Report on the 2017 NHMFL User Advisory Committee Meeting Held in Gainesville, FL, from October 20th to 21th, 2017

Chair: Madalina Furis, Department of Physics, University of Vermont
DC/Pulsed/High B/T Vice-Chair: Sara Haravifard, Department of Physics, Duke University
NMR/MRI/ICR/EMR Vice-Chair: Dane R. McCamey, School of Physics, The University of New South Wales

User committee members:

DC/High B/T Committee: Madalina Furis (Users Committee Chair, University of Vermont), Malte Grosche (Cambridge University), Zhigang Jiang (Georgia Institute of Technology), Lu Li (University of Michigan), Philip Moll (Max Planck Institute for Chemical Physics of Solids), James Williams (University of Maryland), Elizabeth Green (Dresden High Magnetic Field Lab), Sara Haravifard (Chair for DC/ High B/T Duke University), Haidong Zhou (University of Tennessee)

PFF Committee: Chuck Agosta (Clark University), Kirsten Alberi (National Renewal Energy Lab), Nicholas P. Butch (NIST Center for Neutron Research), Krzysztof Gofryk (Idaho National Lab), Jamie Manson (Executive Committee Member, Eastern Washington University), Filip Ronning (Los Alamos National Lab), Zhiqiang Mao (Tulane University), Pei-Chun Ho (California State University, Fresno)

NMR/MRI Committee: Brian Hansen (University of Aarhus), Eduard Chekmenev (Chair, Vanderbilt University), Oc Hee Han (Korea Basic Science Institute), Doug Kojetin (Scripps Research Institute), Len Mueller (Exec. Committee, UC Riverside), David Bryce (University of Ottawa), Paul Ellis (Doty Scientific, Inc.), Richard Magin (University of Illinois at Chicago), Doug Morris (National Institute of Neurological Disorders and Stroke), Aaron Rossini (Iowa State University)

EMR Committee: Chris Kay (University College, U.K.), Dane McCamey (Chair, University of New South Wales, Australia), Stefan Stoll (University of Washington), Joshua Telser (Roosevelt University), Hannah Shafaat (Ohio State University), Stergios Piligkos (University of Copenhagen), Lloyd Lumata (University of Texas), Erik Cizmar (P. J. Safarik University)

ICR Committee: Jonathan Amster (Chair, University of Georgia), Michael L. Easterling (Bruker Corporation), Ying Ge (University of Wisconsin), Kristina Hakansson (University of Michigan), Ljiljana Paša- Tolić (Pacific Northwest National Laboratory) Michael Freitas (Ohio University Medical Center), Elizabeth Kujawinski (Woods Hole Oceanographic Institution), Forest White (MIT)

On behalf of the User Committee, we would like to thank the magnet lab leadership and staff, especially the representatives of the high B/T facility for the flawless organization of the User Committee meeting. The meeting was very productive with highlights that included an extended brainstorming on the possibility of tapping into future mid-scale instrumentation funding opportunities at NSF, exciting new experiments in development at the pulsed field facility, the first architectural renderings of the user housing projects and a very interesting workshop on the progress of spectroscopy techniques at the lab organized in response to a user committee request from the previous year. We are very grateful to all three hosting institutions (FSU, UF and LANL) for their unflinching support of high magnetic field science. We are very confident that all three branches of the magnet lab will to be involved in transformative research across many disciplines, and we are excited and optimistic to see how the three sites will evolve in the future.

(1) Executive summary

Before addressing issues pertaining to the individual facilities which arose from the various subcommittees, we would like to first discuss general developments which affect all the subcommittees at the NHMFL (and the broad user community). The remainder of the report details specific issues which are unique to the different subcommittees.

(i) Outcome of the Renewal

The User Committee was pleased to hear that NSF will continue to support the high magnetic field science. However, the user committee members unanimously expressed their concern about the future of new magnet technologies developments that were originally projected to make significant headway in the next five-year funding cycle.

The User community strongly supports the lab's broad vision for the future of high magnetic field science. Unlocking the quantum world of strong electronic interactions must remain a priority for the lab. It demands the exploration of a large thermodynamic parameter space that requires pulsed magnetic fields as high as 135T and DC fields of 60T.This vision cannot be realized without a new generation of revolutionary magnet technologies coupled with complementary experiments that push forward the frontiers of sensitivity, spectral resolution or vibration control.

