NATIONAL HIGH MAGNETIC FIELD LABORATORY

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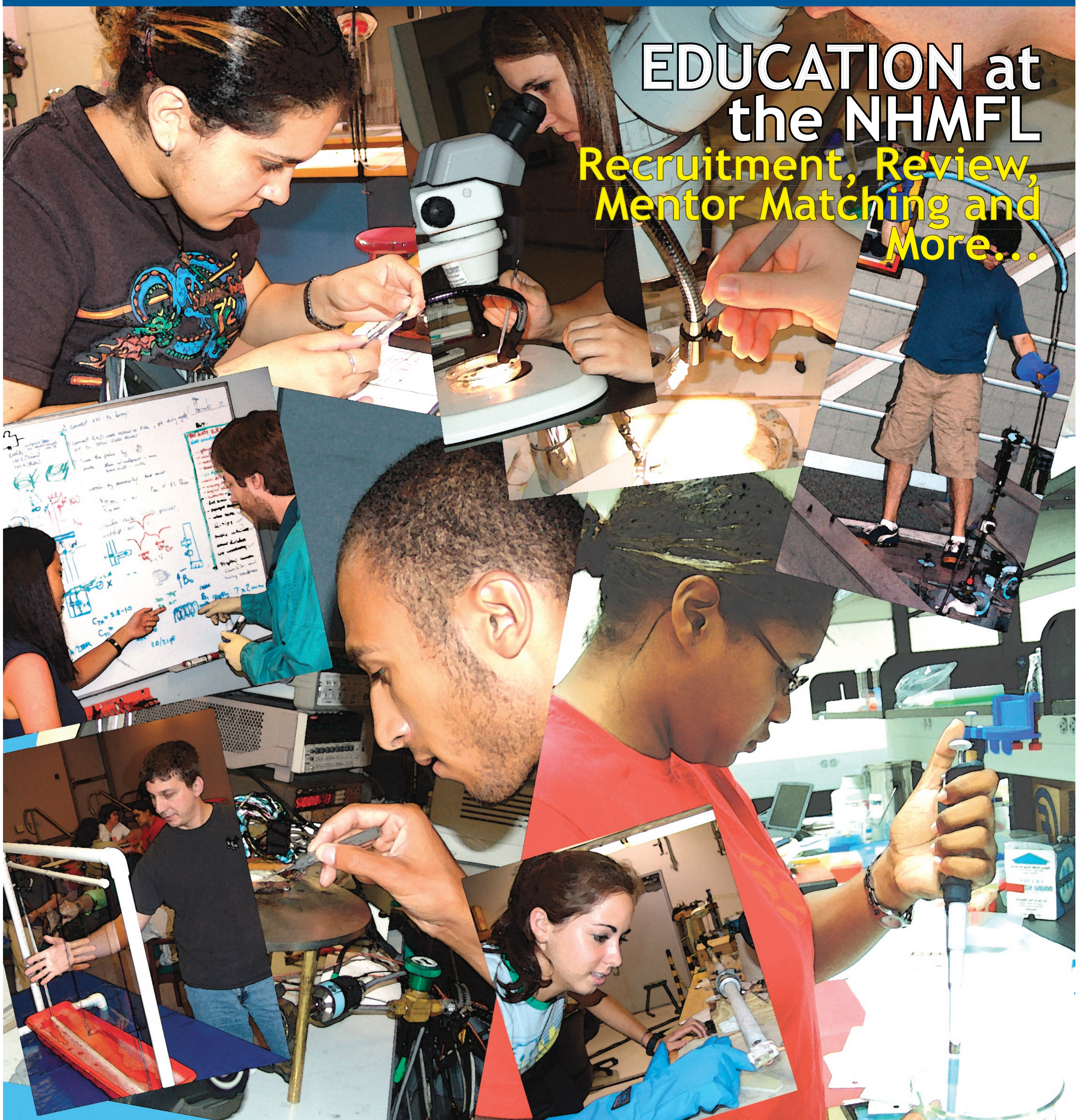

EDUCATION at the NHMFL

Recruitment, Review, Mentor Matching and More...

OPERATED BY: FLORIDA STATE UNIVERSITY • UNIVERSITY OF FLORIDA • LOS ALAMOS NATIONAL LABORATORY

NHMFL REPORTS

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FROM THE DIRECTOR'S DESK

Greg Boebinger

If the first quarter of my tenure as Director of the Magnet Lab foreshadows the years ahead, we are ***ALL*** in for a wild ride…but "wild" is a good thing. There are several notable events to share with readers. Let me first acknowledge and thank NHMFL colleagues, users, members of the External Advisory Committee, our FSU, UF, and LANL institutional leaders, and our NSF program managers, for their support, responsiveness, candor, ***and patience*****,** during the transition.

In mid-May, the National Science Board (NSB) accepted the recommendation of the National Science Foundation to **extend the award for operation of the NHMFL for two additional years**—through December 31, 2007. We were certainly prepared—even eager—to submit a renewal proposal by the end of this year, but the extension allows us time to refine our vision for the future of the laboratory and to incorporate ideas contained in the upcoming **report by the National Academy of Sciences Committee on Opportunities in High Magnetic Fields.** This report is due to be released later this year and is expected to address the current state and future prospects of high-field magnet science and technology in the United States; to assess the current status of U.S. high-field efforts in the international context; to identify particularly promising multi-disciplinary areas for research and development with respect to high magnetic fields; and to discuss and prioritize any major new initiatives in the construction of high-field magnets for the coming decade. As part of their discovery, the NAS committee visited the laboratory for two days in December 2003. We are looking forward to their report.

On the heels of the NSB decision, on May 25-27, the recently reconstituted **NHMFL External Advisory Committee** met in Tallahassee to assess the "State of the Laboratory" and to offer insights and guidance on scientific opportunities, user facility operations, and the three-institutional NHMFL partnership. The committee held fruitful discussions with Pete Nanos (Director of LANL), T.K. Wetherell (President of FSU), and Win Phillips (Vice President for Research at UF) and noted in their report the critical nature of inter-institutional support to the future growth and stability of the laboratory. We are sincerely grateful for the outstanding support we continue to receive from FSU, UF, and LANL and are indebted to the members of the EAC committee for their time and commitment. I am very pleased to recognize them in this space, and to thank them publicly for their service:

Science—Condensed Matter Members

- Meigan Aronson, University of Michigan (2004 Meeting Chair)
- Dimitri Basov, University of California, San Diego
- Paul Chaikin, Princeton University (Congratulations to a new National Academy of Sciences member!)
- George Crabtree, Argonne National Laboratory
- Rui Rui Du, University of Utah
- Donald Gubser, Naval Research Laboratory
- William Halperin, Northwestern University
- Frank Steglich, Max-Planck Institute for Chemical Physics of Solids
- Nai-Chang Yeh, California Institute of Technology

Science—Biological & Chemical Members

- Anthony Cheetham, University of California, Santa Barbara
- Jean Futrell, Pacific Northwest National Laboratory
- Robert Griffin, Massachusetts Institute of Technology
- David Hendrickson, University of California, San Diego
- Stanley Opella, University of California, San Diego

Magnet & Magnet Materials Technology Members

- Alexis Malezomoff, American Superconductor Corp.
- Ronald Scanlan, Lawrence Berkeley National Laboratory
- Albert Zeller, Michigan State University

User Committee Chair, Ex Officio

- W. Gilbert Clark, University of California, Los Angeles (Represented at the May 2004 EAC by Chuck Agosta, Clark University)

As we were catching our breath following the EAC meeting, we learned that the Florida Legislature and Governor Jeb Bush had approved the one-time **$10 million appropriation to address urgent infrastructure needs at the laboratory**. This much-needed supplemental funding sends a very powerful message of Florida's continuing support to the National Science Foundation and strengthens our position during the next renewal. On page 7, DC Field Facility Director Bruce Brandt describes how $7.5 million of the new support will be used to improve magnet power supplies and cooling systems, and to build additional space for new user instrumentation and staff research. The remaining $2.5 million will be spent at UF, split about equally between the High B/T User Facility and the Advanced Magnetic Resonance Imaging Facility. A new high field superconducting magnet is planned for the High B/T laboratory, and a new 600 MHz wide bore imaging magnet will be purchased for AMRIS. Both research facilities will also see other improvements that enhance capacity and user operations. In this era of many competing interests and tight budgets, extraordinary collaborative efforts were required by the joint UF and FSU leadership, by the local legislative delegation, and by my predecessor Jack Crow to secure this additional funding.

