

Report on the 2011 NHMFL User Advisory Committee meeting held in Tallahassee from Thursday, Oct. 13 – Saturday, Oct. 15, 2011

Chair: Janice Musfeldt, Department of Chemistry, University of Tennessee.

DC/Pulsed/High B/T Vice-Chair: Ian Fisher, Department of Applied Physics, Stanford University

NMR/MRI/ICR/EMR Vice-Chair: Tatyana Polenova, Department of Chemistry, University of Delaware

Full list of user committee members: Jonathan Amster, Dmitri Artemov, Steve Beu, Christoph Boehme, Ari Borthakur, David Britt, Joanna Collingwood, Linda Columbus, Nicholas Curro, Myriam Cotten, Enrique del Barco, Ian Fisher, Nathaniel Fortune, Michael Greig, Paul Goddard, Roy Goodrich, Conggang Li, Aimin Liu, Manish Mehta, Vesna Mitrovic, Gavin Morley, David Muddiman, Jan Musfeldt, Cy Opeil, Tatyana Polenova, Cedomir Petrovic, Oliver Portugall, Scott Prosser, Marek Pruski, Mark Rance, John Schlueter, Rob Schurko, Alexandra Stenson, Michael Sumption, Joshua Telser, Fang Tian, Ivan Tkac, Evan Williams, Sergei Zvyagin

The committee thanks the staff of the NHMFL for their hospitality in Tallahassee, for organizing and presenting a day-long workshop on solid state NMR science, and for the scientific efforts of the NHMFL staff in supporting the user community. A summary of the NMR workshop is included as an appendix. We also thank the National Science Foundation, the State of Florida, Florida State University, the University of Florida, and Los Alamos National Laboratory for their generous, long-term support of the Lab.

Highlights and key recommendations:

The NHMFL continues to be a world leading facility with truly unique capabilities that enable ground breaking science. We commend the management and staff of the NHMFL for their recent impressive achievements, including the implementation of a 97.4 T non-destructive pulsed field magnet and the completion of the split coil 25 T magnet – both achievements that open new frontiers for fundamental science. We also commend and strongly endorse the balanced long term plan codeveloped by users and NHMFL personnel as presented in the renewal proposal, which seeks to increase user access to high fields while simultaneously driving ambitious advances in magnet technology. The committee was particularly excited by the prospect of the 36 T Series Connected Hybrid, the advent of low-power 41 T resistive magnets, and the 32 T all-superconducting magnet – implementation of new magnets in these classes will significantly reduce energy demands and ultimately lead to increased user hours, benefiting a wide community of users. Moreover, we remain excited about future opportunities including piercing the 100 T barrier. The committee greatly appreciates the opportunity to weigh in on these scientific priorities on a regular basis. The need for additional user hours at the dc facility, revealed by the series of 2010 user community surveys, is a directly reflection of the unique capabilities available at the NHMFL. This need has been taken seriously in the on-going scheduling process and in the renewal proposal budget, and we are confident that the improved proposal evaluation and prioritization process combined with the new magnet systems coming on-line will ease these oversubscription rates. The committee praises the high level of technical support available to users, the willingness of the staff to develop signature capabilities and try new things, and their broad scholarly scientific impact. Because the staff's leadership-class science and strong can-do attitude continues to characterize the laboratory, we encourage continued investment in personnel. The committee has long recognized the importance of hiring a Chief Scientist for Chem/Bio and hopes that the recruitment of Dr. Lucio Frydman is successful. His international stature will inject new opportunities for cutting edge science, instrumentation development, and diversified

funding for the resonance programs. We fully support the vision to pull together unique NHMFL assets in NMR, MRI, and EMR to pioneer new approaches to dynamic nuclear polarization (DNP). We note that combining the management of the NMR and MRI programs will increase program synergy and provide for a single strategic vision. The committee also thanks the NSF Chemistry Division for their help in securing a 21 T magnet for the ICR program, an initiative that affects a number of high-priority environmental issues for the nation. We recommend that the highly successful NHMFL summer school should be replicated to provide a similar winter school for the theory community. In summary, the NHMFL remains the foremost laboratory in the world for research using high magnetic fields, with more than 500 PIs (and 1200 participating scientists) served, and the laboratory continues to be responsive to the needs, requests and suggestions of the user body, which is one of the most diverse groups in terms of scientific backgrounds, geography (representing multiple states in the nation and many countries), race and ethnicity, gender, as well as age distribution. The user committee therefore strongly and unanimously endorses the 2013-2017 Strategic Plan.