The user committee members will encourage the entire user community to assist the Maglab leadership in their quest for alternative sources of funding to realize this vision, that include the mid-scale instrumentation programs at NSF. A survey was launched shortly after the UC meeting ended, polling the users on their view of the future magnet technology that is critical for the central science theme in their field of research. The responses received so far converge towards a central theme that transcends almost all disciplines and research communities represented in the user pool: understanding electron interactions and complex emergent behavior in quantum systems.

The future of electronic materials lies beyond Moore's Law, a realm where strong electron interactions cannot be understood without a well-controlled energy scale that is comparable to crystal field splittings and other relevant interactions. In the past, similar considerations were applied to semiconductors where these energy scales were of the order of 30T or less.

A 60T superconducting magnet with larger bore sizes and long operation times would revolutionize electronic materials and devices in a similar way, introducing quantum systems such as high Tc superconductors, organic semiconductors and magnets, topological 2D systems into an entirely new generation of devices. Such a magnet would also accommodate new techniques that were either incompatible or limited with the old hybrid, resistive or pulsed technologies. The range of interdisciplinary experimental approaches that combine thermodynamic measurements with spectroscopy techniques (NMR, EPR, MRI, Optics, X-ray) will be dramatically enhanced by the superconducting technologies.

Fundamental understanding of quantum processes in complex molecules (including those involved in processes in live organisms) and molecular assemblies emerged as the second interdisciplinary area where there is a critical need for understanding quantum electronics processes with fields of the order of 60T.

In many cases the strong interactions in quantum systems far exceed the 100 T magnetic field range. This is reason why the pulsed field technologies must grow in parallel to the DC field technologies. While more restrictive as far as the experimental techniques they can accommodate, pulsed fields remain essential in providing insight into the next revolutionary step in quantum materials and a direction for future DC field technology development.

In conclusion, we firmly support the MagLab's plan to develop 60T DC superconducting magnet and 135T pulsed magnet technologies in tandem, in order to maximize the thermodynamic parameters space and accelerate discovery in this broad class of materials and systems that respond to a large variety of societal needs.

(ii) Staff Performance

We commend user support staff (technical and admin) for their excellent performance throughout the year. The post-experiment user feedback is overwhelmingly positive. Users report minor issues such as equipment malfunctions that are usually addressed by staff in a timely manner. Their expertise is recognized and much appreciated.

(iii) Housing

The entire user community is extremely grateful for the institutional support provided by FSU in funding the guest house. One of the main concerns has been accommodation, specifically for early career investigators with limited funding. This will be a great opportunity to reduce travel expenses. The close proximity of the guest house to experiment hall will significantly ease the transportation cost and provide secure and safe environment for users 24hrs a day/7 days a week. The committee is pleased with the amenities considered for the guest house which can further lower the costs and improve the productivity of the users significantly. The committee applauds the plans for the guest house to be managed by MagLab and very much appreciates the non-profit nature of the operations as these measures will ensure low per night stay cost. The users enthusiastically are looking forward to the opening day on January 1, 2019.

(iv) Future hiring strategies

NHMFL is currently in a fortunate period of exciting new experimental techniques developments that are merged into the users program at all three facilities. At the DC facility new magnets are coming online in a matter of months. This expansion of technical infrastructure will require adequate technical support as well as scientific guidance and leadership. We are certain these unique scientific opportunities, enabled by the cutting-edge technologies, will attract exceptional talent at the lab. We are therefore delighted to hear about new possible faculty hires at UF with ties to the AMRIS and high B/T facilities and the new mid-career NMR scientist search. We strongly emphasize the need for a similar hiring plan at the DC facility.

(v) Diversity & Outreach

The User Committee is once again impressed with the maglab continued commitment to their long term for increasing diversity. The outreach staff is doing a fantastic job. The increasing media presence is really good. The new website, podcasts, youtube channel, the summer school for girls and graduate students the K-12 activities, the twitter feed are all fabulous. Keep up the good work!

(vi) Safety

The new risk management and safety policies and procedures implemented a few years ago are strictly observed. Users feedback indicate all staff observed this procedures across the board and the users are adequately trained and briefed by the NHMFL staff upon arrival. Users feel very safe while conducting research at the lab.