"We are confident that the transition in leadership will continue and further advance the established pre-eminence of the NHMFL in magnetic field-based scientific and engineering research, in pioneering magnet technology, as a national and international user facility, and as an important resource for the State of Florida and the Cities of Tallahassee and Gainesville for promoting scientific education and outreach."

Report of the External Advisory Committee, May 2004

Throughout the process, I was reminded again just how ***absolutely imperative*** it is for members of the science and engineering communities to be able to communicate how research, science, and technology drive economic growth and underpin developments that will improve the quality of life for generations to come.

And to celebrate a key date in our past! **A decade ago, on June 22, 1994, the first DC resistive magnet designed and built by the NHMFL was completed and reached a peak field of 27.1....breaking the previous world record by 2 teslas.** This was the first of numerous world records that the NHMFL has achieved, including, among others, the 33 T resistive magnet in 1996, the 25 T Keck magnet in 1998, the 60 T long-pulse magnet in 1998, the 45 T Hybrid in 2000, and the 65 T user magnets in our pulsed magnet program in late 2003....

These magnets have, over the past decade, played a critical role in establishing the NHMFL as the leading facility for high-field research. In so many ways, we look forward to the next 10 years and beyond....

Rock and roll

Greg Boebinger

FROM THE CHIEF SCIENTIST'S DESK

J. Robert Schrieffer

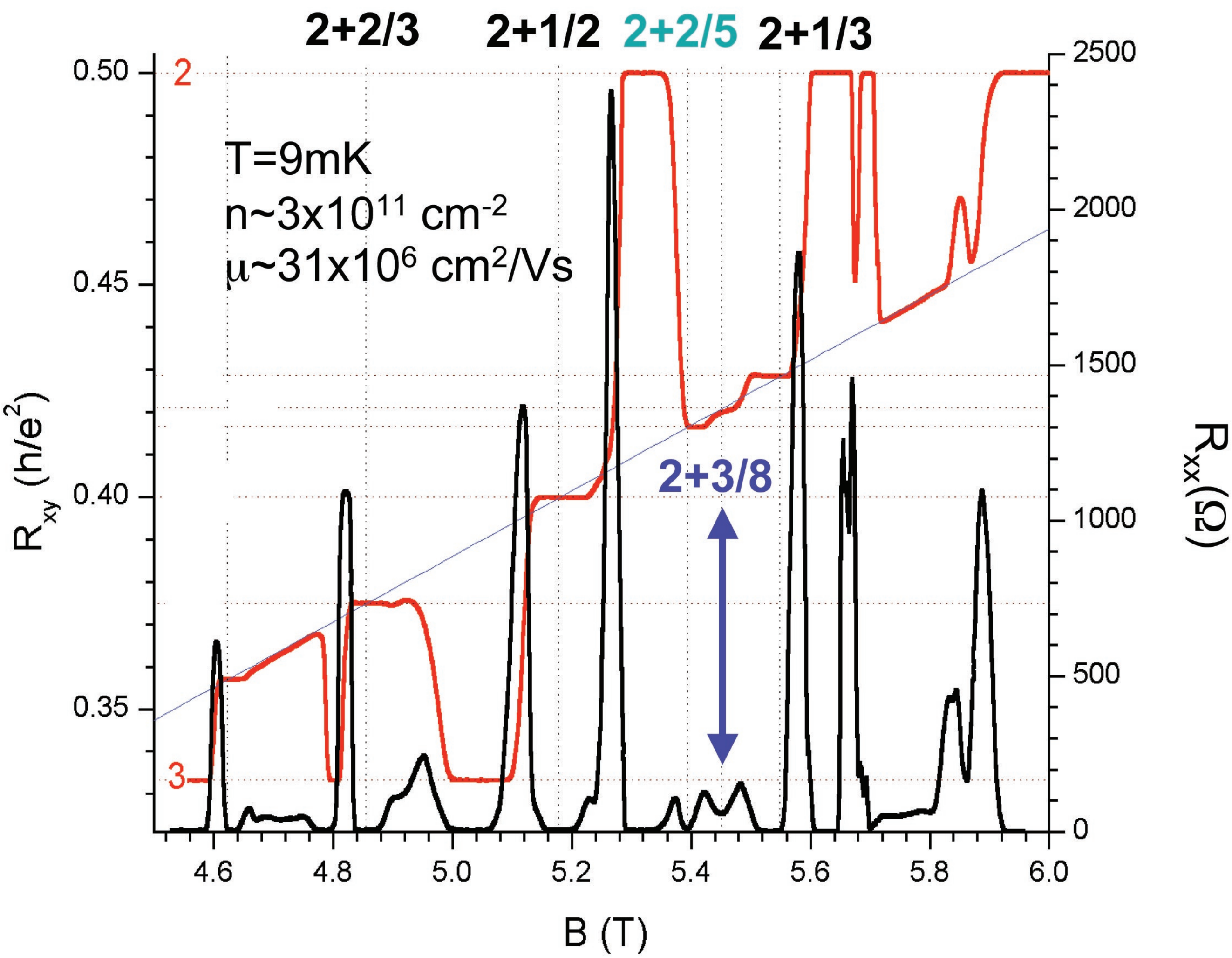
Two-dimensional electron systems continue to reveal new science as researchers push the limits of experimental parameters to lower temperatures. A unique aspect of the NHMFL is its commitment to providing the extremes of parameter space, i.e., pressure, magnetic fields, and temperature. The success of the NHMFL High B/T Facility located at the University of Florida in Gainesville is an example of the laboratory's commitment to this objective.

New Results for Nearly Degenerate Quantum Phases in Two-Dimensional Electron Systems

J.S. Xia, University of Florida, Physics and NHMFL
W. Pan, NHMFL and Princeton University, Electrical Engineering
C. Vicente, University of Florida, Physics and NHMFL
E.D. Adams, University of Florida, Physics and NHMFL
N.S. Sullivan, University of Florida, Physics and NHMFL
H.L. Stormer, Columbia University, Bell Labs, Lucent Technologies
D.C. Tsui, Princeton University, Electrical Engineering
L.N. Pfeiffer, Bell Labs, Lucent Technologies
K.W. Baldwin, Bell Labs, Lucent Technologies
K.W. West, Bell Labs, Lucent Technologies

Interesting new results have been obtained from measurements of a two-dimensional electron system at the intersection of the region between the electron liquid state corresponding to the lowest Landau levels and the charge density wave or liquid crystal-like states at high Landau levels. The recent data was obtained at very low temperatures (sample temperatures as low as 9 mK) for a very high mobility 2D electron system. The results show strong evidence for new fractional quantum Hall effect (FQHE) states that compete with the reentrant integer quantum Hall effect (RIQHE) states.

The sample studied had an electron density of 3×10^{11} cm^{-2} with a mobility of 31×10^{6} cm^2/Vs. The measurements reveal well-quantized FQHE states at filling factors of ν= 2+1/2, 2+1/3, and ν= 2+2/3 in coexistence with the RIQHE, and significantly a new FQHE state at ν= 2+2/5. There is also evidence for a second even-denominator FQHE state at ν= 2+3/8.



The figure shows the diagonal resistance and the hall resistance between filing factor ν=2 and 3 as measured at 9 mK. The most unusual feature is that the Hall trace of R_{xy} instead of moving monotonically from $h/3e^2$ to $h/2e^2$ returns to the value of the neighboring IQHE plateaus. These are the features expected for RIQHE states. Fully developed FQHE states are observed at ν= 2+1/2, 2+1/3, and 2+2/3, all with wide Hall plateaus. There is also a clear Hall plateau at ν=2+2/5 with a vanishingly small R_{xx}. A new even dominator FQHE state is appearing at ν=2+3/8.

From the temperature dependence of the new ν=2+2/5 state, one infers an energy gap of 70 mk. This is much smaller than that observed of the gap for ν= 2+1/3. The origin of the 2+2/5 state is not clear, as within the composite fermion model, the traditional 2+2/5 state is unstable, and numerical studies by Morf and d'Ambrumenil indicate that no hierarchical daughter state of the 2+1/3 state is stable between 2+2/3 and 2+1/3. The results strongly suggest that the new 2+2/5 state is not a conventional FQHE state.

Bruce Brandt, Director

Major Facility Upgrades – *Thanks to New State Funding*

The DC High Field Facility in Tallahassee has received $7.5 M in State of Florida funds to improve the magnets' power supplies and cooling systems, and to build additional space for new user instrumentation and staff research. (See "From the Director's Desk" on page 3 for information about the grant.) The "wish list" of upgrades has been accumulating for a long time. Suggestions have come from users, who always want to run longer at higher field, staff members who have had a hard time finding parts for ten year old equipment, and magnet operators, user support scientists, and instrumentation engineers who have had ideas about how things could be improved. So, how can we make the DC Facility even better?

