Report on the 2013 NHMFL User Advisory Committee meeting
Held in Gainesville from Thursday, Oct 17 – Saturday, Oct. 19, 2013

Chair: Ian Fisher, Department of Applied Physics, Stanford University.
DC/Pulsed/High B/T Vice-Chair: Nicholas Curro, Department of Physics, UC Davis
NMR/MRI/ICR/EMR Vice-Chair: Robert Schurko, Departments of Chemistry and Biochemistry, University of Windsor

User committee members for 2014:
I. Jonathan Amster (University of Georgia); Dmitri Artemov (Johns Hopkins University); Steve Beu (S. C. Beu Consulting); Ari Borthakur (University of Pennsylvania); Kenneth Burch (University of Toronto); Joanna Collingwood (University of Warwick); Linda Columbus (University of Virginia); Myriam Cotton (Hamilton College); Nicholas Curro (University of California Davis); Ian Fisher (Stanford University); Nathanael Fortune (Smith College); Michael Greig (Pfizer Global R&D); Michael Harrington (Huntington Medical Research Institutes); Jeanie Lau (UC Riverside); Conggang Li (Wuhan Institute of Physics & Mathematics); Manish Mehta (Oberlin College); Gavin Morley (University of Warwick); David C. Muddiman (North Carolina State University); Cedomir Petrovic (Brookhaven National Laboratory); Tatyana Polenova (University of Delaware); Scott Prosser (University of Toronto); Marek Pruski (Ames Laboratory); Mark Rance (University of Cincinnati); Rob Schurko (University of Windsor); Stefan Stoll (University of Washington); Makariy Tanatar (Ameslab); Joshua Telser (Roosevelt University); Fang Tian (Penn State University); Ivan Tkac (University of Minnesota); Evan Williams (UC Berkeley); Sergei Zvyagin (Dresden High Magnetic Field Laboratory).

Committee members who served in 2013, and are now retiring:
Christoph Boehme (University of Utah); David Britt (UC Davis);Roy Goodrich (George Washington University); Janice Musfeldt (University of Tennessee-Knoxville); Oliver Portugall (Laboratoire National des Champs Magnétiques Intenses); Alexandra Stenson (University of South Alabama)
(Thank you for your service!)

The User Committee thanks the NHMFL director, management, scientific staff and administrative assistants for their time, energy and hospitality in hosting the recent User Advisory Committee meeting in Gainesville. We also thank the lab management for accommodating the Committee's requests with respect to content and scheduling (both in advance of the meeting, and also on-the-fly during the meeting), which we felt lead to an especially productive meeting as a consequence.

The NHMFL continues to enable cutting edge, ground-breaking science with a user program that encompasses a truly impressive number of users. In 2012, the MagLab hosted experiments by more than 1350 users from 159 institutions across the United States, and a total of 277 institutions throughout the world. The statistics for 2013 are still accumulating, but look like they will equal or surpass those of 2012. On behalf of this enormous and vibrant user community, we sincerely thank the host institutions (UF, FSU & LANL), the NSF, and the State of Florida, for their continued support of the NHMFL.

1. Executive Summary

At the User Advisory Committee Meeting, several issues were discussed that affected the broad user base, as well as topics specific to individual labs or programs. The following bullet points summarize some of the major themes, which are discussed in greater detail in the remainder of the report.

- Safety. The committee is entirely satisfied with the safety procedures and training at the NHMFL with respect to the user program. We discussed several additional ideas that we recommend be implemented to ensure that users have additional opportunities to ask safety questions while in their experimental cells and enhance feedback following the completion of their experiments.

- Leadership for the CMP program / DC Director Search. Building on our recommendation from last year, the committee continues to strongly recommend that the lab partner with FSU to identify funds and a faculty line to attract a faculty scholar of international standing to fulfill the role of chief scientific officer for CMP. This is a different position to the ongoing search for a director/manager of the day-to-day running of the DC program.

- Acknowledging user support in performance reviews. The committee felt very strongly that user support needs to be formally recognized and rewarded at the time of staff performance reviews and promotions uniformly across the lab, and that this be implemented by all of the host institutions.

- NAS Report. In response to its specific charge, the NAS Committee to Assess the Current Status and Future Direction of High Magnetic Field Science in the United States recently published its findings and recommendations in a report entitled “High Magnetic Field Science and Its Application in the United States: Current Status and Future Directions”. This comprehensive report provides a vision for the development of challenging magnet technologies far in to the future, and describes many of the associated scientific drivers. The charge of the NAS committee did not, however, include a determination of the user priorities for a national high field facility. In order to complement the vision expressed in the report, we provide a broad description of user priorities for a national high magnetic field facility.

We emphasize that the current NHMFL meets all of these criteria. We also note that assessing the technical feasibility of any of the magnets proposed in the NAS report requires a deep appreciation of magnet technology, and we strongly recommend that experts on magnet technology/engineering be asked to participate in any future proposal review.

- Housing in Tallahassee. The committee expressed the user priorities of access to safe, convenient and affordable accommodation. As a long term solution, we proposed working with FSU and Innovation Park to build the case for a guest house on the Innovation Park site at which University, Maglab, and Innovation Park visitors would be able to stay. As a short term solution, in so far as it is feasible, we recommend funds be allocated to partially offset the cost of users staying at local hotels (i.e. contributing towards the difference in cost between the condo, which has been let go, and local hotels).

- Training. Finally, we commend the lab for continuing to run their highly successful summer school. We urge the lab to continue hosting this superb training event, which acts to draw new users to the lab, advertise the range of available experiments and facilities, and educate students and post-docs from a broad range of backgrounds.

2. Report on issues affecting the broad user community

The following (somewhat unpolished) bullet points are copied directly from the text used at the out-brief session at the end of the user meeting, in which the committee presented its suggestions to representatives from the host institutions as well as NHMFL management and program/facility directors.

2.1 Safety

- The User Committee expresses satisfaction with safety training & precautions for the user program. (In particular, we note that no major events have occurred that have involved the users.)
- We recommend the lab institutes the following minor measures in addition to the established safety training and protocols:
  (a) brief conversation with users in the cell on the first day of magnet time (does the user have any specific safety questions now that they are in the cell?) – in parallel with the usual technical questions at the start of magnet time;
  (b) brief conversation after magnet time finishes (does the user have any specific suggestions/recommendations for improving safety based on the week's experience);
  (c) explicitly include safety query as part of debrief email after magnet time, and link to safety comment website.