(vii) User Committee Changes

The UAC elected a new vice-chair for resonance (Stefan Stoll). There was also a discussion related to the scheduling of the out-brief with institutional representatives. It was agreed that the committee can accommodate a change in the schedule such that the out-brief can happen at the end of the business day on the first day of the meeting.

(2) Report of the DC/High B/T Facility Users Committee

Contributors to the DC/ High B/T report:

The committee is comprised of:
Sara Haravifard (Chair for DC/ High B/T Sub-Committee, Duke University)
Malte Grosche (Cambridge University),
Zhigang Jiang (Georgia Institute of Technology),
Lu Li (University of Michigan),
Philip Moll (Max Planck Institute for Chemical Physics of Solids),
James Williams (University of Maryland),
Elizabeth Green (Dresden High Magnetic Field Lab),
Haidong Zhou (University of Tennessee)
Madalina Furis (Users Committee Chair, University of Vermont)

Progress Report

During the 2017 annual User Meeting the DC field user subcommittee was briefed on the current status of the facility as well as on the ongoing efforts and developments aimed to address prior user recommendations and to expand and improve the capabilities for the user program. The DC Field user subcommittee particularly applauds the progress achieved in the past year in:

millikelvin Facility Expansion where space for two 32 T all SC magnets has gone under construction with copper screens installed in walls for improved shielding and noise reduction, and non-magnetic bars and reinforced concrete used in the pits for enhanced magnet safety. The subcommittee is very pleased with the on-schedule progress for the magnet development and testing for the 32 T all SC, as well as the simultaneous planning for the needed sample environment to avoid any unforeseen delays, with major cryostats already arrived onsite and projected to be installed in summer 2018.

Enhanced Safety Measures in the infrastructure maintenance and new design efforts with the installation of double block and bleed values in high pressure magnet cooling water circuit; consideration of an isolated space, separate instrumentation grounding system, and the gas-escape route in the pit design for the two 32 T all SC magnets to address safety concerns in case of magnet quench and compete failure; design and construction of dedicated trenches to hold instrument cables in place in order to prevent tripping hazards. The subcommittee acknowledges and further supports the constant efforts by the NHMFL in reviewing and refining the Integrated Safety Management procedures on case by case bases with the goal to eliminate work space hazards both for the NHMFL staff and users.

Development of the Series Connected Hybrid (SCH) Magnet with 36T achieved in November 2016 and stability of 1 ppm reached in April 2017. The subcommittee is very excited about the prospect of having the SCH system available in the user program for the 2018-1 cycle.

Development of the 41.5 T Resistive Magnet specifically with the upgrade in the vibration isolation system anticipated to be delivered early in 2018. Subcommittee specifically supports the the planning efforts by the

NHMFL for the needed sample environment with cryostats already being ordered and scheduled to be installed in 2018. The subcommittee is looking forward to having the 41.5T magnet ready for the user operation in 2018.

General Infrastructure Upgrade efforts with improvements made in powder supply operations to reduce noise; purchase of additional lock-in, amplifier, voltage control units to facilitate supply-demand cycle; and plans for heat exchanger in magnet cooling water to be installed during the next shut-down.

Outreach Activities specifically the efforts in hosting annual MagLab Summer Schools for graduate students and postdocs, organizing regular public tours and various educational programs for undergraduates and high school students. Subcommittee also is grateful for the innovative outreach programs developed during the last year, specifically the launch of the Fields Magazine in which various NHMFL capabilities are introduced. Moreover, featuring user interviews in the magazine not only provides exposure for young investigators but also facilitates the formation of a network of users with mutual research interests and enhances collaborations.

Recommendations

Expressing deep appreciations for the ongoing efforts by the NHMFL in proving the cutting-edge facility for diverse network of users, the DC field subcommittee provides following recommendations:

Ensuring Adequate Staff and Support, especially with the expansion of the milliKelvin facility and addition of new magnets to the user program, it is of vital importance for the MagLab to consider new hires both for technical and scientific support to balance the workload and maintain the high level of support it has been providing to users. Furthermore, the subcommittee recognizes the need for a new hire to fill a vacant position to provide user support for thermal transport measurements. This is an important recruitment as it will enable users to take full advantage of the unique capabilities available in the MagLab to perform thermal transport measurements such as heat capacity and thermal conductivity under high magnetic fields. Such addition will not only help the community in obtaining better understanding of quantum emergent phenomena in condensed matter physics but will also result in attracting new users with diverse research interests to the facility.