The first step has already been taken. The Distributed Control System by which magnets are selected, controlled, and cooled was replaced with a new system that can accommodate many more controlled items. (See description of DCS Upgrade on p. 9)

The next step will be to replace our unreliable power transformers with new ones with current and voltage ratings high enough for 30 years of power supply and magnet improvements. The immediate benefit will be increased reliability for everyone and increased time at high fields for those who hold fixed fields for long times. NMR, heat capacity, far-infrared spectroscopy, and temperature sweep users will notice the biggest difference in performance. No more will such users have to ramp down from the maximum field after each hour of running. They can sit until the end of their shift, or until the capacity of the cooling system is exhausted; which brings us to the next item.

The cooling system's ability to remove heat from the magnets must be increased to allow magnets to sit at full field for 8 hours instead of the 6 or fewer hours that are now possible. We expect to purchase additional chillers, more chilled water storage tanks, or some combination of both. More subtle improvements to the cooling system are needed to move heat out of an operating magnet faster in order to lower its operating temperature and extend its useful life.

The circuit boards that control the operation of the rectifiers that provide the basic muscle for our magnet power supplies are of a discontinued design. Newer designs with more sophisticated controls are available that will bring the rectifiers back up to the state of the art and provide quieter power to the magnets. Users will be able to measure smaller signals with the reduced magnet ripple.

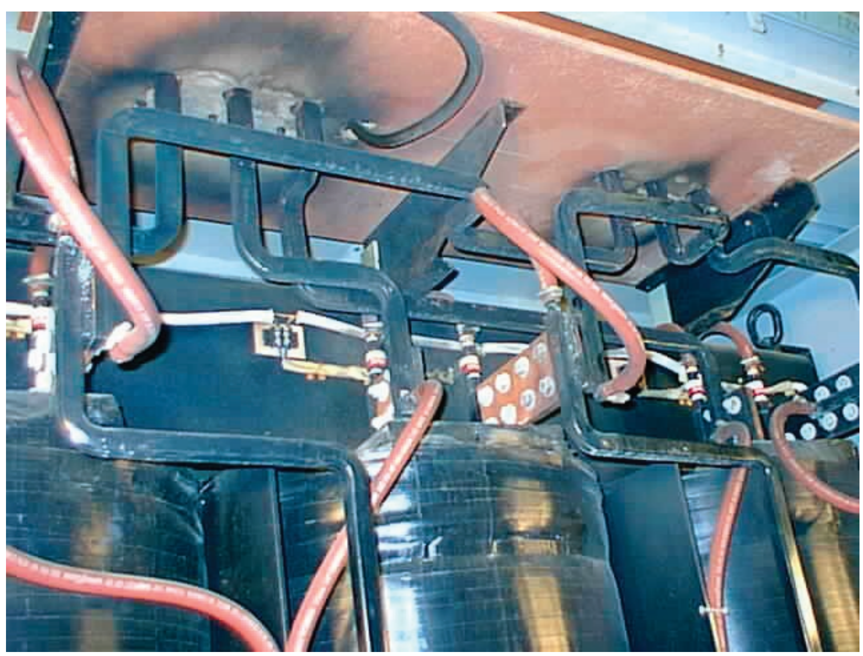
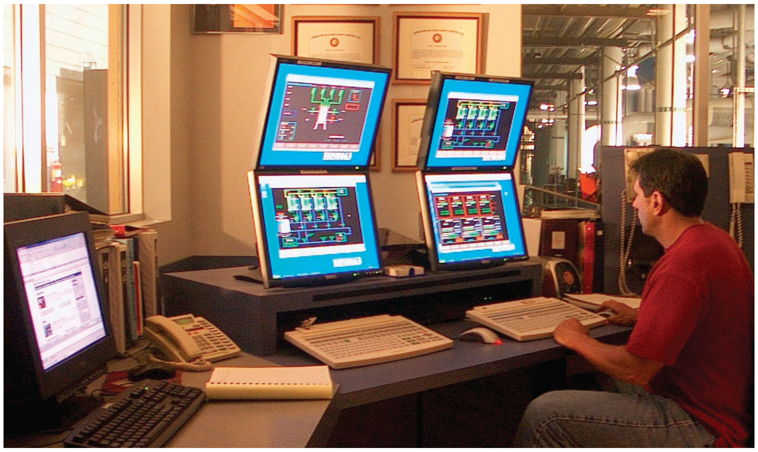


Figure 1. Burns caused by high voltage arcs in transformers.

We will also begin the process of increasing the power of our magnets. Voltage increases of up to 20% are possible at reasonable cost, yielding up to 10% increases in magnet fields. Current increases over about 10% appear to be expensive, but would also give users increased field. The fields delivered depend strongly on the choice of magnet design. Magnet design choices also affect the measurements that can be done because those measurements are affected by the bore size, whether the magnet is a single solenoid or split solenoid with a gap between the halves, the distance from the field center to the outside of the magnet, field homogeneity, and field stability. Some experiments cannot be done without the highest possible field, which is provided only by the four power supply hybrid. Decisions about the desired future mix of magnets and measurements will also constrain the choices along the power supply and cooling system upgrade paths.

The work that we have done to date to analyze our needs has been sufficient to identify possible solutions and budgetary estimates of cost. Now we must dig into the details.



Here is the plan:

Now through October, 2004 we will determine:

- The limits to upgrading the existing power components and cooling system
- The limits on increasing the voltage or current of powered magnets of known and proposed designs
- The capital and long term operating costs of identified options
- The scientific impact of identified options

November, 2004:

- Determine the path and schedule for upgrading power and cooling systems through 2016
- Request proposals for transformers
- Request proposals for cooling system improvements
- Request proposals for rectifier controls
- Set the budget for and complete the specifications of the User Services Building
- Design and install components needed to increase power supply voltage

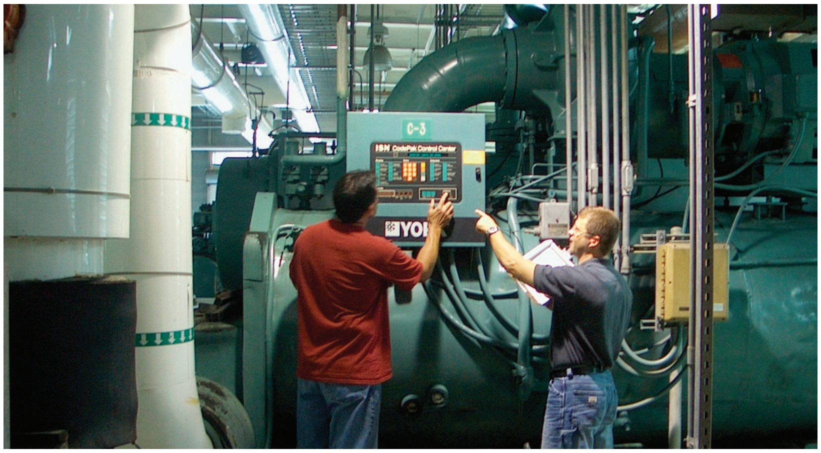
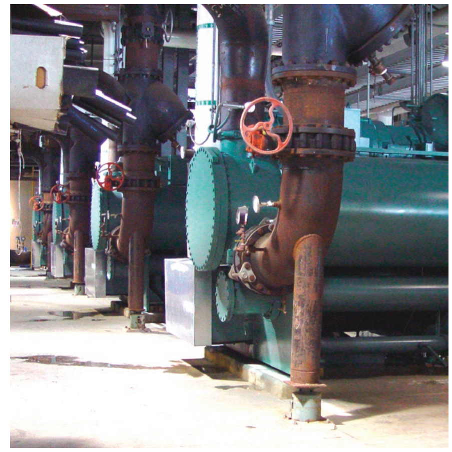
Throughout 2005:

- Select manufacturers for and order transformers, cooling system components, and rectifier controls
- Work closely with manufacturers on design, manufacture, and delivery of ordered equipment
- Work with FSU major projects team and architects on design and construction of User Services Building
- Design, purchase, and install power supply components that are needed to increase the output voltage and/or current

March 2006 (regular maintenance period):

- Install new transformers, new control system, increased voltage
- Install first components of expanded cooling system

Consultants have been hired to help us analyze the transformers, other power supply components, and the cooling system. People within the NHMFL are tackling the magnet design and scientific questions. We are excited about the prospects and look forward to making the users' dreams real.