2.2 Intellectual leadership for the CMP program

- The CMP program broadly construed has historically been the flagship for the lab (largely within the DC program)
- It is crucial for the lab's success going in to the recompetition that there is a strong intellectual leader for the CMP program to articulate the scientific vision & opportunities
- We strongly encourage the lab, in partnership with the host universities, to raise to the highest priority finding the resources and faculty line for a senior CMP faculty hire who would play the role of Chief Scientific Officer for CMP (defacto intellectual director for the DC/PFF programs). Should be widely publicized and made attractive to the very best in the field.
- This is a separate/different role to the current DC Director search, but just as important.

2.3 Housing in Tallahassee

- User priorities: access to convenient, safe and affordable accommodation
- Many users have enjoyed access to the condo; at the same time, we understand the driving forces that have led to letting it go
- No strong support for continued access to the Alumni Village (primary concern safety)
- Long term, a guest house in the Innovation Park could be an ideal solution (addressing both convenience and safety), and we strongly encourage any partnership between FSU and Innovation Park that might lead to such an outcome. We note that this is not a recommendation for the Maglab to have its own guesthouse, but rather to partner with the community in Innovation Park to attract a facility that serves a broader community, including Maglab users/visitors.
- Short term, the broad consensus is that it would be valuable to the user community if the lab could partially support/offset hotel costs (partially addressing the difference in cost between the old condo and more expensive hotels). Could be used as a method to encourage new users. We can help work out a sensible way to configure this depending on the level of support that is feasible (flat rate; scaled in some way with amount of magnet time received, etc).

2.4 Comment/discussion on the NAS "Magsci" Report

- We note, and add our voices to, the high level of praise voiced for the NHMFL in providing world-class facilities, enabling world-class science, and driving new magnet technologies.
- We strongly endorse the main finding and recommendation of the report; that the highest priority is to providing continued support for a centralized facility.
- The report clearly contains a vision of exciting but technologically challenging magnets, with a commensurate cost.

- Assessing the technical feasibility of any of these magnets requires a deep appreciation of magnet technology, and we strongly encourage that experts on magnet technology/engineering be asked to participate in any future proposal review.
- We also note that the committee that drafted the report were charged to address three specific questions:

  1. What is the current state of high-field magnet science, engineering, and technology in the United States, and are there any conspicuous needs to be addressed?
  2. What are the current science drivers and which scientific opportunities and challenges can be anticipated over the next ten years?
  3. What are the principal existing and planned high magnetic field facilities outside of the United States, what roles have U.S. high field magnet development efforts played in developing those facilities, and what potentials exist for further international collaboration in this area?
- We aim to provide in our report a balancing set of statements that convey user priorities for any national magnet facility. For our community these are perhaps statements of the obvious, but our concern is that if we don't make these statements we potentially risk having the bold vision of the Magsci report dominating any future conversation about perceived user needs. We note that the current NHMFL is delivering on all of these user priorities. Any national field facility should…

  (1) Provide access to high-field magnets
  - huge demand for continued access to existing magnet systems: "work horses" that enable cutting edge science (i.e. exciting new science is still being done on existing magnets)
  - commensurate ongoing need for instrumentation, and instrument/technique development
  - users require a transparent and fair proposal review procedure

  (2) Provide a high level of user support and training
  - provide expert technical advice for planning and implementing experiments
  - provide clear avenues for instrument development in collaboration with Maglab scientific staff & in cooperation with external grants
  - provide training for new users and our students/post-docs (summer/winter schools are excellent; repository for good low-temperature practices in a time of off-the-shelf cryogenics!)
  - user support needs to be formally recognized and rewarded at time of staff performance reviews and promotions (See comment in Executive Summary)

  (3) In house science
  - beyond the implicit intellectual outcomes, a strong in-house science program drives a vibrant intellectual community (attractive to visitors), drives technique development

(enables new tools and techniques for all users), and publicizes the sort of science that can be done at the lab (effectively reaching out to new users)

- needs to be balanced with user support

(4) Develop new magnet technologies in consultation with the user community.

- new science is enabled by new technologies, as envisioned/articulated in the magsci report
- the report describes several very ambitious proposals for new magnet technologies, which could open new research avenues and/or vastly change the landscape of research in existing field regimes. To develop all of these systems simultaneously is likely infeasible, and we therefore strongly recommend that any decisions to invest in these directions be taken in consultation with the user community in order to maximize the research benefit associated with the initial investment.
- development of appropriate instrumentation in parallel with the new magnet technologies

- In our considered opinion, the current NHMFL is delivering on all 4 of these requirements for a national high field user facility.

3. Report on DC-pulsed field- high B/T facilities:

Contributors to the DC-pulsed field – high B/T report:

The committee comprises…
Nicholas Curro (UC Davis; UC; vice chair for DC/Pulsed/High B/T),
Kenneth Burch (University of Toronto),
Jason Cooley (Los Alamos National Laboratory),
Ian Fisher (Stanford University),
Nathanael Fortune (Smith College),
Jeanie Lau (UC Riverside),
Janice Musfeldt (UT Knoxville),
Makariy Tanatar (Ames Laboratory),
Chris Wiebe (University of Winnepeg),
Cedomir Petrovic (Brookhaven National Laboratory),
and Oliver Portugall (Laboratoire National des Champs Magnétiques Intenses, CNRS).

Overall the user committee for the DC/Pulse Field/High B/T facilities found that the NHFML continues to do an excellent job to support the broad user base for these unique facilities. The upcoming commissioning of the series connected hybrid will enable a new generation of experiments beyond the current frontier, and the committee commends the leadership for their continued work bringing this new capability online. Furthermore, we enthusiastically support the development of the 32 T superconducting magnet scheduled for the 3rd quarter of 2015, which will exploit new technology to achieve high fields at a fraction of the electrical cost of the traditional Bitter magnets. We also encourage the lab to continue planning for a 42T 28MW DC magnet, which would provide a second DC magnet above 40 T, with the added advantage over the existing hybrid magnet that it can easily go to zero field, and reverse field.

As discussed in earlier statements, the committee expressed satisfaction with the changes made to the safety training. The anonymous email server (*safemag*) for addressing safety concerns has clearly engaged the entire community of users, staff scientists, and technicians. The committee feels that the safety needs of the **users** are being adequately met. In fact, the safety training and practices that have been put in place at the magnet lab have provided inspiration for similar efforts at various users' home campuses.