Measures to Address Oversubscription and Shorten Waiting for Magnet-Time, remain as one of the key concerns of the user community. With the conclusion of the upgrade phase, normal user operation is expected to resume beginning in January 2018. However, the subcommittee reiterates the importance of new recruitments both for technical and scientific support to ensure full implementation of the new magnets in the user program, address growing number of new users, and maintain the high productivity of the magnet-times. Moreover, the addition of new magnets to the facility and the increased demands for magnet time, calls for reconsideration of weekend operations in order to ease the scheduling limitations.

Data Management Plan, is an important component of the user program. Subcommittee recommends specific clarifications to be issued to the user community with details about the Data Management Plan at the DC facility including the timeline for local data storage and back up process. It is specifically important to modernize the data collection and storage process for MagLab owned local computers in order to facilitate possible future data recovery – for example unique extensions can be automatically assigned to data collected during each magnet-time. The subcommittee also recommends strengthening security measures for accessing the stored data on MagLab owned computers – for example the stored data can be encrypted and only accessed through sign-in process by team members assigned to each proposal/experiment.

Proposal Review Process, and particularly the peer-review aspect of it has been one of the key components of the successful user program, ensuring the high scientific merits for the projects approved for magnet time at NHMFL. The subcommittee notes the need for development of a standard procedure for the review process in order to establish a timeline for the reviews to be submitted. The subcommittee recommends all review requests sent to potential referees to specify due dates by when the reports need to be submitted. Furthermore, the subcommittee recommends that automatic reminders to be sent to the referees in case the due date is missed. This process should ensure that all new proposals are reviewed on time before scheduling period for each cycle.

Tracking User Progress and Accurate Citation of work produced from data collected at MagLab, is an important measure to assess the science enabled by the facility. For that matter the subcommittee recommends a step to be added to the magnet-time request process, in which the submitters are asked to acknowledge and agree to the terms and specific wording needed for the proper citation of the work resulted from data collected at the NHMFL. Additional reminders can also be included at the time when a magnet-time request is approved and scheduled, as well as when an annual report is submitted. The subcommittee also supports MagLab's proposal to request all users to register for an ORCID number and add their number to their user profile, so that their related publications can automatically be tracked and easily be cited whenever appropriate. The subcommittee suggests that MagLab provides online tutorials and additional help for users who are not familiar with the ORCID database to prevent any unforeseen technical complications specially in case of common names. The subcommittee also recommends that the ORCID number entry to be optional for the first couple of magnet-time cycles in order to avoid any last-minute surprises for the users who are not familiar with ORCID.

Sample Environment, has always been one of the strongest and most important aspects of the user program at MagLab. Expanding the high pressure capabilities to include uniaxial pressure, in addition to further developments for hydrostatic pressure will certainly be of a great interest to the user community.

Development of the 60 T DC Magnet, will for sure maintain the DC field's world-leading instrumentation and the subcommittee fully supports these efforts. Addition of a 60 T DC magnet will be a game changer for sure, as it will enable new science to emerge in high fields under a quieter environment compared to pulsed field setting. From studies of normal states of high temperature superconductors, to emergent new states of matter such as Bose-Einstein condensation in quantum magnets at high fields, to quantum oscillations in topological systems, all will tremendously benefit from the 60 T DC magnet development. Such capability not only provides a calm environment needed to probe the critical quantum phenomena but also enables lower temperatures compared to pulsed field setting, critical for any quantum phase transition study.

High B/T Facility

Progress Report

The subcommittee has been very pleased with the on-going progress at the High B/T facility, specifically the unique vibration isolation, and high magnetic field-low temperature sample environment. High B/T is one of a kind facility in the world that operates 24 hours-7 days a week, with 39% registered international users requesting to perform experiments. The subcommittee is grateful for the supports provided by the host institution, especially the considerations for new faculty recruitments at UF with research interests matching the current goals of the lab.

Sample Environment progress in the past year has not been limited to low temperatures down to ~ 7mK but the new effort in development of high pressure capabilities at mK temperatures has been of great interest to the user community. Furthermore, the subcommittee is grateful for the development of LHe purifier by undergraduate students.