Magnet Plant Control System Upgrade

by Bryon Dalton

In mid-2000, John Kynoch and I began working in earnest on a project I had started with Sean Maney in 1999. The distributed control system (DCS) that controls the magnet power supplies and magnet cooling water system in the DC High Field Facility needed to be replaced. The DCS was of an early 1980s design, had been upgraded once, but was now at the end of its useful life. All the circuits were full, data flow was slow, hardware and software could be purchased from only one vendor, the manufacturer had stopped making new parts in 2000, and support would stop in 2007.

The new DCS contains all the old timing and control circuits, plus several hundred more—a 60% increase that will permit us to expand our facility in the future without purchasing a new control system. Installation of new plant equipment (see Bruce Brandt's "Attention Users" on page 7 for some examples) will require that we purchase Input/Output boards and signal conditioning nests and add wiring, but that is all.

The new Yokogawa CS3000 DCS is built with a more open architecture than its predecessor, with more available off the shelf software, equipment drivers, and instrumentation. The operator stations and servers are MS Windows based PCs. The old system required expensive, proprietary console style operator stations with custom parts. When one of the 500 MB operator console hard drives failed in January 2004, the replacement part cost $1,800 and caused magnet operations to stop for a day. The new system permits replacement of a hard drive in two hours for about $100. Other parts like the alarm printers (remember dot-matrix printers?) were similarly expensive and hard to get.

Another feature that users, managers, and other interested parties can use is the Web Monitoring Package. A person with the necessary permissions can use a web browser from any computer inside the NHMFL fire-wall to check on the status of the magnet plant or view graphs of magnet current, chilled water temperature, or anything else that the DCS measures.

The new DCS will definitely prove itself when we go through our infrastructure upgrade, since we will be able to readily add Input/Output and control logic with minimal expense, and with proven technology and expertise.

EDUCATION at the NHMFL
-Recruitment, Review, Mentor Matching & More-

Six months of preparation has culminated in the start of another exciting summer at the Center for Integrating Research and Learning. A record 170 applications were received online for the **Research Experiences for Undergraduates (REU)** program. The Magnet Lab Florida State University site will host 16 talented undergraduates, three will reside at the University of Florida, and three are hosted at Los Alamos. The 22 students represent 17 universities from around the country. Two students are presenting their research at the Sandia National Laboratory Student Symposium in Albuquerque, New Mexico, in August, meeting one objective of the program: to encourage students to present at national conferences. In addition to all of the features of the REU program, an online REU Network has been established to provide a means through which students can keep in touch with one another and through which the Center can track students who update their profiles (see *http://reu.magnet.fsu.edu*).

Tallahassee Participants

Intern	University	Mentor
Colin Ashe	Northeastern University	Peter Fajer
Charles Bosse	University of Oregon	Jim Brooks
Christopher Bradley	Florida State University	Arneil Reyes
Ran Chang	University of Maryland	William Brey
Kianna Ferguson	University of Florida	Peter Fajer
Julia Giblin	Florida State University	Vince Salters
Jesus Gonzalez	University of Colorado-Denver	Chris Hendrickson
Sahara Hernandez	Smith College	Stan Tozer/Eric Palm
David Lehr	The Pennsylvania State University	Jim Brooks
John Macaluso	The Richard Stockton College of NJ	Luis Balicas
Jason Mantei	University of Wisconsin-Madison	Justin Schwartz
Shaun Murphy	Florida State University	Peter Kalu
Jonathan Sobota	Cornell University	Vladimir Dobrosavljevic
Ben Thayer	Florida State University	Vladimir Dobrosavljevic
Mary Warren	University of Massachusetts, Amherst	Justin Schwartz
Stephanie Wolin	Florida State University	Mike Davidson

Gainesville Participants

Intern	University	Mentor
Christine Amwake	Florida State University	Tom Mareci
Westin Kurlancheek	Harvey Mudd College	Alex Angerhofer
Lingyun Xiong	Duke University	Alex Angerhofer

Los Alamos Participants

Intern	University	Mentor
Jennifer Kirchhoff	Carnegie Mellon University	Scott Crooker
Winston Okraku	Occidental College	Victor Correa
Brian Haines	New York University	Charles Mielke

The **Research Experiences for Teachers (RET)** program began on June 14, a week after the REU program. Seventy applications were received for 14 positions, and teachers came from as far away as Hawaii to take part in the 6-week internship experience. The NHMFL RET program is unique among other national laboratories in that elementary school teachers are accepted into the program. CIRL's infrastructure supports the features of the program that help teachers translate their experiences into the classroom. The Center is proactive in dealing with rapid local, state, and national policy changes in science education. The RET program provides professional development for science teacher leaders who return to their schools and districts and provide workshops, activities, information, and strategies for other teachers. RET 2004 hosts teachers from four states who will share their experiences with others at local, regional, and national conferences. The education Web site now includes an RET Network that encourages continued interaction among teachers after they leave the program (see *http://ret.magnet.fsu.edu*). This new feature also provides the Center with the means to keep in touch with educators to further research into how the experience influences teacher practice and how it changes students' attitudes toward science.

RET

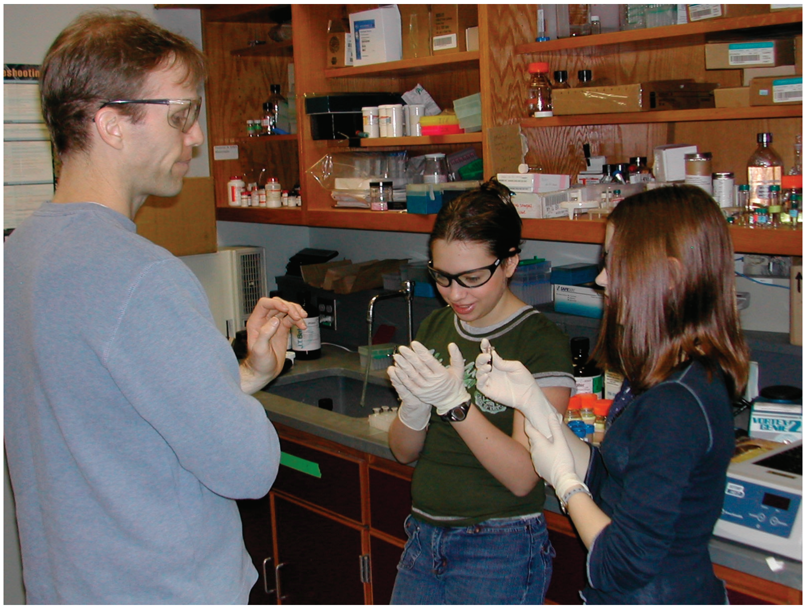
Tallahassee Participants		
Teacher	**School**	**Mentor**
Jeri Martin	Thomas L. Sims Middle School	Jim Brooks
Amber Matthews	Pre-Service	Jim Brooks
Farrell Rogers	Marshall Middle School	Jim Brooks
Lavonda Deale	Niceville High School	Mike Davidson
Josh Underwood	Deming Middle/High School	Mike Davidson
Nancy Reddick	Buck Lake Elementary	Philip Froelich
Marcy Steele	Ruediger Elementary	Philip Froelich
Rhonda Gordon	Pre-Service	Bob Goddard
Robert Krouch	Winston Park Elementary	Bob Goddard
Jodie Martin	Pre-Service	Bob Goddard
Soon Young Kim	Moanalua High School	Eric Palm
Amanda Underwood	Robertson County School	Eric Palm
Linda Ford	Seven Hills School	Justin Schwartz
Mark Johnson	Lake Weir High School	Justin Schwartz

In addition to REU and RET, 50 local teachers attended two 4-day summer institutes at the NHMFL during which they learned how to implement new strategies to introduce complex science concepts to elementary, middle, and high school students. Teachers constructed equipment for their classrooms and learned the content behind the technology. *The World Is Your Classroom II* and *Changing Perspectives II* deal with the processes of science, chemistry, physics, and life science.

Science Night at Borders Bookstore is a great success among children of all ages. On the first Wednesday night of each month, discovery-type activities are set up for children. The event has its own following and, at the children's request, CIRL will continue the activities through the summer months. Each activity has a reading that accompanies it and enhances the science concept covered.

In partnership with Florida A&M University's RIMS Project (Regional Institutes for Math and Science), CIRL is providing nine high school students brief research placements at the NHMFL. The two-week experience matches high school students interested in pursuing math and science majors in college with REU students and their mentors. This is a unique experience for high school students to work in a national laboratory and provides a mentor that is one step ahead of them in the career path.

