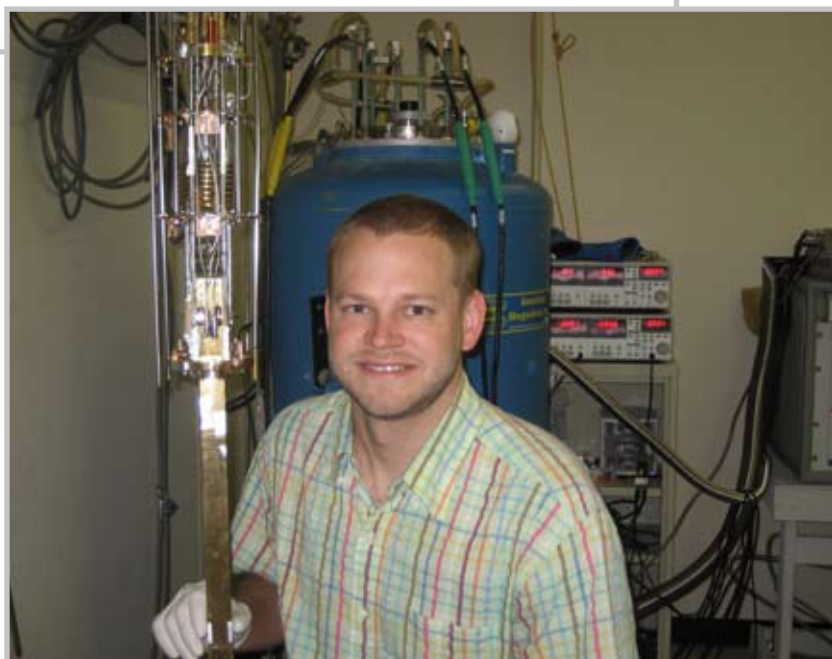
**IN HIS WORDS:**

"The Mag Lab is such a collaborative environment that you cannot spend time there without recognizing the value of working with other scientists. Collaboration can often turn a good publication into a major breakthrough."

**HOW MENTORS MAKE A DIFFERENCE:**

"There are two Mag Lab scientists who have really inspired me. The first is my Ph.D. adviser, Naresh Dalal, who taught me how to be a competitive scientist. Even while busy as the chairman of the chemistry department, Naresh always had time to discuss science, football, or life. I hope to have the same approach to managing people in the future."

"My second inspiration is Steve Hill, whose career I have followed from nearly the beginning. Steve is a model for the amount of dedication and ingenuity it requires to make a name for yourself as a young scientist."



**"I study molecular magnets, primarily single-molecule magnets, which are about a billion times smaller than a basketball."**

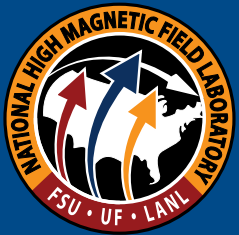
*"Science Starts Here" showcases young scientists whose career paths have been greatly shaped by their experiences at the Magnet Lab.*

SUPPORTED BY: THE NATIONAL SCIENCE FOUNDATION

1800 EAST PAUL DIRAC DRIVE  
TALLAHASSEE, FL 32310-3706

TEL: 850 644-0311  
FAX: 850 644-8350  
[www.magnet.fsu.edu](http://www.magnet.fsu.edu)

*Non-Profit  
Organization  
U.S. Postage  
PAID  
Tallahassee, FL  
Permit No. 55*



SUPPORTED BY: THE STATE OF FLORIDA