A serious challenge that the magnet lab will be facing in coming years is the ever-decreasing supply of helium. The lab leadership continues to address this issue with commendable foresight. The upgrades to the recovery system at the DC field facility are a clear improvement and will provide security against the types of shortages that have been devastating to other institutions in recent years. We are also encouraged by the efforts underway at the pulsed field facility at Los Alamos to implement similar recovery systems, and express our recommendation that the LANL management team support these efforts via any necessary infrastructure upgrades.

The new developments at the high B/T facility include Mössbauer capabilities and new low-temperature preamplifiers. We recognize the need to utilize the remaining Bay 1 system in order to increase user access to these unique facilities and reduce the long wait times after proposal submission. <u>Future user committees should comprise an increased representation by high B/T users</u>.

We commend the lab leadership for their careful consideration of balancing the need to invest in new technologies versus maintenance of current facilities. The development of the 25T superconducting magnet for the Helmholtz-Zentrum Berlin facility for neutron scattering is an excellent example of how new experiments will be enabled by the phenomenal magnet design team at the NHMFL. We encourage the lab leadership to continue to think as broadly as possible to not only continue to push the frontier of high magnetic fields, but also to enable new technologies at the currently available fields. This can be done by expanding the range of measurements - for example pulsed-field NMR and high resolution optical scanning --- and by upgrades to the facilities — such as the proposed Quantum Limit Lab — that would provide improvements in electrical, magnetic, and vibrational stability and signal to noise at these fields. The coupling of these high-risk/high-return investments with steady improvements in measurement performance and capability at existing fields will help the magnet lab to maintain its leadership role in the international scientific community.

Finally, one specific issue that emerged in conversations was the need for quality of user support by NHMFL staff members to be emphasized <u>with equal weight</u> by all of the NHMFL sites. The committee felt very strongly that strength of user support needs to be formally recognized, recorded, and rewarded at the time of staff performance reviews and promotions uniformly across the lab, and that this be implemented <u>by all of the host institutions</u>.

4. Report on the Magnetic Resonance Division

Sections: NMR, EPR and ICR

I. <u>Nuclear Magnetic Resonance</u>

Contributors to the NMR section of this report:
Robert Schurko (University of Windsor, UC Chair, MR division)
Linda Columbus (University of Virginia)
Michael Harrington (Huntington Medical Research Institute)
Manish Mehta (Oberlin College)

1. Overview

The NMR Users' Committee (NMRUC) is happy to report that we are pleased with progress at the NHMFL over the last year. There are significant advances in fundamental and applied research, continued development of new technologies, and expansion of the user base into an increasingly wider set of sub-disciplines. The promise of the launch of the 36 T Series-Connected Hybrid (SCH) NMR system in 2015 was the focus of a workshop prior to the meeting – this system has the potential to make enormous impacts in NMR research on biomolecules, materials and small molecules, as well as in magnetic resonance imaging. The continued development of the DNP research instrumentation and programs (dissolution, *in vivo* and solids) is impressive, and the impact of Lucio Frydman and co-workers is extraordinary. Older spectrometers have been repurposed for new applications, and construction of a plethora of different probes is enduring. A wide range of research areas are again being supported, including chemistry, biochemistry and materials science, and target research areas in biostructural characterization, pharmaceuticals, metabolomics, energy (batteries and fuel cells), and magnetic resonance imaging. Again, there are concerns about budget constraints and their influence on user programs, technical staff and support/acquisition of instrumentation. However, given the sustained improvements and advancements being made at the NHMFL facilities, it is still apparent that there is a bright future ahead for this facility, and that numerous scientific breakthroughs will continue to be made in the coming years.

2. Personnel

Despite some turnover, the NMRUC notes that the overall stability in staffing in the NMR/EMR section of the lab has led to reliable operation for the external users. We are particularly delighted to see greater cooperation between the staff at UF and FSU, spurred by the DNP initiative. The efficient partitioning of resources and enhanced communication between these two sites strengthens the program and benefits the end user.

The appointment of Lucio Frydman as chief scientist has proven successful on several fronts. The departure of Rafael Brüschweiler from FSU, however, has created a vacancy that needs to be filled. The Committee encourages the NHMFL management team to work with FSU officials to appoint a replacement without delay.

The appointment of three staff scientists (Malathy Elumalai, Sungsool Wi and Srinivasan Shekar) is working out well. Two additional staff scientists (Ilya Litvak in probe engineering and another in DNP) are currently being supported by external grants (so-called soft money). These are important positions that complement existing expertise at the Mag Lab, and, as such, a way should be found to retain them in the long run. It is anticipated that the new Southeast Center for Integrated Metabolomics (SECIM), spearheaded by Arthur Edison, will result in a cluster of faculty hires. We note that Joanna Long has been appointed as a new co-PI at UF, while Art Edison will have more focus on activities at the SECIM. A new initiative in brain MRI is expected to result in a similar cluster of hires at UF. These additional faculty lines may place new demands on staffing at the AMRIS facility and other parts of the Mag Lab, to which careful thought should be given. It is our impression that growth areas (DNP, imaging, SCH, metabolomics) are creating new pressure points at the staffing level. This issue is compounded by aging instrumentation, as the MagLab is passing its second decade of operation: the staff is dividing their time between servicing existing and innovating new hardware. For example, the production queues for the probe development team have now lengthened to over a year. The NMRUC encourages the NHMFL management team to incorporate sustainable staffing into its overall growth model of the Mag Lab. In general, the NMRUC is pleased with the level and quality of support the staff are providing for the Lab's external users.

3. Infrastructure & Safety

3.1 *Current instruments and facility*

The current instrumentation is serving the user community well with many instruments near 100% usage (e.g. 750 MHz). The space has accommodated the two new DNP (one at each site) magnets well. The low E and HST probes have facilitated exciting new research. The synergies between Tallahassee and Gainesville groups, as well as between the NMR and EMR groups) has significantly advanced the facilities and research conducted. The repurposing of equipment and purchasing of used equipment (e.g. magnets) to gain more capabilities was very successful for the 800 MHz instrument and the dissolution DNP and should be continued as a model.

3.2 ***Development/acquisition of new instrumentation.***

User access for the dissolution DNP instrument will be on-line in the coming months for magnetic resonance experiments and within the year for imaging. The SCH development is promising and exciting with users already designing probes and collaborating with staff to begin test measurements as soon as the instrument is available. The HTS probe development is essential for the metabolomics work as well as many solution applications. The infrastructure needed for these developing technologies is in place to facilitate usage.