Throughout the school year, Gina LaFrazza, Assistant Director; Carlos Villa, Outreach Coordinator; Dave Sheaffer, Webmaster; and Pat Dixon, Director of the Program interact with a large number of people. 6,000 schoolchildren took part in outreach activities during the 2003-2004 school year; more than 1,500 people toured the laboratory; and the annual Open House attracted over 2,500 visitors. We regularly receive letters, phone calls, and e-mails from students, parents, and other interested parties expressing their appreciation for the openness of the laboratory and the willingness of educators, scientists, researchers, administrators, and staff to share the excitement of real-world science. We are proud to facilitate these experiences and are planning new programs and activities to further engage students, teachers, and the general public.



For more information, contact Pat Dixon, who contributed this article. She can be reached at 644-4707 or pdixon@magnet.fsu.edu.

Insights into Enzyme Dynamics During Catalysis of Cyclophilin-A

E.Z. Eisenmesser, Brandeis University, Biochemistry
W. Lebeikovsky, Brandeis University, Biochemistry
D.A. Bosco, Brandeis University, Biochemistry
D. Kern, Brandeis University, Biochemistry
J. Skalicky, University of Utah, Biomolecular NMR Center (previously with NHMFL)
T. Logan, NHMFL and FSU, Chemistry and Biochemistry
O. Millet, University of Toronto, Biochemistry
D.M. Korzhnev, University of Toronto, Biochemistry
L.E. Kay, University of Toronto, Biochemistry

Though protein structure is correlated with function such ties to protein dynamics have only been made recently. Structural characterization using spectroscopic techniques such as X-ray crystallography and nuclear magnetic resonance can illuminate areas of a protein exhibiting multiple conformations under different conditions or bound with different ligands or inhibitors. NMR offers the distinctive advantage of being able to measure motions on a broad range of timescales from picoseconds to days. Our main interest is to bridge the gap between the three-dimensional static structure of a protein and its corresponding function by understanding the motions it exhibits, e.g., dynamics. We have been characterizing the dynamics exhibited by the enzyme cyclophilin-A (CypA) using NMR and have focused on those time scales relevant to catalysis, namely the micro-milliseconds regime.

CypA exemplifies one of three classes of prolyl-isomerases that also include the FKBP-binding proteins and the parvulins such as pin1.[1] Beyond its involvement in protein folding, often catalyzing the rate-limiting step of prolyl-isomerization, CypA is the target of the immunosuppressive drug cyclosporin. CypA also plays a role in HIV virulence, where it has been shown to interact with at least two HIV proteins that include the Capsid protein and VPR.

With the recent advent of several Carl-Purcell-Meiboom-Gill (CPMG) pulse sequences, molecular motions in the micro-millisecond time scale can be probed with a much higher sensitivity than was previously possible.[2] Briefly, by altering the time delay between CPMG refocusing pulses and measuring the resonance intensity in the corresponding 15N-edited 2D spectrum, the effective relaxation rate, Reff, can be determined. This results in what is referred to as a dispersion curve from which both the exchange contribution and its corresponding rate can be extracted.

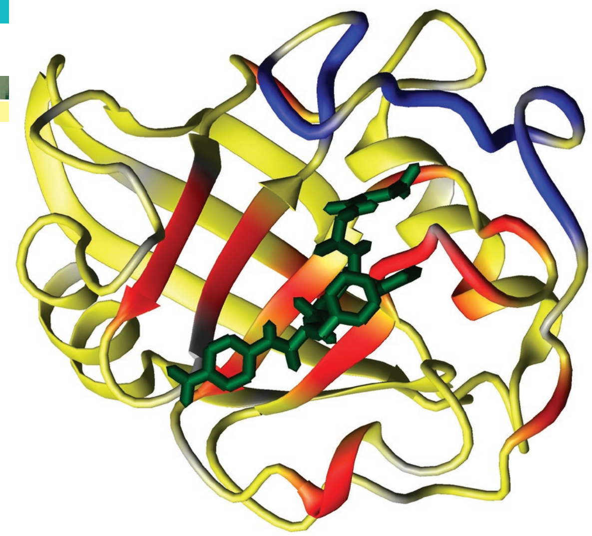


Figure 1. Residues of CypA exhibiting exchange both in the presence and absence of a peptide substrate, suc-AFPF-NA at 10 °C. In the free enzyme the slower process is ~1000 s^{-1} (residues in red) and the faster process is ~2000 s^{-1} (residues in blue). During catalysis both processes adopt a rate of ~2000 s^{-1}. The structure was taken from the PDB data bank with accession number 1RMH and colored in Molmol.

Thus, as opposed to simply determining the existence of chemical exchange from standard experiments such as R1 (longitudinal relaxation rate), R2 (transverse relaxation rate), and heteronuclear-NOE measurements, CPMG sequences offer the advantage of ascertaining the rates of these exchange processes. This, in turn, can offer striking insights into the correlations of protein motions since residues involved in a single event should have similar rates. Our previous work on CypA proved chemical exchange measured by NMR can be used to understand motions at the atomic level on a working enzyme, but only several dynamic "hot spots" were detected.[2] Thus we have applied 15N-CPMG experiments to this prolyl-isomerase both free and during turnover using a model peptide substrate to gain further insights into its mechanism.

To our surprise nearly all of the residues exhibiting chemical exchange during turnover exhibit exchange in the absence of substrate, Fig. 1. Most of these residues are found within the active site where the substrate is catalyzed. In the free form there are two apparent processes that can each be globally fit (colored blue and red in Fig. 1) resulting in two very different exchange rates, yet in the active complex these rates are uniform. Thus, the data suggest that, in the absences of substrate, critical residues for catalysis are already undergoing conformational exchange. Furthermore, the two processes that occur in the free enzyme (corresponding to the two rates measured in Fig. 1) may be correlated during catalysis.

Correlated Motions Probed by Mutagenises

Several mutations of CypA are currently under investigation. The impetus behind such work can be understood as follows. If correlated motions exist within a protein (e.g., CypA) then a change at one site may bare dynamic consequences to other sites. Studying dynamics on the wild type CypA revealed numerous residues with similar exchange rates yet this alone does not prove they are correlated. Only by changing the dynamics at one site and detecting changes at distal sites can the existence of a correlated network be proven. This was exactly the case for several mutants found including the mutant CypA^{K82A} (lysine at residue 82 in CypA was mutated to alanine).

From previous work on CypA several residues were found effected by the presence of the substrate.[3] Lys82 appeared to undergo a large chemical shift upon the addition of substrate despite its relatively large distance to the active site (over 10 angstroms). Furthermore its transverse relaxation rate was shown to be strongly dependent on substrate binding. The mutant CypA^{K82A} has about 80% activity relative to the wild type enzyme which is likely due to its weaker binding affinity. Though the exchange rates of this mutant were found to be similar to the wild type enzyme, the amplitudes were found to approximately double as shown in Fig. 2. Because the amplitude is proportional to the product of populations sampled, this global increase is readily explained by an increase in the minor population. Thus networks of residues undergoing correlated motions have been revealed by combining mutagenesis with NMR dynamics.

Chemical Exchange in the Presence of the Inhibitor Cyclosporin A

A reduction in chemical exchange for two regions of CypA, residues 101-104 and 65-72, in the presence of the inhibitor cyclosporin A, has previously been observed.[4] We too see a reduction in exchange for the amides of these regions at 10 ^{o}C yet several residues still exhibit measurable exchange that was not found previously. This is most likely due to the higher sensitivity of CPMG experiments relative to a simple R_2 experiment. For example Asp^{66}, Asn^{71}, Gly^{72}, and Gly^{74} (found within the loop region colored blue in Fig. 1) all exhibit exchange in the inhibitor bound complex and their dispersion profiles give similar exchange rates as wild type. In fact there are several residues within the inhibitor binding site, which is also the active site, that also display chemical exchange yet their amplitudes are too low to be accurately fit. Thus, once again there is a global change in amplitudes that supports a global change in populations. But as opposed to the mutant CypA^{K82A} that induces an increase in the minor conformation sampled with a concomitant increase in amplitudes, inhibitor binding shifts the equilibrium the other way. Here, a decrease in the minor population results in diminished amplitudes. Both of these cases are shown in Fig. 3 for Gly^{74}.