DC facility:

User demand: The dc facility offers world leading magnets for user research, including the flagship 45 T hybrid magnet, as well as a series of 30-35 T resistive magnets. These work-horse magnets enable cutting edge research in condensed matter and materials physics, chemistry, and biology, and regularly lead to a large number of highly cited publications in high impact journals. Access to such a facility is absolutely crucial for continued advances in fields ranging from high temperature superconductivity, to quantum magnetism, to topological phases of matter. The committee praises the laboratory for maintaining these magnets and continuing to upgrade and improve the associated cryogenics that is necessary to perform world class research. However, the essential nature of the magnets offered by the dc facility also means that they are massively oversubscribed. The Laboratory is to be commended in consistently achieving a high rate of new users (typically ~ 20% of the PIs are new each year), but this necessarily leads to a rising level of demand from an ever-increasing user community that cannot easily be sustained. Consequently, as revealed by the recent user survey, most users are not getting as much time as they believe they need to perform their critical research (research that is often already funded by agencies such as the NSF). Associated delays not only reduce the pace of key scientific breakthroughs in important fields, but also directly impact graduate students, for whom the work is often a core part of their thesis work. A large limiting factor in determining the number of user-hours that can be granted each year is the high electricity cost associated with running the resistive magnets.

The user committee commends the NHMFL management for being responsive to the need for increased user time in the renewal proposal, and in particular for their focus on developing and implementing more efficient magnets, that will enable more users to perform their essential experiments. In the meantime, the committee commends the NHMFL for the continued efficiency of the unified online user portal and the external peer-reviewed proposal system that ensures optimal use of the existing magnets.

Improved cryogenics, probe development & thermometry: The users committee was especially pleased by the recent improvements in cryogenic technology made available to magnet users, as well as the new liquefier and cryogenic distribution system. From the user perspective, we note that implementation of top-loading VTI and He-3 cryostats significantly improves ease of use, enabling users to focus more on the materials being measured, and also significantly reduces the time taken to change samples, ultimately leading to more efficient use of magnet time. We applaud the magnet lab for their leadership in this regard, and strongly recommend that the continued development and maintenance of probes (and associated thermometry) for the user community should remain a high priority of the user program.

25 T split coil magnet: The 25 T split coil magnet that came on line this summer was the culmination of a project initiated several years ago at the suggestion of the user community. Combining innovative magnet

design and cryogenics, the new magnet enables optical access to the field center over a large range of angles. Initial user experiments have already begun to demonstrate the range of exciting measurements that are now possible. We encourage the lab to continue to prioritize the completion of this project, including implementation of the necessary cryogenics. The committee notes that funding delays pushed back the scheduled implementation of some aspects of the initial instrumentation, and hope that these difficulties can be avoided in the future.

Development of 36 T Series Connected Hybrid (SCH): The committee was uniformly excited by the prospect of the 36T SCH magnet. The reduced power consumption relative to the 45 T hybrid is especially attractive in terms of enabling more users. In addition, the larger inductance results in an increased stability, important for NMR and EPR measurements. Longer term, the committee was excited by the possibility of a SCH magnet in the 40 T range, running at a considerably lower power than the current 45 T hybrid. The committee encourages the laboratory to keep development and implementation of the SCH as a high priority.

In addition, the committee is pleased to see NSF investment in the SCH being leveraged by a similar project for the Helmholtz Zentrum Berlin. This helps to mitigate the considerable uncertainties of such a high risk project and benefits the broader high magnetic field scientific community. There were fundamental concerns with all high-field cable-in-conduit magnets, including those for the ITER plasma fusion project that the NHMFL helped address. The NHMFL remains well positioned to solve any related problems.