Outreach: High B/T has continued its active outreach and educational program with on-going REU programs as well as regular public lab tours. Currently five recent PhD students are using the facility for their thesis research.

Recommendations

Long wait time and oversubscription has been a recurring concern of the subcommittee and the user community in general. Access to higher fields certainly is also of great interest to the user community.

The subcommittee recommends nomination of new members with specialized expertise in ultra-low temperature physics for future user committee elections, aiming to add expert members in the field to better represent the needs of the High B/T facility.
Parking limitation has been of great concern to the users. The subcommittee recommends resources to be provided to address the lack of dedicated parking space for the users of the High B/T facility.

(3) Report of the PF Facility Users Committee

Contributors to the PF report:

The committee is comprised of:
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Kirsten Alberi (National Renewal Energy Lab)
Nicholas P. Butch (NIST Center for Neutron Research)
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Jamie Manson (Chair, PFF Sub-Committee, Eastern Washington University)
Filip Ronning (Los Alamos National Lab)
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Pei-Chun Ho (California State University, Fresno)

During the meeting the pulsed field user committee was presented with current status of the facility and its existing measurement capabilities. A significant part of the review has also been devoted to ideas and future plans for advancing magnet technology and measurement techniques. The pulsed facility at Los Alamos National Laboratory is the world leader in generating the highest (non-destructive) magnetic fields up to 100 T. Despite the millisecond time scale of the peak field, the facility offers a wide selection of experimental techniques that can be performed at low temperature and under pressure. We commend the LANL pulsed field facility (PFF) for providing consistent and reliable performance. Last year close to 8000 pulses were generated for ~180 users. The cutting edge research conducted at the pulsed facility is only possible through their outstanding support to the users. Pulsed field facility users recognize and appreciate the support they receive at the PFF. We also recognize generous support from LANL of nearly $1.5M for facility upgrades (breakers and capacitor banks). This ensures the sustainability of the program. The mixture of outstanding expertise and involvement of exceptional staff creates a unique and very successful research environment.

The committee is pleased with the PFF's ongoing effort to repair the 60 T long pulse magnet. This measurement capability is critical for a variety of experimental efforts and is needed to enable future scientific discoveries. We commend the PFF's strong efforts to identify failure mechanisms and make design improvements throughout the re-build. However, the extended timeline for replacing the damaged coils (with an estimated two year total timeframe) highlights a greater challenge to maintain measurement capabilities at high pulsed fields in the event of a magnet failure. The PFF has expressed a desire to have spare coils on hand to accelerate re-builds of the 60 T long pulse and 100 T magnets, an approach that has helped to keep 65 T short pulse magnetic capabilities going amid magnet failures. The user committee fully supports this approach.

The user committee recognizes that there are critical materials that are needed to keep the pulsed magnet program operational and moving forward. Specialized wire, in particular wires made of Glidcop and copper-niobium are high on the list of materials that are necessary to construct magnets, that are single source, and that have very long lead times. We urge the NHMFL to fund sufficient wire purchases to make spare magnet shells available to repair failed magnets. These specialized wires are also necessary for the development of new higher field magnets. Finding other sources for these wires, or forming collaborations with other facilities in the US or around the world may help securing a supply of advanced wire into the future. We also urge the NHMFL to continue to support and expand the facilities in Tallahassee to be able to do as much custom modification of wire in-house.

Regarding ongoing efforts to improve measurement capabilities at the PFF, we were updated on the status of the development of pressure cells for use in pulsed field magnets. Substantial progress has been made on the development of specialized diamond anvil cells that are capable of applied pressures up to 6 GPa and temperature stability in a liquid cryogen environment. The diamond anvils have been designed to incorporate electrical leads with an eye toward reliability and ease of use when they are deployed in the user program. This development was performed in response to request from users last year. Despite not having been included in the renewal proposal, this was carried out through the generous support from Los Alamos National Laboratory, which continues to back the pulsed field user program. There was a promising demonstration of this concept with a graphite sample and measurements under pressure will be proven soon. We look forward to the deployment of these cells in the user program, which will, for example, make possible studies of pressure-tuned physics in quantum materials. Lithography, etching, and other processing are fundamentally important to these small and complicated sample environments, and we encourage the exploration of applying focused ion beam techniques to anvil and sample preparation. We also encourage the development of uniaxial strain clamps and hydrostatic piston-cylinder clamps for use in pulsed magnetic fields.