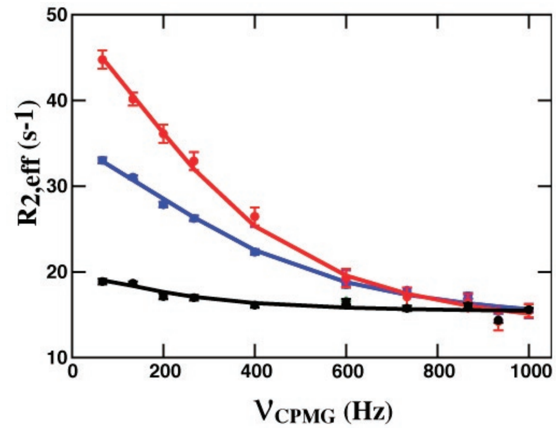


Figure 3. Dispersion curves for Gly^{74} for wild type(blue), CypA^{K82A} (red), and CypA bound to the inhibitor cyclosporin-A (black). The majority of residues exhibiting chemical exchange follow a similar trend lending support to a global process

Conclusions

In an effort to probe motions in proteins we have combined mutagenesis with NMR investigations to study correlated motions. We have found (i) that the majority of residues exhibiting chemical exchange during catalysis have measurable exchange in the absence of substrate, Fig. 1, and (ii) evidence that at least a subset of these motions are correlated by either shifting the populations sampled by the enzyme with a single mutation, Fig. 2, or completely shifting the equilibrium with the addition of the inhibitor cyclosporin-A, Fig. 3. Current work includes both dynamic and structural investigations of several CypA mutants, including active site mutants, both free and during turnover with the ultimate goal of discerning the networks important for catalysis and the enzyme mechanism.

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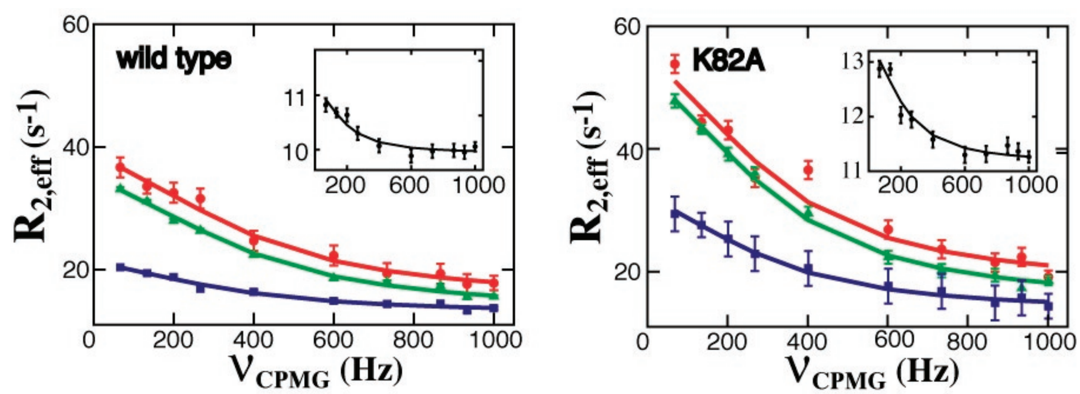
1 Dornan, J., *Current Topics in Medicinal Chemistry*, **3**, 1392-1409 (2003).
2 Mulder, F.A.A., *et al., Nat. Struct. Biol*., **8**, 932-935 (2001).
3 Eisenmesser, E.Z., *et al*., *Science*, **295**, 1520-1523 (2002).
4 Ottiger, M., *et al*., *J. Mol. Biol*., **272**, 64-81 (1997).

Figure 2. Dispersion curves for both wild type CypA and CypA^{K82A}. A global increase in chemical exchange is found for the amides of CypA^{K82A}. Data are shown for the amides of Phe^{67}(blue), Gly^{74}(red), and Lys^{76}(green) found within the loop region as well as for Phe^{46} (inset) that lies outside this region.



PULSED FIELD USERS PROGRAM

ATTENTION USERS

C.H. Mielke, Head of the NHMFL/Los Alamos Users Program

M. Jaime, V. Correa, N. Harrison, C. Batista, and an international team of co-workers have used a combination of experimental tools in pulsed and DC magnetic fields, modeling, and state-of-the-art numerical methods to study a quasi-2D quantum spin system, also an ancient man-made pigment known as Han purple. Their impressive results, just accepted for publication in the *Physical Review Letters*, suggest that $BaCuSi_2O_6$ is the best candidate to date for the realization of a new phase-coherent state of matter: a Bose-Einstein condensate of spin degrees of freedom.

Search for Phase Coherence in Quasi-2D Quantum Spin System $BaCuSi_2O_6$

M. Jaime, LANL
V. Correa, LANL
N. Harrison, LANL
R. Stern, NICPB, Tallinn, Estonia
C.D. Batista, LANL
N. Kawashima, Tokyo Metropolitan University, Physics, Japan
S.A. Zvyagin, NHMFL
K. Uchinokura, University of Tokyo

$BaCuSi_2O_6$ is a quantum magnet where the spin lattice is provided by Cu^{2+} ions (S = 1/2), grouped in mutually parallel dimers arranged in a square lattice. The ground state of these Cu-dimers is a spin singlet state, separated by an energy gap $\Delta \approx 4.45$ meV from the spin triplet excitations. When a magnetic field is applied, the spin triplet component (Sz = 1) splits and approaches the spin singlet (S = 0) ground state. If the applied magnetic field is large enough, the low energy degrees of freedom on a given dimer are the spin singlet and the spin triplet states that form a strongly correlated spin gas moving in a square lattice. Upon cooling these states can undergo condensation, as predicted by Bose and Einsten back in 1925.

Magnetization vs. field measurements performed at Los Alamos show that the spin triplet coherent-phase is formed at magnetic fields between $H_{c1} = 23.5$ and $H_{c2} = 49$ T at T = 1.5 K. In this range of magnetic fields, H is effective in controlling the spin triplet gas, i.e., the chemical potential of the system. Fig. 1 displays magnetization vs. field data and a roughly parabolic (H,T) phase diagram constructed from M vs. H, magnetocaloric effect and specific heat measurements. Compelling evidence for a transition into a low temperature coherent state is found in the excellent agreement between specific heat vs. temperature data taken at 37 T in a 45 T Hybrid magnet (Fig. 2) and predictions of an effective Hamiltonian (Fig. 2 inset). For more details see Jaime, *et al.*, *Phys. Rev. Lett*. to be published (cond-mat/0404324).

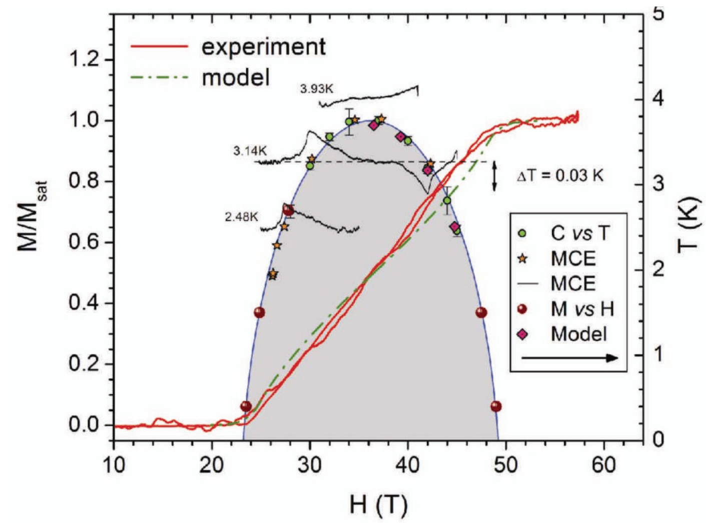


Figure 1. Left y-axis: Magnetization normalized to the saturation value (M/Ms) vs. magnetic field along the c-axis, measured at T = 1.5 K (red line) and results for our model (green line). Right y-axis: Transition temperature from specific heat vs. temperature, magnetocaloric effect (MCE), and magnetization vs. field data.

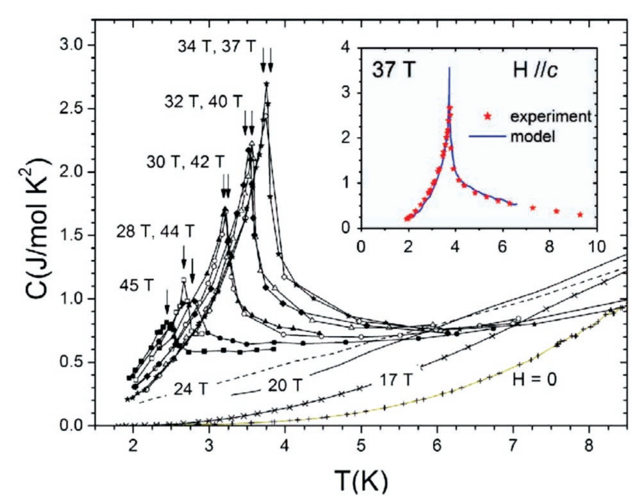


Figure 2. Specific heat vs. temperature at constant magnetic fields *H*. A low temperature λ-anomaly is evident at $H \geq 28$ T. Inset: Specific heat vs. *T* at *H* = 37 T after subtraction of a small contribution due to the Sz = 0 triplet level only relevant at higher temperatures, and phonons. Also displayed is the result of our Monte Carlo calculation.