Development of 32 T superconducting magnet: Implementation of an all-superconducting magnet in the 30+ T range, with the associated dramatic reduction in power consumption over traditional resistive magnets, has the potential to significantly impact the number of users that could be supported. It would also confirm the NHMFL as a truly world leading center for superconducting magnet technology and development. Such a magnet would also represent an important step on the way towards higher homogeneity magnets in this field range. The user committee urges the Laboratory to continue to prioritize the development of this magnet technology.

Longer term plans for advanced dc magnets: The user committee was very pleased by the forward-looking stance of the magnet lab. Audacious plans for a 60 T hybrid magnet continue the NHMFL's tradition of developing magnets that completely outclass all competing labs. Ten years ago it would have been unthinkable to propose a 60 T dc magnet, but the continued innovation at the laboratory and in materials technology makes such a proposition entirely credible, if technically extremely challenging. The scientific pay-off associated with the implementation of such a magnet would be enormous, with access to such large dc fields. In addition, ideas to develop additional dc magnets that operate in the 40 T range (including a 28 MW 40 T all-resistive magnets, or a 14 MW SCH) would relieve some of the strain on the flagship 45 T hybrid, providing more users with access to dc fields above 35 T. The committee strongly encourages the laboratory to continue this forward-looking and adventurous approach to magnet technology and hopes that the level of funding achieved in the renewal will be sufficient to support this activity at the high level that it deserves.

High B/T facility:

Increased user base: The committee was pleased to hear that the number of users of the high B/T facility has steadily grown over recent years. It is the nature of ultra low temperature to be very time consuming, limiting the number of experiments that can be performed over the course of a year. The committee therefore applauds efforts to expand the capacity of the High B/T facility to service this growing user community.

Enhanced facilities: The committee enthusiastically endorses plans to open Bay 1 to NHMFL users, and to upgrade Bay 2 to full-time user support. The committee was also pleased to hear about development of new measurement capabilities in the high B/T facility which will be available to users, including high-sensitivity susceptometers and a high-pressure cell. The committee hopes that resources can be found to support additional user support personnel, which will be especially important with the opening of the additional bays.

Pulsed field facility:

97 T pulsed magnet: The user committee congratulates the scientists and staff at the pulsed field facility for their recent achievement of a 97.4 T peak field pulsed magnet. This achievement underscores the world-leading status of the NHMFL in development of new magnet technologies, and opens new horizons for experiments probing complex quantum materials. Acknowledging that operating at such extreme conditions represents a major technical challenge, the user committee was impressed that the magnet has already generated exciting new scientific results in the field range above 80 T. These plans will keep the NHMFL pulsed field facility as the world's leader. The committee endorses the laboratory's plans to improve signal to noise in these extreme conditions and to provide a high level of technical support to the nascent user community. The committee also recommends that the NHMFL continues with its plan to implement upgrades to the outsert coil, leading eventually to pulsed fields in excess of 100 T. The committee also recognizes the need to maintain the generator and other critical laboratory infrastructure, noting urgency indicated by recent failures in the cooling system that lead to several weeks for which this highly-oversubscribed magnet was unavailable.

Other magnets: The committee also notes the impressive science that continues to come out of the workhorse 55, 60 and 65 T pulsed magnets. The committee welcomes the new rapid cool 65T magnet (cell 3) which essentially doubles the number of shots that can be fired in a day, of considerable value to users who travel a long way for such experiments. Beyond the pulsed fields, the committee also notes that access to the 18/20 T superconducting magnet with new He-3 and dilution refrigerator inserts will be of considerable value to users who do not have access to this field/temperature range in their own institutions.

Cryogenic systems: The committee commends the plan for the pulsed field facility to become Helium self sufficient by 2012, with the associated substantial reduction in operating costs.

User support: The committee noted the continued improvement in user support at the pulsed field facility, both in terms of assigning two local points of contact for users, and in terms of support for probe design and storage. The committee also appreciates the flexible approach to assigning magnet time for external users working at the facility given the challenging nature of experiments in these extreme conditions. The committee encourages the laboratory to continue the development of this high level of user support with continued investment in support staff, including a dedicated post-doc for the 200 T single turn magnet.