3.3 ***Facilitating future research and development***

Staff needs support in focusing their expertise towards development and interactions with users rather than maintenance. In-house fabrication and outsourcing should be reassessed. For instance, reliable stator sources are lacking and the purchases of a mill would enable the facility to make their own. Alternatively, certain other fabrications can be outsourced if the manufacturer is reliable and the cost feasible. There should be a mechanism for recommendations and evaluation of current procedures (what should/can be home built and what can be standardized and outsourced) driven by staff and user input in order to have these operations assessed on a regular basis.

3.4 ***Access and expanding the user base***

Remote access has been implemented for many of the spectrometers enabling even more user access and reducing costs for users. Remote access should continue to be a priority for increased access to the facility. Creative recruitment of users should be pursued; such as organization of workshops at society meetings profiling user results and low cost targeted public relations for the facility.

3.5 ***Facility management***

There is a need to begin to think about satellite instruments to increase access and users. The remote capabilities on instruments do not need to be duplicated as satellite instruments; however, there may be synergies with existing laboratories that can handle the maintenance of non-commercial instruments (or probes) at other geographical locations. Planning and discussions about these possibilities should begin. The NMR and MRI staff has made significant efforts to obtain supplemental funds for the purchase of equipment and personnel support. These efforts and collaborations should be incentivized and continue with the user community and serve as a model for the other user groups.

3.6 *Partnerships*

Currently, there are productive active partnerships with Agilent, Bruker, Revolution, and JEOL. Industrial and academic partnerships are very important and should continue to be a priority.

3.7 *Safety*

The safety training and on-site training are sufficient and adequate for the safety of NMR/MRI users. The accessibility to materials online is improved from past years and will continue to bring awareness to the user community.

4. Technological Accomplishments and Future Directions

4.1 *HTS Probes*

The repair and continued development of the HTS probes is exciting and crucial for the solution NMR and specifically in supporting the new metabolomics center. The increase in sensitivity gained with the use of these probes is very important to the NMR community. These applications and probe development should be continued. The 2012 1.5 mm HTS probe optimized for ^{13}C detection is extremely important to the metabolomics and biomolecular user group. An area of development may be for a LC/MS/NMR flow probe for metabolomics.

4.2 *900 MHz Imaging Spectrometer*

Use of the unique 21.1 T, 900 MHz imaging spectrometer (Tallahassee) has continued to accomplish “firsts”, such as ultrafast spatiotemporally encoded imaging sequences of a stroke rat model, and “functional” imaging *in vivo* of rat brain sodium-23 and chloride-35. Continued access to this imaging spectrometer is encouraged for the MRI field to take advantage of the increased SNR for protons and other biologically informative nuclei. The AMRIS group (Gainesville) is adapting the 17.6T, 750 MHz vertical system for rodent imaging. Initial experiments with an excised rat brain imaged overnight at 150, 150, 300 microns, interpolated to 75, 75, 75 microns, demonstrated the potential to examine white fiber tracts in the hippocampus, thalamus, and surrounding cortex. Coil development is underway for *in vivo* imaging.

4.3 *Magnetic Resonance Imaging Probes*

Probe development for both Tallahassee and Gainesville imaging spectrometers involves active collaboration with the expertise of the two centers. The AMRIS-centered group has utilized 3D printing technology, some in collaboration with the UF Architecture School, to produce rat and mouse birdcage coils based on the designs of the sliding ring volume birdcage probes designed originally in Tallahassee for the 21T system. Proton linear, circular, and dual ^{1}H/^{13}C linear birdcage coils are in development and user access is predicted for the summer of 2014. Modifications for other nuclei for user projects, such as for ^{23}Na resonance, can be readily implemented on these probes.

4.4 *MAS and static probes*

Further development of MAS and static probes are needed for the 830 and 900 MHz NMR spectrometers. The NMRUC recommends that (almost) all new probes should be double resonance (H/F-X) at a minimum, and tunable over a broad range of frequencies on the X channel, except for probes designed specifically for $^{13}C/^{15}N$ applications. In particular, probes with larger coil sizes should be able to access frequencies well below that of ^{15}N (i.e., so-called low-gamma probe frequencies), to enable access to a wide range of low-gamma nuclides. The H/F channel is necessary for providing a source of decoupling, and to enable cross polarization experiments, both of which are crucial for most multinuclear SSNMR studies conducted at high field. Single-resonance probes (i.e., X-channel only) are of limited use by comparison, since proton decoupling is necessary for most experiments involving CPMG echo trains; as well, new broadband CP techniques cannot be applied without a proton channel.

The NMRUC was happy to hear of the development and use of several new probes, and the proposal for future probes including:

- Low *E* 3.2 mm MAS probes, spinning speeds of 18-22 kHz, good for $^{13}C/^{15}N$ applications, available up to 900 MHz
- A fast MAS probe must be developed for the 36 T SCH; this will require even higher spinning speeds, which are important for J-based 2D correlation experiments, ^{1}H detection in HMQC-type experiments, and of course narrowing of lines in 1H NMR spectra and increasing the efficiency of homonuclear dipolar coupling.
- Low *E*, 1.6-2.0 mm fast-MAS probe for $^{13}C/^{15}N$ applications; spinning speeds of 70-110 kHz for high-resolution ^{1}H NMR applications

5. Series Connected Hybrid

The challenges surrounding the anticipated 36T Series Connected Hybrid magnet, as well as potential research innovations, were discussed at a one-day workshop on October 17, 2013. The 36 T SCH (40 mm bore, 1 ppm field inhomogeneity) should be operational in 2015. Continued innovations in stability, induction field regulation and water-cooled shims, continue to be developed. Major concerns were expressed over getting the field homogeneity of the magnet as low as possible, to permit studies of organic and biomolecules; high resolution is extremely important.

5.1 *Applications to Materials Science and Unreceptive Nuclides*

The SCH magnet is ideal for the development of ultra-wideline (UW) NMR techniques, and the study of a wide-range of unreceptive nuclides that were previously thought to be inaccessible to routine NMR experimentation. There are growing communities of NMR spectroscopists in the U.S., Canada and Europe who are increasingly using these techniques, and would certainly be interested in access to the 36 T SCH system for such experiments. Unreceptive nuclides constitute a large proportion of the periodic table, and are so-called due to their low gyromagnetic ratios, low natural abundances (or dilution in samples of interest), anisotropically broadened patterns, unfavourable relaxation characteristics, or some combination of all of these properties. UW NMR, which generally refers to acquisition of SSNMR powder patterns with breadths of 250 kHz or greater, is well suited for the 36 T SCH magnet, as there are no real concerns with resolution. Zhehong Gan and Ivan Hung have already demonstrated the usefulness of the 25 T resistive Keck magnet for the acquisition of broad powder patterns (*SSNMR* **2009**, *36*,159–163).