PEOPLE IN THE NEWS

Jennifer Ascher, a graduate research assistant with the NHMFL ICR Program, received a 2004 Presidential Research Fellowship from FSU. She has been honored with this award each year since 2001. She received her B.A. in Chemistry and B.S. in Science Education from the University of South Florida. She is a Florida teacher who uses magnets for her research into protein patterns in cells in diseases like Alzheimer's, cancer, and schizophrenia. When Ascher graduates this summer with her M.S. degree, she plans to return to teaching chemistry at the high school or community college level.

Michael Chalmers, a postdoc in the ICR Program at the NHMFL, has been hired by the Scripps Research Institute in Florida. He will join their advanced technologies division and work on designing more effective drugs to combat disease through the use of a mass spectrometer to create precise depictions of protein molecules. The data will be used to determine how drugs can latch onto the protein and change its effects. Chalmers earned his Ph.D. at the University of Manchester Institutes of Science and Technology.

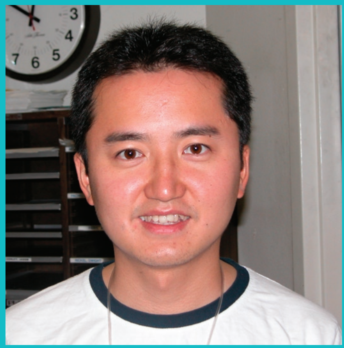
Xuan Gao, a postdoc working with Scott Crooker in his lab at NHMFL/LANL, has been awarded the 2004 Robert Simon Memorial Prize by Columbia University's Department of Applied Physics and Applied Mathematics. This annual award is given to graduate students who have completed the most outstanding dissertation. Gao has been working with Crooker and NHMFL Director Greg Boebinger on transport and terahertz experiments on two-dimensional hole system physics.

A special issue of the *International Journal of Mass Spectrometry* honors **Alan Marshall,** NHMFL Ion Cyclotron Resonance Program Director and FSU Kasha Professor of Chemistry and Biochemistry. The 232-page issue (Volume 234, Issues 1-3) includes 22 contributed articles, and celebrates Marshall's seminal contributions to FT-ICR mass spectrometry on the occasion of his 60th birthday. The issue was presented to Marshall at the 2004 American Society for Mass Spectrometry annual conference in Nashville, Tennessee on May 25, 2004. Marshall assumes the presidency of ASMS this year. He has also been designated as one of the inaugural group of Fellows of The Society for Applied Spectroscopy. SAS Fellows are honored for their service to the Society and for their exceptional contributions to spectroscopy. These first Fellows will be recognized at a reception in Portland, Oregon, on October 5, 2004 at the Federation of Analytical Chemistry and Spectroscopy Societies.

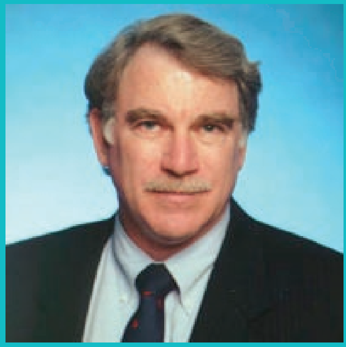
Jarrod A. Marto, a member of the inaugural group that designed and built the first 9.4 T FT-ICR mass spectrometer at NHMFL in 1994, has accepted a position at Dana Farber Cancer Institute (Boston) and a faculty appointment in the Department of Biochemistry and Molecular Biology in the Harvard

Jennifer Ascher

Michael Chalmers



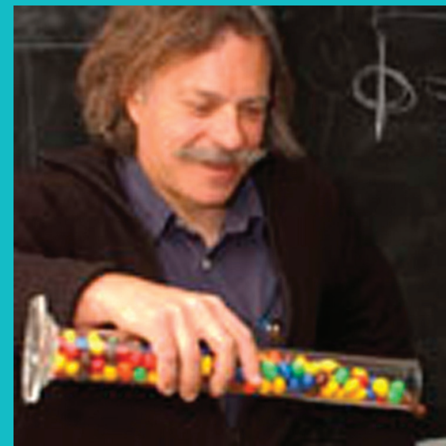
Xuan Gao



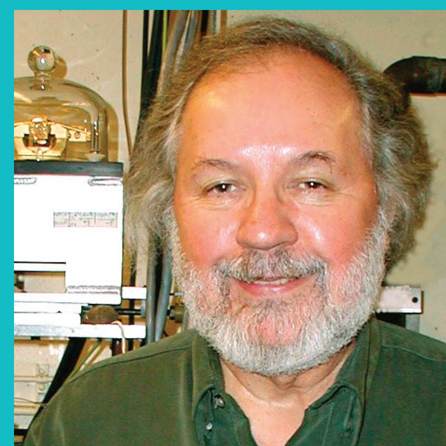
Alan Marshall

Bob Schrieffer

NATIONAL ACADEMY OF SCIENCES SELECTS TWO NHMFL USERS



PAUL CHAIKIN



M. BRIAN MAPLE

Paul Chaikin, Henry DeWolf Smyth Professor of Physics at Princeton University, has been inducted into the National Academy of Sciences along with 71 other new members and 18 foreign associates. His research interests include soft and hard condensed matter, colloids, nano-lithography with diblock copolymers, and low dimensional strongly correlated electron systems. Chaikin is also a fellow of the American Academy of Arts and Sciences. He was an early NHMFL user who has served the laboratory in various advisory capacities over the years, including as a member of the NHMFL External Advisory Committee that met at the laboratory in May 2004.

M. Brian Maple, Bernd T. Matthias Professor of Physics at the University of California at San Diego, has also been inducted into the National Academy of Sciences this year. Maple is a former member of the NHMFL External Advisory Committee and is the current chair of the LANL Materials Science and Technology Division External Review Committee. He also serves as Director of the Institute for Pure and Applied Physical Sciences and the Center for Interface and Materials Science at UCSD. The focus of his research is in low temperature solid state physics. One of his main objectives is the study of superconductivity and magnetism, and the striking effects that arise from the interplay between these two phenomena. His principal interests are strongly correlated electron phenomena in novel d- and f-electron materials.

VE RI TAS

HARVARD MEDICAL SCHOOL

Medical School. He will start in August, 2004. Dr. Marto completed his Ph.D. at the NHMFL/FSU in 1995. Following graduation, he spent three years as a postdoc with Prof. Donald F. Hunt at the University of Virginia and from 1998-2000 was a Research Faculty member at U.Va. Since 2000, he has been the Director of Analytical Proteomics at MDS Proteomics in Charlottesville, VA. Dr. Marto is the eighth member of the NHMFL ICR Group to hold a university faculty position.

Bob Schrieffer, NHMFL Chief Scientist and Nobel Laureate, has been awarded the FSU Robert A. Holton Medal for Distinguished Research Service. The Office of Research award recognizes individuals whose work reflects the very best in university research. Schrieffer's pioneering contributions began nearly 50 years ago with the BCS Theory of Superconductivity, that was according to Kirby Kemper, FSU's Vice President of Research, "the first plausible explanation of a natural phenomenon that some scientists have called the most remarkable physical property in the universe." Schrieffer, a graduate student at the time, along with John Bardeen and Leon Cooper, won the Nobel Prize in physics in 1972 for this achievement. Through Schrieffer's leadership, FSU has gained an increased international visibility and its undergraduate and graduate students have had the pleasure of being taught state-of-the-art condensed matter physics topics by a science icon. The award was previously presented to Robert Holton, an FSU chemistry professor who synthesized the life-saving cancer drug Taxol.

FAMU Confers First Ph.D. in Physics

Graduate Part of FAMU Research Program at the NHMFL

by Joseph A. Johnson, Director, FAMU Center for Nonlinear and Nonequilibrium Aeroscience (CENNAS)

On May 1, 2004, Kyron M. Williams was awarded the Ph.D. Degree in Physics by Florida A&M University (FAMU). His dissertation "Molecular Sensitivity of Transport Parameters in Turbulent Plasmas" focused on evidence of new turbulent physics in high temperature plasmas produced by hypersonic ionizing shock waves. Using a turbulent energy concept, turbulent fluctuation frequencies, trends in plasma complexity, and a sensitivity of turbulent effects to the atomic weight of the plasma species have been discovered. Dr. Williams is FAMU's first Ph.D. in physics. The research was performed in FAMU's Laboratory for Modern Fluid Physics (LMFP) that is located on the third floor in the NHMFL Building in Tallahassee.