Studying samples under simultaneous extreme conditions of high field, low temperature, and high pressure is vital to our understanding of electronic self-organization. We encourage the PFF to design and build a dilution refrigerator for use in the pulsed field magnets. Initial estimates suggest that the base temperature of measurements will be extended down to at least 0.15 K, which is an important improvement for the study of quantum oscillations, topological superconductivity, and quantum criticality. The investigation of these and other emergent electronic effects will be facilitated by mounting the pressure cells in the dilution refrigerator.

The user committee recognizes the tremendous potential for using focused ion beam (FIB) machining of samples for measurements in high magnetic fields. This is particularly impactful for metallic samples in pulsed magnetic fields, where eddy current heating limits the ability to perform transport measurements in time varying fields, and increases signal to noise in a limited measurement time window. Work on heavy fermions, spin liquids and topological materials over the past year that would not have been possible without FIB machined samples demonstrate the value of this technique. This becomes particularly important as the magnet lab pushes towards higher magnetic fields, which will certainly require higher sweep rates resulting in even larger heating issues. Additionally, FIB micro-machined devices will be advantageous for pressure measurements given the small sample space. As such, we encourage the magnet lab to hire staff to develop this as a capability and make it available to the user community.

Another capability, which we believe would be valuable to the community are ultrasound measurements in pulsed magnetic fields. Ultrasound measurements up to 95 T have been demonstrated in TaAs, and provide thermodynamic evidence for a phase transition, at such high fields. Ultrasound measurements additionally provide directional information, and hence can be used as a symmetry resolved probe, which is particularly valuable for exploring fluctuations and static order which are anisotropic. Given the interest in unconventional superconductivity, electronic nematic orders, spin fluctuations, and topological order could all exploit this capability. We encourage the magnet lab to make this capability available to more users.

The pulsed-field facility continues to do an exceptional job at supporting the needs and requests of the users. In support of the PFF's effort to provide world-class capabilities to users, the user committee also backs the purchase of smaller items that would expand those capabilities. Among other items, we encourage the purchases for improving the infrastructure and the reliability of the pulsed field magnet program, as well as enhancing the magnet lab's ability to fully exploit the unique capabilities of this world class facility, which cannot be found elsewhere in the US or the world.

The user committee supports the plan to extend pulsed fields to beyond 100 T. High magnetic fields are critical to the study of many areas of condensed matter physics. Broadly the committee is excited about expanding the phase space of extreme conditions by ~ 35%. This is tremendous and will certainly lead to new, unanticipated discoveries in a similar fashion that extending to 100 T had done previously. Of note, there is an exponential increase in the amplitude of quantum oscillations with an applied field. Higher fields will enable studying the normal state of cuprates, enhanced effects due to Zeeman splitting, mixing of spin-orbit coupled states, and quantum magnets. Of particular current interest is the field of topological materials. Discoveries of three-dimensional topological materials, including Dirac and Weyl semimetals, have attracted enormous interests because they represent new topological states of quantum matter and opened a new era of condensed matter physics and material science. The unique topological properties of the electronic band structures of Dirac/Weyl semimetals result in useful exotic properties such as extremely high carrier mobility and large linear magnetoresistance, which carry great promise for future applications in energy and information technologies. Quantum oscillation measurements under high magnetic fields have been extensively used to characterize the Dirac/Weyl fermion properties, such as effective mass, quantum mobility and Berry phase. One big open question in this emerging field is what new exotic properties will be found in the ultra-quantum limit under extremely high fields. Some current high-field (<92T) studies on 3D topological semimetals have revealed exciting properties near the quantum limit, e.g. quantum Hall effect. If these materials could be pushed to the ultra- quantum limit in the fields above 100T, new quantum states are expected. This includes fractional quantum Hall effects and exotic ordered states due to enhanced correlation. Building a new magnet offering fields greater than 100 T would have significant impact on the understanding of new topological physics, and accelerate the pace of quantum materials' applications in technology.