The 36 T SCH magnet and spectrometer should enable acquisition of SSNMR spectra of nuclides that have either sparingly or never been observed before, including those with very large nuclear quadrupole moments and/or low gyromagnetic ratios, (e.g., $^{79/81}$Br, ^{105}Pd, ^{127}I, ^{197}Au), and certain spin-1/2 nuclides with low n.a., low Larmor frequencies and broad patterns arising from CSA (e.g., ^{57}Fe, ^{103}Rh, etc.). The 36 T SCH magnet also serves to narrow the central transitions of the SSNMR spectra of the half-integer quadrupolar nuclei, which leads to further enhancement of S/N. UW NMR techniques have permitted the study of many new NMR nuclides in solid materials – but the 36 T SCH will increase the rapidity with which spectra can be acquired, reduce experimental time frames, and enable the study of unreceptive nuclides which have been diluted (e.g., molecules grafted to surfaces, metal centers in biomolecules, etc.).

The sheer variety of materials and nuclides that will be opened to study by the 36 T SCH spectrometer is stunning. This spectrometer will be of great interest to many of the NMR researchers who develop and apply UW NMR methods, and will be very attractive to materials, inorganic and organometallic chemists.

5.2 *Applications to Biosolids*

From the standpoint of the end user interested in conducting NMR experiments on biosolids, the main challenge will be to squeeze in full data collection in the approximately 8-10 hours the magnet will be in operation during a typical run. Given the magnet's design parameters and its hourly operational cost, the first round of experiments will necessarily be those that are relatively short and do not require high field homogeneity (1 ppm). Samples with short relaxation times may prove ideal for the first round of experiments. For bio-solids, samples that demand maximum spectral dispersion will be good candidates. A complement of six probes is in the design and planning stages, including four MAS probes, a static probe, and a dielectric resonator for MR microscopy. The NMRUC encourages the planners to assure that one of the MAS probes has a standard triple-resonance configuration, capable of spinning samples to at least 40 kHz. At the SCH workshop, the possibility of removing the DC insert was discussed. This would make available an approximately 80 mm bore within the 30T outer magnet, which would allow RT shims to be inserted in its place, much as in a traditional 89 mm wide bore NMR magnet. Members of the NMRUC in attendance were encouraged by this prospect and thus encourage the magnet design team to keep this possibility on the table. The magnet design team has already done an impressive amount of work toward field stabilization, shimming, console, and safety.

With improvement of stability, the areas of 2D spectroscopy, heteronuclear experiments, analysis of complex solutions (e.g. metabolomics), and field-induced alignment should be explored to determine the feasibility and applications with biomolecules. Progress towards these applications is already in progress with groups designing probes, developing instrumentation to deal with temporal field fluctuations and other necessary technologies. These efforts should continue and develop along with user needs.

5.3 *Applications to Imaging*

The NMRUC was very excited with the progress made with the SCH and request that the MagLab consider feasibility and cost of adding a larger bore for the SCH than that currently envisaged to enable *in vivo* rodent imaging at higher field strengths than current in the 21 T system. Requirements would be to achieve 1 ppm homogeneity over a 35-mm diameter sphere in the SCH at 30 T. To achieve this, an additional resistive coil set may need an inner diameter of ~80mm and achieve 50 ppm at 30T. Users have interest in working with the MagLab to generate additional funds towards costs for this development. Considering this SCH modification would add value for the recommended longer term design and feasibility study to construct a 20 T, wide-bore (65 cm diameter) magnet suitable for large animal and human subject research, for which the required homogeneity is 1 ppm or better over a 16 cm diameter sphere.

6. Dynamic Nuclear Polarization (DNP) NMR

The NMRUC is very pleased with the continued commitment to the development of DNP NMR. This plan recognizes the great potential of DNP in enhancing NMR's sensitivity and the need of further foundational research in this area. The DNP effect was predicted theoretically, demonstrated experimentally and brought to recent prominence in the American universities by A. W. Overhauser, C. P. Slichter and R. G. Griffin, among others. However, as pointed out last year, the United States currently lags behind Europe in this area in view of significant investments made recently in Germany, Switzerland, France and the Netherlands. The increasing number of DNP NMR workshops in the US and Europe, and the growing number of publications describing applications of DNP NMR to wide range of materials, continue to illustrate the pressing demand for user access to DNP instrumentation. There must be a continued pledge for further development of DNP instrumentation and methodology in the United States – and the MagLab is the place that this should occur.

Last year, the future of developing DNP NMR looked bright, due to the hiring of Lucio Frydman, and the proposal of three new DNP initiatives: (i) shuttled DNP NMR at low temperature, (ii) DNP MAS NMR for solids, and (iii) pulse DNP NMR (Overhauser NMR) at room temperature.

6.1 ***Dissolution and in vivo DNP NMR***

Interesting advances in dissolution and *in vivo* DNP are being made that really distinguishes the instrumentation at NHMFL from the commercial Hypersense DNP equipment.

The NHMFL dissolution DNP polarizer operates at 1.2 K, requires 1 to 2 L of liquid He, has a 140 GHz MW source, operates with a 5 T/89 mm bore magnet, and has a 2.8 GHz SW (considerably larger than the Hypersense). Importantly, the increased SW does not affect the choice of polarization radical; rather than using tritylOX063, which is expensive and proprietary, it is possible to use radicals like 4-oxo-TEMPO. The instrument also boasts a 92% liquid He recovery level, which is impressive. Transfer of samples can be made to any NMR or MRI spectrometer (though there are some problems with the stray fields of the latter that have to be resolved). The NMRUC is impressed by the versatility in terms of radical choice, higher S/N enhancements at higher fields (and lower temperatures), the absence of sample heating at optimal microwave powers, and the potential for ^{13}C MRI imaging. There is also much interested in future prospects involving optimization of polarization parameters for narrow line radicals, injection time minimization and the introduction of NMR and MRI animal studies.

6.2 *MAS DNP NMR and Overhauser DNP NMR*

As discussed last year, a single gyrotron source will service both the MAS DNP (solids) and Overhauser DNP (liquids) NMR spectrometers. An existing console was used to jump start this program, and progress has been made in developing both of these areas. The system will feature a 600 MHz magnet and a 395 GHz gyrotron source. An NIH application has been put in for a field-swept magnet, which is essential for the successful operation of these systems. In addition, a high-volume, liquid nitrogen MAS NMR system has been ordered for solids experimentation. The development of low-E, high power, 80-100 K DNP MAS probe and the necessary cryogenic system is an essential resource for many users with interests in studying low-gamma nuclei in materials science, battery materials, catalysts, etc.