Dr. Williams is a native of Pensacola, Florida. He received his B.S. (1997) and his M.S. (2000) degrees in physics from FAMU. Prior to his tenure as a FAMU Graduate Research Assistant in LMFP, he was an undergraduate Distinguished Scholarship Award recipient at FAMU. He has also been a FAMU Undergraduate Research Assistant in the Department of Mathematics, a Ronald McNair Fellow, and an Undergraduate Intern at the Advanced Photon Source at Argonne National Laboratory.

Dr. Williams is one of five doctoral dissertations supervised by FAMU's Prof. Joseph A. Johnson III in the FAMU LMFP facilities at the NHMFL since he arrived in August 1991. The four others include Upul DeSilva (FAMU-FSU COE, 1995), along with Jean Bio Chabi Orou (1994), Ephrem-Denis Mezonlin (1998) and Charlemagne Akpovo (2004) whose degrees were awarded by the National University of Benin, Cotonou, Benin (West Africa). The research in these dissertations touched on a broad spectrum of topics in turbulence, ranging from studies of turbulence in the internal combustion engine, turbulence in laser induced plasmas, and experimental and theoretical studies of viscosity and vorticity in compressible turbulence in supersonic free shear layers. Dr. DeSilva is now Director of a Combustion Research Laboratory at Caterpillar Tractor Company. Dr. Chabi Orou is a member of the Faculty at the National University of Benin having recently served a term as Minister of Secondary Education for Benin. Dr. Akpovo has just been appointed an Instructor at the Institute for Mathematical and Physical Sciences at the National University of Benin. Dr. Mezonlin has returned to Tallahassee and is now a Research Associate in the FAMU LMFP in charge of a new FAMU experiment on the SSPX fusion device at LLNL.

Dr. Kyron M. Williams

The FAMU LMFP continues in scientific workforce development. The Director, Prof. J.A. Johnson, and the Deputy Director, Dr. L.E. Johnson, have funded research projects for several current students including two Ph.D. candidates, Chavis Raynor and Stephen Roberson, a new graduate student beginning Fall 2004, Brandon Alexander, and a current student at Godby High, Carmen Johnson, who has her sights set on a FAMU Ph.D in Physics during May 2014.

For more information, Dr. Johnson can be reached at 850-561-2471 or johnsonj@cennas.nhmfl.gov.

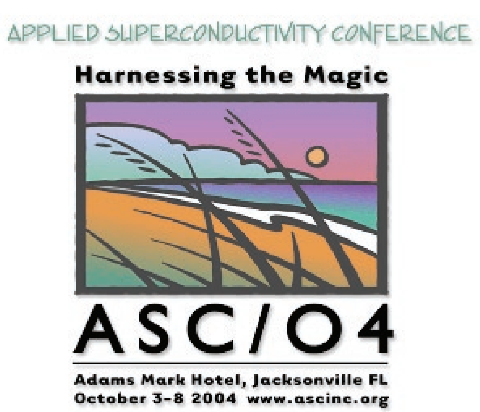
2004 Applied Superconductivity Conference

Plans are shaping up for this conference to be held October 3-8, 2004, in Jacksonville, Florida. Over 1,400 oral and poster presentations are planned for the week. The following plenary lectures have been scheduled:

Greg Boebinger	Superconductivity and High-Field Magnet Research
Jiri Vrba	SQUIDS in Brain Research
Cathy Foley	SQUIDS in Geomagnetism and Prospecting
Shirabe Akita	Superconducting Technologies of the Power Grid
Joe Minervini	Review of ITER and Other Fusion Programs
Chang-Beom Eom	Nanotechnology and Superconductors
Hasan Padamsee	Accelerating Applications of RF Superconductivity, A Success Story…

Special sessions are planned in cryo-packaging and integration of superconducting electronics, cryo-power electronics for large scale superconducting devices, and integration of superconducting devices to the utility grid. In addition, a special memorial session honoring the late John Hulm, a key figure in the discovery of superconducting materials and their applications, and marking the 50th anniversary of the discovery of A15 superconductors is planned.

Conference registration is now available on the Web site, *www.ascinc.org*. For additional information, please check the Web site or contact the Local Conference Chair, Ysonde Jensen, NHMFL (*ASC04LocalChair@magnet.fsu.edu*, 850-644-0807).

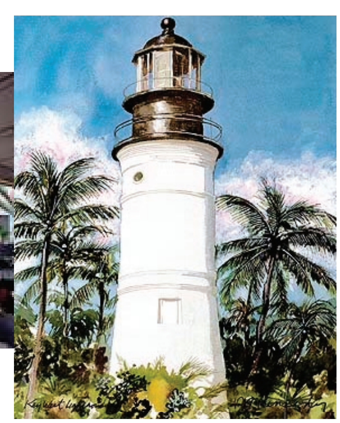


5th North American FT-ICR Conference

This conference has been scheduled for April 17-20, 2005, in Key West, Florida. This conference is organized and supported by the NSF Funded FT-ICR User Facility at the NHMFL in Tallahassee and draws together the top scientists in the field of FT-ICR MS. Presentations range from pure instrumentation advancements to biomedical applications.

The Doubletree Grand Key Resort will be the official conference hotel. The new expanded conference facilities of the Doubletree Grand Resort will allow more flexibility for poster presentations and vendor exhibits than in past years.

As in the past, the conference will consist of 24 invited speaker presentations and one plenary presentation. There will also be 25 student awards for poster presentations. The awards will waive student registration fees and provide housing for awardees to encourage student attendance. Attendance will be limited to 150 conferees and is expected to fill up quickly. Initial interest was high when the first announcements were made at the recent American Society for Mass Spectrometry Meetings in Nashville, Tennessee (May 23-27, 2004). Regular registration will be $300.00 and student registration will be $100.00. More information on the 5th North American FT-ICR Conference and the Double Tree Resort Conference Site can be found on the NHMFL Web site: *http://www.magnet.fsu.edu*.



National High Magnetic Field Laboratory

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Tallahassee, FL 32310-3706
Tel: 850 644-0311
Fax: 850 644-8350
www.magnet.fsu.edu

CONFERENCES & WORKSHOPS

2004

16th International Conference on High Magnetic Fields in Semiconductor Physics (SemiMag16)
http://SemiMag16.magnet.fsu.edu
August 2-6, 2004
Tallahassee, Florida
Contact: Yong-Jie Wang
SemiMag16@magnet.fsu.edu
850-644-1496

Applied Superconductivity Conference (ASC04)
http://www.ASCinc.org
October 3-8, 2004
Jacksonville, Florida
Contact: Justin Schwartz
ASC04ConfChair@magnet.fsu.edu
850-644-0874

15th Conference of the International Society of Magnetic Resonance (ISMAR 2004)
http://www.ismar2004.org/
October 24-28, 2004
Ponte Vedra Beach, Florida
Contact: Tim Cross
mail@ismar.org
850-644-0917

2005

5th North American FT-ICR MS Conference
http://www.magnet.fsu.edu/FT-ICR
April 17-20, 2005
Key West, Florida
Contact: Mark Emmett
emmett@magnet.fsu.edu
850-644-0648
or Karol Bickett
bickett@magnet.fsu.edu
850-644-0535

Electronic Properties of Two-Dimensional Systems (EP2DS-16)
http://ep2ds-16.sandia.gov/
July 10-15, 2005
Albuquerque, NM
Contact: Jerry Simmons
ep2ds-16@sandia.gov
505-844-8402

Physical Phenomena at High Magnetic Fields-V (PPHMF-V)
August 5-9, 2005
Tallahassee, Florida
Contact: Alice Hobbs
aclark@magnet.fsu.edu
850-644-3203

24th Low Temperature Physics Conference
http://www.phys.ufl.edu/~lt24/
August 10-17, 2005
Orlando, Florida
Contact: Gary Ihas
lt24@phys.ufl.edu
352-392-9244

Sixth International Symposium on Crystalline Organic Metals, Superconductors, and Ferromagnets (ISCOM 2005)
http:ISCOM2005.magnet.fsu.edu
September 11-16, 2005
Key West, Florida
Contact: Jim Brooks
850-644-2836
ISCOM2005@magnet.fsu.edu
or Diane Nakasone
850-644-9186