(4) Report of the Magnetic Resonance Division User Committees

Sections: I. NMR and MRI, II. EPR and III. ICR

I. NMR and MRI

NMR/MRI UAC and contributors to this section of the report:

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Len Mueller (Exec. Committee, UC Riverside),
David Bryce (University of Ottawa),
Paul Ellis (Doty Scientific, Inc.),
Richard Magin (University of Illinois at Chicago),
Doug Morris (National Institute of Neurological Disorders and Stroke)
Aaron Rossini (Iowa State University)

Overview:
The NMR/MRI user subcommittee (USC) is pleased with the continued progress being made at NHMFL/AMRIS: they are pushing the boundaries of sensitivity and resolution and advancing science that simply cannot be done anywhere else. A major accomplishment this last year has been the acquisition of NMR spectra on the 36 T SCH magnet – this initial work is already demonstrating the incredible insights into chemical structure and dynamics that will be possible. The USC notes some concerns with how this exceptional resource will be made available and scheduled for magnetic resonance community. Additional highlights included reports on the incredible sensitivity of the HTS probe for metabolomics, the continued development of solid-state NMR probes with unparalleled performance, the awarding of the P41 center grant, news of the on-site housing to be constructed adjacent to the Tallahassee site, and the multiple, exciting developments on DNP. For the latter, the USC notes the synergy between the NMR and EPR groups that has contributed to this programs success.
The USC has noted several concerns regarding staffing and its impact on core support and equipment

development. We have identified the following as the three highest priority items:

1. Positions needed to be filled: (i) An RF staff scientist to work with Peter Gor'kov **(highest priority)**, (ii) an MRI RF engineer, and (iii) an SCH operator.
2. Fast (>50 kHz) and ultra-fast (>100 kHz) MAS probes need to be developed or purchased for the high-field spectrometers.
3. The magnet lab should re-establish itself as a world leader in micro-imaging.

Personnel:
There are several recommendations for future hires that are essential (and these recommendations echo the recommendations from the previous year report): (i) Another staff scientist is needed like Peter Gor'kov. This has been a severely underfilled niche. Peter is a very talented scientist but is stretched far too thin. This is a key hire to relieve the bottleneck for probe development and construction. This position is the **highest priority**. (ii) An MRI rf engineer is also needed (see notes on establishing Magnet Lab as the leader in the field of micro-imaging). This is crucial for building new coils for the 900 MHz (and other lower fields) and to extend MRI to the Series Connected Hybrid magnet. (iii) the SCH is a huge success both scientifically and engineering wise. Additional staffing is certainly required for the operation of SCH and facilitating the scheduling and working with the users. This additional staff person would help alleviate the overload of the Magnet Lab leadership, which has done a great job of getting the SCH project where it is today: way ahead of the USC expectations.

Fast magic-angle spinning (MAS) probes:
The Magnet Lab is an established leader in providing ultrahigh magnetic fields for NMR applications. In order to maximize the potential of these high-field systems, it is critical to ensure also that users have access to the latest in very fast magic-angle spinning (MAS) probe technology. These probes are essential for users to be able to carry out the latest biosolids experiments, in particular those that rely on proton detection, as well as experiments on quadrupolar nuclei in biosolids and materials. The USC recommends that all high-field solid-state NMR instruments be equipped either with commercial or home-built very fast MAS probes, e.g., probes for 1.3 mm and/or 0.7 mm rotor-diameter. It should be a top priority to develop analogous very fast MAS probes which spin in the 100 to 150 kHz range for the SCH system. Such developments may place additional strains on the time and resources of Peter Gor'kov, and this is another reason why it is essential to hire additional staff with expertise in rf electronics and probe construction. This may also present an opportunity to bring in trainees through an rf probe construction program analogous to what has been implemented for building MRI coils. Fast MAS infrastructure is an area where the Magnet Lab is deficient, and could jeopardize the Magnet Lab's ability to attract users in the future. Laboratories in Europe, for example, are far better equipped in this regard.

Micro-Imaging:
The Maglab employs some of the world's leading experts in MR microimaging and MR microscopy (MRM). However, due to challenges related to both hardware and scanner software these programs have been hampered. We strongly recommend that the NHMFL should make it a priority to re-establish its position as a world-leader in micro-imaging and MRM. The impressive developments in magnet technology at the Maglab provide ideal circumstances for this effort. Previous MRM programs have relied on collaborations with commercial NMR vendors. However, currently these companies do not have a strong interest in hardware development for MRM (due to this being a limited market). We therefore recommend that the Maglab supports collaborative fabrication with small businesses which focus on the development of strong and fast gradients and micro-rf coils (ideally double tuned) coils for MR microscopy applications at > 14.1T. Such a collaboration would have as it end objective a technology transfer to MRM programs within the Maglab. In this connection we note that the MRI coil workshop progress has been a great success and very valuable for training and knowledge transfer.
MR imaging is an iconic technique which has revolutionized clinical medicine and biomedical research. There is a strong potential for new discoveries in these arenas if imaging related research is prioritized in relation to the Maglab's new magnets (especially the upcoming 32T). Because of the medical potential inherent in this

line of research, the Maglab should consider vetting the level of commitment from the medical departments at UF in relation to the inherently multidisciplinary imaging research.