The NMRUC was also interested to hear of new developments in the area of Overhauser DNP NMR, in particular, for observing molecules that are tumbling in super-critical fluids (e.g., CO_2). The correlation times for such rotations are proportional to viscosity; hence, in the non-viscous SCFs, the correlation times can be very low, and accordingly, line widths very narrow. A high-pressure probe with a 5 mm ZrO2 cell is currently under construction. This system will permit the studies of proteins in reverse micelles, a variety of large molecules in SCFs, and even the nature of the super-critical phases themselves.

Finally, the NMRUC is also impressed by the large number of collaborators that were involved in the proposal for the 600 MHz instrument; this list features a veritable “who’s who” of biological solids NMR. The NMRUC was also impressed with the list of potential future projects, including applications in metabolomics, SCF chromatography, study of protein aggregation, and identification of natural products and active pharmaceutical ingredients. There is also great potential for collaborations with the materials and solid-state chemistry communities, especially for study of small molecules that are absorbed or adsorbed on porous support materials (e.g., heterogeneous catalysts).

7. Summary: Diversity of Projects and Disciplines

The NMRUC is impressed with the wide range of projects covering numerous disciplines, including:

- Biosolids
- Structural characterization of biomolecules in solutions
- Materials science, inorganic chemistry, solids-state chemistry
- Energy-targeted research (batteries, fuel cells, etc.)
- Metabolomics
- Magnetic resonance imaging (MRI, fMRI, MRS, physiological/medical studies, etc.)

Equally important are the developmental projects that will help make great strides in all of the aforementioned research areas:

- DNP NMR (dissolution, *in vivo* and MAS for solids)
- Development of the 36 T SCH magnet, console and probes
- 900 MHz MRI spectrometer
- HTS probes
- New probes for MAS and static solids experiments at ultra-high fields

It was also very impressive to see that major research proposals involving MagLab personnel have been submitted to or supported by federal granting agencies, including:

- High-end instrumentation for a rampable 600 MHz NMR spectrometer and associated cryogenics – $1.2 M
- Membrane proteins for mycobacteria tuberculosis (PI's: Cross and Opella) – $9.7 M
- R21 proposal for HTS/LTS demonstration (PI's: Trociewitz and Brey) - $657 K
- Establishment of the Southeast Center for Integrated Metabolomics (PI: Edison)

The NMRUC also notes that the record of peer-reviewed publications from the Magnetic Resonance group is again excellent, both in quality and number of papers (143 reported at the time of the meeting).

8. Prioritized List of Recommendations

8.1 Synopsis

The NMRUC is pleased to see all of the great progress that has been made over the past year, and the coherent set of future plans made for development of key project areas, and acquisition/construction of instrumentation. We are aware of the financial constraints facing the MagLab, and make the following recommendations with this is mind:

8.2. General management (recommendations from 2011 and 2012 reports are still pertinent)

The NMRUC strongly recommends that the following recommendations be carried out:

- Management must continue to strive for infrastructure support, including maintenance and upgrades of existing equipment, along with support for future mid- to ultra-high field strength magnetic resonance spectrometers.
- The continued purchasing and repurposing of older NMR magnets and systems should continue to be supported (this year, an 800 MHz system from Minnesota was arriving on site). The MagLab is better equipped than anywhere in the world to give these systems second lives – which is a very cost effective way of ensuring NMR spectrometer availability to large use base with a wide array of interests.
- If budget constraints are not too tight, it would seem that the hiring of additional technical staff is a necessity – we hope that management can continue to push for this. Current staff seems occupied halfway between development of new projects, instruments, etc. and the maintenance and repair of older systems. The obligation of keeping older systems running can severely hamper progress on new systems, probes, etc.
- Ongoing collaboration between NMR and EMR areas should be continued, to ensure the success of the DNP research programs.
- Management must continue to improve outreach to attract a wide user base. Many of the meeting attendees (from all committees) were unaware of the great work that has been done in revising the MagLab web site. Regularly updated advertisements, mail outs, email lists and web site pages are essential for this. <u>This is key for attracting the best users to the MagLab to use the ultra-high field NMR instrumentation</u>! See also §8.4.

8.3 Budget

We did not have as detailed a budget discussion as that at the 2012 Users' Meeting, and specific line items and cuts were not examined in great detail. However, we understand that there are financial constraints on all areas. With this in mind, the NMRUC would like to make the following recommendations:

- As in the past, maintain funding for NMR/MRI experiments at close to previous levels.
- DNP NMR research is just getting off the ground – continued support of this area is essential.
- There has been past success in the development of *HTS probes*, and future developments and applications should be supported.
- As mentioned in §8.2, if possible, additional technical staff should be supported; certainly, no cuts to current technical staff should be made. See also §8.4 below.
- The SCH workshop demonstrated that the presence of the 36 T SCH system will have a major impact on many areas of NMR; support should be kept at a steady level to ensure the construction of probes, set-up of instrumentation and launch of first experiments in 2015.

8.4 User base and administrative issues:

Once again, the NMRUC is concerned that the total number of base users will be difficult to increase given the limited technical staff and scientist-scholars available on site. This staff is crucial for assisting users with experiment design and execution, as well as for the development of the new methods, instrumentation, etc. discussed over the course of this report. We make the following recommendations:

- The SSNMR spectrometers are largely oversubscribed in terms of users time, the only exception being the 830 MHz spectrometer at Tallahassee. However, the continued construction of new probes (Peter Gorkov) for the 830 should see the usage increase on this spectrometer as well, and alleviate some of this strain. Once again, we mention the clever purchasing and repurposing of older spectrometers from other institutions as something that should continue.
- It is crucial that new users are recruited for the newer application areas like all three DNP areas, the 36 T SCH system (both materials and biosolids users), and the HTS probes.
- As in 2011 and 2012, we feel that the continued support for infrastructure, new spectrometers, development of new MR hardware and probes, repurposing of old spectrometers, along with the hiring and retention of scientific/technical personnel, are absolutely necessary for the continued development of a strong user base.

In addition:

The NMRUC would like to suggest that the MagLab host **<u>annual workshops</u>** (at least one per year) in several key areas of NMR, similar to the SCH workshop this year. This would include, but not be limited to (i) SSNMR applications to materials science; (ii) biosolids characterization; (iii) low-gamma/metal nuclides in SSNMR; and (iv) ultra-high field applications in MRI. This would be sure to attract a much wider user base into emerging areas of research interest.