NMR Magnet Facility and AMRIS Program:

Overview: The Committee is very pleased with the excellent progress made at the NHMFL in the past year in technology development, science, and broader impacts. A major success is the recruitment of the Chief Scientist for the Chem/Bio program, who is a world leader in the field of magnetic resonance and who will provide outstanding scientific leadership. The Lab continues to serve a diverse base of domestic and international users, who are attracted by its unique instrument capabilities bringing transformative science in the areas of energy, materials, and human health. The committee is pleased by the progress being made on the 32 T all-superconducting magnet system and is quite excited about the potential for 30

T high-resolution NMR. This is one of the grand challenges laid out by COHMAG several years ago which now appears accessible given the new HTS magnet technologies.

Infrastructure:

- Hiring of Dr. Lucio Frydman, one of the world leading figures in NMR and MRI at 25% would be an outstanding development, and his vision would invigorate transformational science and technology developments at the Lab. The NMR research community consists of a diverse base of scientists representing Physics, Chemistry, and Health Sciences communities. These researchers use solid and liquid, spectroscopy, MRI and MRI-S, and work on a broad range of problems in materials science, energy, and human health. Dr. Frydman would bring outstanding leadership to these diverse communities. Dr. Frydman's seminal contributions to the field and his vision would invigorate transformational science and technology developments at the Lab.
- The committee is pleased to see that the budget for NMR instrumentation maintenance and upgrades is on track to be restored in 2013 as part of the renewal proposal. We recognize that maintenance had to be deferred due to tight budgets and hope that this needed maintenance will be funded as planned.
- Commitment of NHMFL to invest in infrastructure for electronic resources to keep up-to-date records and dissemination of information is timely.
- AMRIS has built outstanding infrastructure for MRI and made excellent use of NHMFL seed funding to attract external federal support for their biomedically relevant imaging research. AMRIS brought together unprecedented PI and staff expertise. The research output is outstanding.
- Hiring an animal imaging specialist at AMRIS is an excellent development, and altogether, the synergy between clinical and basic science is unique and provides opportunities for attracting translational medicine research funding.
- Commitment to an MRI physicist in AMRIS is a very logical and positive development to reinforce the current strengths.
- Synergy between Tallahassee and AMRIS facilities is beneficial for the success of the NMR program.
- Intermediate field NMR instruments are unique technology development platforms for the higher field NMR magnets and boost user productivity, and these instruments should continue to be supported by the Lab.
- The Committee notes excellent diversity of users in terms of demographics (gender, ethnicity), geographical distribution, and academic background (size and type of institutions).

Technological accomplishments:

- The 900 MHz instrument remains an outstanding platform for cutting edge science, with an eye towards solution and solid state NMR, MRI, and MRI-S applications at very high fields.
- The probe technology development program is unsurpassed, and is a unique strength of NHMFL. In particular, both the HTS NMR probe and the 900 MHz low-E 3-channel MAS probe show superior sensitivity and resolution compared to commercial probes, while 900 MHz live animal imaging probe, surface and volume coils, low-G MAS probe do not have commercial counterparts and provide users unique applications unavailable elsewhere.
- Development of the dielectric resonator and waveguide technology for ultrahigh field MRI is a highly promising and exciting direction in the Lab.

Science: The Committee notes the excellent diversity of projects/disciplines that benefit from technological developments. These include:

- Magnetic resonance program aimed at investigation of new materials for energy storage is a very important and timely effort.

- Inorganic chemistry and biosolids NMR programs remain a major strength, in particular due to the availability of low-G and low-E enhanced-design MAS probes whose sensitivity and resolution dramatically exceeds any commercial probes.
- The imaging and microscopy programs are truly innovative and represent transformative science. The range of systems under analysis ranges from live animals to individual cells, in the latter case the resolution limit is unsurpassed in any other facility worldwide.
- Metabolomics and solution NMR of mixtures is a very promising direction.
- Publication record is excellent, both in quality and number of papers.