The NMRUC also like to suggest that a set of governing rules be developed for the Users' committee to ensure that productive committee members are retained, and new and enthusiastic committee members are added on a regular basis. We note that on our committee contact list, there are members who have not attended a Users' meeting in years – this is certainly not optimal for obtaining useful input or broadening the user base. Ideas regarding term limits for committee members, development of new mailing lists, and how proposals should be reviewed have been tossed around, but perhaps should be treated with more gravity and formality at next year's meeting.

II. <u>Electron Magnetic Resonance</u>

Electron Magnetic Resonance (EMR) User Committee 2013 Meeting Report – Summary

Attendees (18 October 2013)
User Committee: Christos Lampropoulos (incoming, chem/bio area), Gavin Morley (in part, by Skype; outgoing, physics area), Stefan Stoll (continuing, chem/bio area), Josh Telser (Chair; outgoing, chem/bio area), Kurt Warncke (incoming, physics area; Chair-elect), Sergei Zvyagin (continuing, physics area), Alexandra Stenson (in part, ICR user committee).
FSU/NHMFL: Steve Hill, Jurek Krzystek, Andrew Ozarowski, Likai Song, Hans van Tol, Sebastian Stoian
UF: Alexander Angerhofer, Gail Fanucci

General/User Support: The EMR program at the NHMFL with its outstanding instrumentation and staff is world-leading. The user committee is enthusiastic and congratulates the members of the EMR program on their continuing extraordinary success. Most impressive is the EMR program's high scientific productivity (46 papers already published or in press in 2013), relative to its small share of the NHMFL budget. The tremendous support given by EMR scientists to users, from start (or even pre-start in terms of assisting with magnet time proposal writing) to finish (publication) is especially noted. The user base is very broad, covering physics, materials science, chemistry, and biophysics/biochemistry.

Instrumentation:
HiPER: The committee is impressed by the progress with the HiPER spectrometer over the past year, despite shipping damage. It has been operational since January 2013 and already outperforms the Bruker E680 in terms of signal to noise (S/N). The committee is especially pleased that last year's recommendation of securing funding for a 1 kW high-power amplifier was followed. Funding was provided by NHMFL, and the amplifier was already delivered in July 2013. However, the integration of this amplifier will require field service from the vendor of HiPER (University of St. Andrews, Scotland) and additional components (e.g., a fast switch). The committee urges that funding be found for these and other improvements (e.g., ENDOR accessory for HiPER, EMR improvements, see below). Once implemented, HiPER with the 1 kW amplifier will allow additional increases in sensitivity and smaller sample sizes that are critical for high-field biostructural studies (spin labeling, DEER). The HiPER spectrometer provides capabilities that are unique in the U.S., and will likely expand the EMR user base significantly.

EMR: The committee is supportive of proposed, relatively simple hardware improvements in the 120/240/336 GHz pulsed-EPR system that will make this equipment even more powerful for users, such as a new sample holder, a protection switch and a phase-stable reference source.

These developments will allow phase sensitive detection in pulsed-EPR experiments as well as increased S/N, faster repetition times, shorter pulse lengths, and improved phase stability. The phase sensitive detection will be particularly useful for quantum information work carried out with this spectrometer, which has produced papers in *Science*, *Nature*, *Nature Materials*, and *PRL* in the last four years. Access is also an important issue. Although EMR facilities are booked at or near capacity, no concerns were raised about user access. The proposal review process and magnet time allocation is smooth (see comment in first section above). However, due to this heavy utilization, any downtimes are potentially damaging. Therefore, the committee recommends that sufficient funds are provided to cover routine repair and maintenance of aging equipment.

In particular, the Oxford 15/17 T SC magnet power supply was down in 2013, but fortunately was able to be locally repaired. The associated VDI source is approaching the end of its usable life: failure of this source would make the spectrometer unusable. Replacement of the VDI source (including a new set of multipliers) is estimated at $66,000.

Other improvements that would make the spectrometers more attractive to users include a crystal rotator on the SC system and the integration of laser excitation into the pulsed EPR system. The continued development of high pressure HFEPR is also a strong point. Another physical parameter that can be extended is temperature. There is interest in the condensed matter physics user community for EMR at temperatures below 1.5 K.

DNP: The committee is strongly supportive of the continued progress in DNP development, and the resulting close collaboration with the NMR facility. Recent hardware developments include purchases of a (no longer in service) 600 MHz NMR magnet from UF and a gyrotron (joint with NMR) from Bruker (demonstration model). Basic EMR-based research on organic radicals and solvent systems, that efficiently create and transfer polarization to the nuclei, thus enhancing DNP effect, is also strongly encouraged. This will bring aspects of the large organic chemistry community into EMR-related areas, from which they have been largely absent for the past several decades.

Mössbauer/Magnetic Mössbauer: The committee is supportive of the expansion of the EMR facility into the magnetic resonance technique of Mössbauer spectroscopy in magnetic fields (maximum 8 T). This has been achieved at low cost (including equipment donated from Emory Univ., Physics). The potential for supporting current users and attracting new ones, who may often become EMR users as well, is great, given the current dearth of Mössbauer facilities and expertise in the U.S. The committee also supports the extension of this technique to nuclei other than ^{57}Fe, e.g., ^{151}Eu and ^{161}Dy, which have great relevance to the latest research in molecular magnetism as well as to materials/condensed matter physics.

DC: The committee is also supportive of EMR users taking advantage of the NHMFL's remarkable capabilities in resistive and hybrid magnets. EPR experiments are being done in the

Keck, 31 T, and 35 T resistive magnets, and the 45 T hybrid. Therefore, EMR users share the concerns of other DC Field users regarding competition for magnet time on these oversubscribed systems. The EMR users join with others in urging that technological, staffing, and other measures be taken to ensure maximum DC magnet time availability. The committee is also very excited about the coming (2 – 3 years) low-power Series-Connected Hybrid (SCH) magnets, which will offer high-resolution – crucial for many EMR applications. Techniques to enhance the homogeneity of high-field resistive and hybrid magnets for NMR and EPR are encouraged (e.g., P.J.M. van Bentum et al., *Chem. Phys. Lett*. 376, 338 (2003) and Z. Gan et al., *J. Magn. Reson*. 191, 135 (2008)).

Funding: The committee is impressed with EMR Director Hill's success in obtaining external funding, such as for DNP (NSF-MRI) and high pressure EMR (NSF-CHE), which helps keep the lab on its trajectory of technological advance in parallel with high scientific impact. The committee urges the EMR staff scientists to similarly leverage core grants by seeking external funding, especially in conjunction with collaborative projects with EMR users. For example, as suggested by G. Fanucci, the NIH-SIG program could provide a mechanism for obtaining funds that extend NHMFL EMR equipment to run experiments in biomedical research.

Staffing: The committee is extremely pleased with the recent (September 2013) hiring of an EMR/NMR engineer (B. Trociewicz, funded 1:1 by Hill's NSF grant and NHMFL) whose presence will be crucial in DNP development, but will also help with EMR hardware improvements. This engineer will also be able to interact better with NHMFL machinists in terms of preparing technical plans to their exacting requirements. The addition of a postdoc (T. Dubroca, funded by Hill's NSF grant) with expertise in DNP and the presence of Crow postdoc S. Stoian, with respect to Mössbauer, are also very positive developments.

Administrative: A broader issue that EMR users share with other users is the evolving management structure of NHMFL. There should not be an increase in unneeded layers of management; a direct line of communication should be maintained between the NHMFL Director and Deputy Director and the user programs. Such communication is crucial for maintaining and pushing a clear, strong and coherent scientific vision for the lab.

Recommendations (in Priority Order)

- Increase visibility and recognition of the contributions of EMR to magnet science overall. The MagSci report mentions EMR only in the context of NMR-related applications (DEER, greater *g* dispersion) and not in the context of (bio)inorganic and materials chemistry or solid-state qubits.
- Continue support for the operation and improvement of pulsed and CW EPR spectrometers at NHMFL/FSU (and supporting instrumentation such as magnetic Mössbauer) for the large number and wide scientific range of users. This includes

ensuring that there are sufficient funds for routine maintenance, repairs, and consumables (e.g., Mössbauer sources).

- Continue the already strong progress toward bringing the HiPER spectrometer online, and thus, to complete this high-field/high-sensitivity EPR user facility, to fully realize a unique user facility in the U.S. The recommended support includes funds that are necessary for integration of the the high-power amplifier (purchased, and on-site) and associated components,
- Make sure that the newly hired engineer is involved in projects that are directly related to EMR facility, in addition to projects related to DNP. This includes better interfacing with NHMFL machinists, who will now have someone who "speaks their language".
- Support the DC facility by contributing to the development and EPR applications of its existing magnets and the future high-resolution, low power SCH magnets. Make continued, and wider, use of the other DC facilities for EPR experiments.
- Support the DC facility in the hiring of a top-level condensed matter scientist (physicist, chemist, materials scientist, or engineer) as an FSU faculty member to lead the DC facility and provide direction in this core mission of the NMHFL that is also crucial for EMR, with its extensive research in materials areas.
- Support the NMR facility in the development of the DNP program.
- Encourage the EMR staff scientists to seek external funding, that comes to NHMFL, rather than simply providing support letters for external users' grant proposals.
- Continue supporting X-/Q-band EPR at UF for regional users.

III. <u>Ion Cyclotron Resonance</u>

21 T: Strongest FT-ICR MS magnet in the world

- The most exciting news this year is that the 21 T magnet has arrived and passed specs.
- The improvements in instrument design (from ions optics to cell configuration) that have taken place in the 14.5 T test-bed in preparation for bringing the new 21 T FT-ICR MS instrument online quickly and maximizing its potential are, once again, pushing the envelope in sensitivity, resolving power, and dynamic range.
- Use of the 14.5 T as the test-bed will therefore not only allow swift bringing online of the 21 T for user experiments, but will also enhance existing instruments.
- Thus, the acquisition of one new magnet resulted in far reaching improvements throughout the ICR facility from which all users will benefit.

Informatics Hires

- Previously, the user committee recommended the hiring of additional in-house informatics personnel.

- Acquisition of extremely complex and information rich datasets is only as valuable as the ability to process, evaluate, and present the data.
- Commercial software is largely incomplete, unsuited to specialized experiments, and unaffordable to most users.
- Therefore, the availability of powerful data processing technology alongside the world-leading data acquisition technology is important to both external and internal users.
- Therefore, the community welcomes the recent hiring of two in-house informatics specialists.

Hiring of World-Class Proteomics Expert

- Previously, the user committee recommended the hiring of a replacement for Mark Emmett to reinvigorate the bio-applications field of FT-ICR MS at the NHMFL.
- The hiring of Nick Young, a world-expert in histones, appears to be doing just that.
- Dr. Young's progress in attracting new users and enhancing visibility of FT-ICR MS in the proteomics field is impressive.
- Under his leadership, the bio-applications FT-ICR MS program at the NHMFL has joined two consortia (one on top-down proteomics and one on H/D exchange of proteins), which not only involve interesting and important science but also serve as an avenue to enhance visibility of the program in the proteomics community.
- Finally, the bio-applications community, in particular, will greatly benefit from the new 21 T FT-ICR MS technology soon to be available at the NHMFL. Getting the word out to this important base of users, maximizes the transformative potential of this powerful new tool.

Commitment to Users

- FT-ICR MS has shown true commitment to user support by not only meeting the previous year's number of external users but exceeding it despite high turnover in personnel and three months unavailability of the 14.5 T during its service as a test-bed for the 21 T magnet.
- The total number of users, number of new users, and diversity of external users illustrate unbiased commitment to serving the user community.

Innovation and Forward thinking

- Being the world-leader in FT-ICR MS and staying the world-leader require continual innovation and forward thinking.
- As mentioned above, the FT-ICR MS group continues to innovate and improve existing instrument design and software technology.
- In addition, the group is already thinking of ways to fund and implement the next big innovation - an 18 T wide bore FT-ICR MS.
- An 18 T wide bore instrument would be a powerful advancement for the characterization of extremely complex mixtures. As the current workhorse instrument, the 9.4 T has proven, a wider bore allows for more ions to be in the cell at the same time. In the

characterization of extremely complex mixtures (as in the hugely successful petroleomic's work), it is an important advantage to look at millions of ions at the same time because each individual analyte is only a minor component in mixtures of thousands of components.
- The FT-ICR MS group at the NHMFL continues to impress with its creative and innovative ways to procure funding outside of the NHMFL core grant from a variety of sources (e.g., NSF, BP, NIH, Skolkovo Tech, etc.)

External Review

- Given that FT-ICR MS is such important and highly successful component of the NHMFL, the user committee would recommend that the NHMFL lobby for the inclusion of more ICR experts on external review committees evaluating the NHMFL and/or science drivers in the field of NHFL-related research.