Proposed future technology:

- (Immediate future) The committee enthusiastically endorses the proposed development of DNP program within NHMFL. This is an area of prime importance in magnetic resonance that gained international attention and strong momentum. NHMFL is uniquely positioned to lead the development of DNP due to outstanding expertise in cryogen technology, magnet design, MHz and GHz radiation sources, and probe technology. Lucio Frydman is a leading expert in the area of DNP, and his leadership is anticipated to result in transformative science. The committee anticipates that major contributions will be made to both basic and translational research by the DNP program.
- The user committee is highly excited about the prospects of future development of HTS 30+ T magnet. It would bring transformative science to all NMR communities- solids, liquids, and MRI. It will permit a variety of novel imaging and spectroscopy, including microimaging, low-gamma MRI and MRIs as well as solids NMR spectroscopy of new materials and biological systems.

Prioritized List of Recommendations:

General: While the users' committee is impressed with how the user programs are running, there are several suggestions from the committee members on how to improve the current operation of the facility. The synergy among the solution, solid-state and imaging aspects of the NMR program has been extremely important, especially in terms of cross-fertilization of ideas and mutually beneficial technological developments. Recognizing that resources are limited, we outline a priority list in five specific areas: general management, budget, technology development, user base and administrative issues, and scientific directions.

General management (recommendations from 2010 are still pertinent):

- It would be highly beneficial to the NMR/MRI programs that NHMFL demonstrates commitment for systematic infrastructure support, including maintenance and upgrades of existing equipment.
- It is essential for the most productive operation of NHMFL NMR program that the Laboratory supports development of both cutting-edge high-field magnet technology and maintenance of the existing intermediate frequency NMR instruments. These intermediate frequency spectrometers are essential for development of novel probe technology and testing of prototype probes operating at the high magnetic fields, as well as development of DNP (see below). Furthermore, the existing intermediate frequency instruments are essential for support of a diverse user base and a broad range of ongoing and future scientific projects in the Laboratory that yield multiple publications in high-quality peer-reviewed journals. It is necessary that appropriate balance is maintained between these two highly important aspects of the NMR program.

Budget:

- The restored equipment and supply budget, as the committee requested in last year's report, is absolutely necessary to maintain the NMR user program. Using newly developed Low E solids probe technology promises to reduce data collection times by as much as 50%.

- The DNP program's focus on technology development for He cooled MAS probes is very exciting and the funding is appropriate.
- (the recommendation was given in 2010 and is still pertinent) With the growth of the biosolids NMR program, it is essential that a full-time Ph.D. level support scientist is hired to work with the expanding biosolids user base. This is even more crucial for the series hybrid, and it would be valuable to accelerate the position this year.
- The small animal imaging 750 MHz probes at AMRIS should be supported if the UCGP is approved.
- Continued support of an RF engineer at AMRIS is critical for the success of the coil technology development program.

Technology developments:

- Development of technologies (probe and lock) for SCH magnet is very timely, and it is important these technologies be transferrable for the projected HTS system.
- The Committee recognizes probe technology development as one of the major strengths of the NMR program and strongly recommends continued development of solids NMR probes with the goals toward sensitivity and resolution enhancements.
- The Committee recommends that the Magnet Lab works with the new Chief Scientist for CHEM/BIO on establishing priorities for major technology development programs.
- The NMR division of the Magnet Lab stands uniquely positioned to make major impacts and advances in the DNP area, due to the combination of outstanding expertise in probe design and construction, magnet engineering, development of MHz and GHz radiation sources, and general cryogen technology. The leadership by Lucio Frydman as the Chief Scientist, for CHEM/BIO and broad interest by the community makes this a formula for success.
- The committee recommends that the NMR division pursues new directions in three key areas of dynamic nuclear polarization (DNP) NMR spectroscopy: (i) DNP MAS NMR (for solid materials), (ii) shuttled DNP NMR (for dissolution and solution NMR studies), and (iii) pulsed DNP technologies.
- The Committee enthusiastically endorses development of MAS DNP probes without taking funds from existing user programs.

User base and administrative issues:

- Continue building the diverse user base and diverse cutting-edge science with the focus on the unique capabilities of NHMFL in high field technology while reaching out to a broad and diverse range of scientists in the US and internationally
- Continue to actively and aggressively recruit users of the high-field NMR facilities, and to make people aware of research initiatives and new instrumentation and infrastructure.

Scientific directions:

- The Committee recommends development of scientific priorities for the planned DNP technology.
- The Committee enthusiastically endorses the current areas of scientific focus of the Lab and recommends that the NMR division works with the new Chief Scientist for CHEM/BIO on establishing scientific directions for the program, with a particular emphasis on emerging ultrahigh field magnet technologies, such as SCH and the projected HTS systems.

EMR Facilities:

Overview: The EMR program at the NHMFL is world-leading and we are pleased to be able to congratulate the NHMFL on this success story.

The experimental EMR systems provide unique abilities to a broad range of users. These include pulsed EPR spectroscopy at the highest magnetic fields available in the world, with both radiation detection and electrical detection. The committee is also very supportive of the proposed developments in pulsed EPR (HiPER) and very high field EMR (using the SCH). Virtually all of the papers emanating from this facility are in high impact journals, covering the range of physics and chemistry/biology, and a small, but steady number are in the highest level journals (*Science, Nature*). Overall, the committee is very pleased with the current situation and feels that the EMR facilities at the NHMFL are truly a world center of excellence.

User service: The magnet time application and review process is going smoothly, with all high quality projects being accommodated. Projects solely involving routine use of conventional EPR are not appropriate for this facility. However, a Bruker E500 CW X-/Q-band EPR spectrometer will be made available to users in the region, including researchers at PUIs and HBCUs, through an NIH SGI-funded grant that will include a small match from FSU.

Contribution to NSF Renewal: The EMR User Committee is very excited by the contribution of EMR to the NHMFL overall vision and its significant role in the renewal proposal. Three directions are of particular relevance: “Spin Coherence and Control” (an area in which the contributions of the EMR facility are long established), “Photocatalysis” with emphasis on Energy and Environment, and “Metalloenzymes” that directly relates to the science driver “*In vitro* to *in vivo*”. Spin Coherence and Control included major sections on molecular magnetism, for which HFEPER measurements are crucial. *In vitro* to *in vivo* included sections on HFEPER measurements of biomolecules and model compounds. Energy and Environment included sections on HFEPER of catalysts.

Science Developments: The committee was pleased to hear about the exciting cutting-edge science:

- HFEPER measurements, which can now be performed on single crystals at high pressure (up to 1 GPa). This fundamental physical parameter, which has been successfully exploited in other forms of spectroscopy, is now available for the first time in HFEPER – only at the NHMFL. A manuscript on a first application of “HP-HFEPER” is nearly complete. Many applications of HP-HFEPER are expected in materials research and coordination chemistry.
- Development of a multi-frequency high-field pulsed HFEPER spectrometer – available only at the NHMFL. The capabilities have recently been expanded to include electrically detected EPR (EDMR) at high frequencies, which is another unique capability (EDMR is traditionally performed only at X-band) and is now being applied to materials research.
- Development of a frequency domain magnetic resonance spectrometer (FDMRS), which provides information that is often complementary to that from HFEPER. The FDMRS, which operates at frequencies up to 1 THz, will also allow more efficient use of both the DC field (Keck) and SC systems by enabling screening of samples to determine the field/frequency range most suitable for their further investigation. Work on the Keck magnet on biological samples was also described (see below).
- Development of a Mössbauer (nuclear gamma resonance) spectrometer. Two such instruments are now available, thanks in part to donations by Bill Reiff (Northeastern U.). One will be for routine use and one for variable temperature/variable field measurements. The Mössbauer system at NHMFL has already led to several publications. This technique is an important complement to EPR and will provide “one stop shopping” for users working on iron-containing systems across the range of materials research, chemistry, and biology.

New Science Initiatives: The committee was excited to hear about efforts to improve the EMR facilities at the NHMFL. Paramount among these, and exclusive to the EMR program, is the installation of the HiPER system which will provide high power, high time resolution, pulsed 95 GHz EPR. Only one such system currently exists (St. Andrews U., Scotland, UK) and the EMR facility and its users will play a major role in developing the science program for this instrumentation.

Two other initiatives are associated with other NHMFL facilities. The first is the development of the 36 T series-connected-hybrid (SCH) magnet by the Magnet Technology facility. Use of this magnet, in combination with mm- and sub-mm wave sources will allow investigation of organic radical sites in proteins that are unresolvable/unidentifiable by conventional EPR. The promise of this technique is highlighted in the work on tryptophan radicals in azurin at 25 T (Keck magnet) and 695 GHz. The availability of 36 T and 1 THz will allow a wider range of systems to be investigated.

Lastly is the development of a dynamic nuclear polarization (DNP) spectrometer by the NMR facility. DNP is extremely important to NMR and the EMR facility will assist in development of microwave components for DNP, provided that additional resources are made available for this support. The EMR User Committee is also very supportive of the hiring of Lucio Frydman and believes that he can be an asset not only to DNP and the NMR facility in general, but also to the EMR facility in areas such as DEER measurements using the HiPER system and in other pulsed EPR areas.

Along these lines, the User Committee encourages the hiring of a technical support staff member, such as in other programs, to work on instrumentation development and maintenance.

Summary of Recommendations (in Priority Order):

- Continued support for the operation of pulsed and CW EPR spectrometers at the NHMFL/FSU (and supporting instrumentation such as FDMRS and Mössbauer) for the large number and wide scientific range of users.
- Bringing HiPER online for EMR facility users.
- Hiring a technical support staff person for the EMR facility.
- Contributing to the development and EPR applications of the 36 T SCH magnet.
- Supporting the NMR facility in the development of a DNP spectrometer.
- Making NIH-funded X-/Q-band EPR at UF available for regional users.

ICR Facilities:

General: The ICR program has continued to maintain a world leading role in high field FT-ICR mass spectrometry and complex mixture analysis.

Infrastructure:

- Delivery of the 21 T FT-ICR magnet is scheduled for 2013
- Further progress on the Future Fuels Institute (with 5-6 major oil companies in a joint partnership, targeting high-profile problems of mutual interest)

Technology:

- Mass accuracy improvement by a factor of 10 since 2006

Science:

- Record for the most peaks in a single spectrum for any frequency range
- Record for the largest protein complex characterized by H/D exchange (NMR or MS)
- Investigation of oil degradation evident in tar balls from the Deep Water Horizon oil spill is a promising collaboration with the Woods Hole Oceanographic Institute that takes advantage of the world-class expertise on petroleomics and complex mixture analysis at the NHMFL.
- Strong external funding (e.g., 21 T FT-ICR (NSF CHE) and FSU Gulf Research Initiative Consortium)

Targeted needs for the ICR Program:

- 12-15 T test bed magnet for 21 T R&D
- Replacement of Mark Emmett as Director of Biological Applications
- A bioinformatics specialist is needed to assist in processing the increasingly large datasets that emanate from ultra-high resolution FT-ICR mass spectrometry. It is a major and constant challenge to effectively process data without losing any of the advantages provided by the high resolution capabilities of ICR at the NHMFL. Although the ICR group at the NHMFL is leading the way on petroleum analysis software (because there are fewer groups/companies involved), it has not been able to keep up with its bio mass spectrometry analysis needs. Specifically, better tools for H/D exchange; site identification for phosphorylation, glycosylation, and other PTMs; mass assignment for large proteins and protein fragments; and lipid identification and characterization are needed. The main challenges here include:
 1. Most of the data generated at the NHMFL is by a custom data station and therefore not typically compatible with commercial software or available freeware.
 2. Most analysis programs available are not written to take advantage of the ultra-high mass accuracy and resolving power available at the NHMFL.
 3. Few analysis programs include all features that are required (e.g., H/D exchange, site identification for PTMs, mass assignment for large proteins and protein fragments, and lipid identification and characterization)
 4. Because the rate of bio mass spec software development is very high, analysis programs are upgraded with high frequency, making upkeep time-consuming and inefficient especially when it is necessary to use multiple programs in combination to obtain desired information.
 5. Using students or postdocs to develop in-house analysis tools has proven not to be an efficient solution because updates and improvement of such tools is problematic after the authors have left the NHMFL.

Scientific directions:

- Maintain and extend world leadership in FT-ICR MS instrumentation and capabilities; highest magnetic field, highest resolution and mass accuracy, new ionization methods, ion optics, automation, data reduction.

NHMFL summer school and outreach efforts:

Taking advantage of unique magnets requires advanced instrumentation and also training of users. Users of the dc, pulsed field and high B/T community enthusiastically support the innovative summer school hosted by the NHMFL. The week-long program mixes academic lectures and hands-on laboratory experience, and is designed to make new students working at the facility more effective and hence more efficient in their use of magnet time. Those of us on the committee whose own students have attended the course can attest to its efficacy, and also to the high level of enthusiasm of the students and post-docs who attend and benefit from it. Responses to the school from attending students and postdocs were uniformly extremely positive. The committee commends the NHMFL for their service to the user community in

offering this course, and strongly recommends that it continue to be offered as long as funds permit. The committee also expresses their support for the proposed winter theory school.

Appendix: Solid State Workshop Agenda:

New Frontiers in High Field Condensed Matter NMR workshop				
Thursday, October 13, 2011, NHMFL Conference Room B101				
Start	Dur (min)		Title	Speaker/Chair
7:00 AM			shuttle from Residence Inn	
7:45 AM			Registration	
8:00 AM	5		Welcome	Boebinger
8:05 AM	15		Introduction	Reyes
			Session I	Kuhns
8:20 AM	15	Tech I	Overview of the NHMFL SCH Project from an NMR User's Perspective	Bird
8:35 AM	15	Tech II	Improving Field Quality in Powered Magnets	Brey
8:50 AM	15	Tech III	CryoMAS NMR - an efficient high magnetic field inspired research tool for various correlated electronic systems	Stern
9:05 AM	35	Tech IV	Scientific and technical issues of the recent high-field NMR activities at LNCMI- Grenoble	Horvatic
9:40 AM	20		Break - at the Atrium	
			Session II	Brooks
10:00 AM	35	Theory I	Phenomena coexisting on a short spatial scale in layered metals	Gorkov
10:35 AM	15	Theory II	Condon Domains (Just what the Doctor Ordered...)	Shivaram
10:50 AM	35	Organics I	Opportunities for high field NMR in molecular solids	Brown
11:25 AM	35	Organics II	Magnetic field driven quantum criticality in S=1/2 antiferromagnetic Heisenberg chains	Klauss
12:00 PM	60		Lunch - at the Atrium	
			Session III	Hoch
1:00 PM	35	Spin I - strong correlations	Big Fat Geek Cryostat: If You Build It, They Will Come	Imai
1:35 PM	35	Spin II- spin liquids	Nature of low energy excitations and spin texture in a frustrated magnet	Mitrovic
2:10 PM	35	Spin III- frustrated systems	Incomplete devil's staircase in the magnetization curve of SrCu ₂ (BO ₃) ₂	Tagigawa
2:45 PM	20		Break - at the Atrium	
			Session IV	Sullivan
3:05 PM	35	Superconductor I - pnictides	Field-dependence and ordered Fe moment anisotropy in underdoped (Ba _{1-x} K _x)Fe ₂ As ₂	Urbano
3:40 PM	35	Superconductor II - cuprate	Pseudogap ground state of high-T _c cuprates: metallic state violating Luttinger theorem	Zheng
4:15 PM	35	Superconductor III - vortex	High Field NMR Investigations: Superconductors and Diffusion	Halperin
4:50 PM	10		Summary	Halperin
5:00 PM	20		Break	
5:20 PM	70	Poster Session/UC Meeting	Parallel sessions	
6:30 PM	60		Banquet	
7:30 PM	60		Maglab Tour (optional)	Reyes
8:30 PM			Dismissal	

Posters

1	NMR Spin-Lattice Relaxation of Dilute ³ He Impurities in the Conjectured Supersolid Phase of solid ⁴ He	Sullivan
2	Origin of the Anomalous Dispersion-Like Lineshape in Resistively Detected NMR in the Quantum Hall Effect: Evidence	Bowers
3	Magnetic properties of Cr based antiferromagnetic ring clusters studied by NMR and high field magnetization measurer	Furukawa
4	Spin Density Modulation Near the Vortex Cores of Bi ₂ Sr ₂ CaCu ₂ O ₈ +	Mounce
5	Volovik effect in the s state of Ba _{0.69} K _{0.33} Fe ₂ As ₂ from high field NMR	Oh
6	2 GHz NMR at the NHMFL	Brooks
7	Information Storage and Qubit Manipulation in Electron-Nuclear Spin Systems at High Fields	Van Tol