Series-Connected Hybrid:
The USC was extremely impressed with the initial results of the SCH and believe that there will be very strong interest from the community to use the system moving forward. The primary concern with the SCH we had is that the magnet time for NMR is limited and that rigid scheduling of time may impede access and lead to inefficient use of the instrument. We recommend that the scheduling of SCH time be done in the most flexible method possible to maximize access to the instrument.

DNP:
DNP, in its many forms, is a core strength of the magnet lab! The USC is pleased with the development of the MAS and Overhauser DNP systems and programs. We are very excited to hear about the perspective of developing additional probes for the MAS DNP system. We strongly support the development of a helium MAS DNP system as this could provide further gains in sensitivity of ca. 2 orders of magnitude. The hiring of Dr. Mentink-Vigier is also a very positive development. He is a world leading expert in the theory of MAS DNP and given his strong EPR background he will contribute positively to enhancing collaborative efforts with the EMR group.

Synergies with EMR:
The USC was impressed by the continuing cooperation/collaboration between the EMR and AMRIS NMR/DNP groups.
NSF RFI:
Regarding the RFI for mid-scale instrumentation, the USC is very supportive of the leadership efforts and places a priority on next-generation, persistent high-field magnets for NMR and MRI.
ORCID:
The USC strongly supports the adoption of ORCID for tracking users' publications.
Automated Time Notification:
The USC would like to encourage that notification be sent out once NMR time is awarded and scheduled. This notification should include a reminder (and the language) about citing the core grant.
Outreach:
The USC would like to highlight the outreach and educational activities by the NMR/MRI staff at the NHMFL. The RF coil development workshop in particular is innovative, and USC suggests that similar outreach be performed on NMR probe technology. We additionally note that Peter Gor'kov should have protected time for teaching the RF-probe knowledge to the broader community through training of students and postdocs, and publicizing the results of his research work on the RF-probe development.
Concluding Remarks:
For continuous progress in NHFML, the USC recommends (i) the flexible scheduling of SCH time to maximize access to the instrument, (ii) a priority on next-generation, persistent high-field magnets for NMR and MRI for the RFI on mid-scale instrumentation, (iii) publicizing Peter Gor'kov's RF-probe development results, and (iv) the continuing collaboration between the EMR and AMRIS NMR/DNP groups. We also note the following three highest priority items:

1. Positions needed to be filled: (i) An rf staff scientist to work with Peter Gor'kov **(highest priority)**, (ii) An MRI RF engineer, and (iii) an SCH operator.
2. Fast (>50 kHz) and ultra-fast (>100 kHz) MAS probes need to be developed or purchased for the high-field spectrometers.
3. The magnet lab should re-establish itself as a world leader in micro-imaging.

II EMR

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Program

- The UC acknowledges the contributions that the EMR staff make to both the operation and development of the EMR capabilities, as well as the significant scientific support they provide to the user community.
- The combination of the world-class equipment and staff with outstanding expertise is crucial to the delivery of the EMR user program.
- The EMR program has ~30% new users per year, indicating a vibrant and expanding program.
- Feedback from users remains uniformly positive. No issues were brought forward regarding the operations of the EMR user program.

Personnel

- The UC is concerned about the impact that the recent departure of postdoc Johannes McKay may have on usability and continued development of the HiPER spectrometer, a particularly sophisticated instrument.
- The UC values the expertise that the EMR scientific staff provide, and appreciates that more cross-training of staff will ensure that unanticipated staffing changes do not impact user operations.

Capabilities

- The lack of tunable optical excitation is limiting the use of the EMR facility, particularly for studying photoexcited states, which are central to quantum and energy materials research. The UC suggest that the lab acquire an appropriate OPO system and integrate it into the various instruments.
- The UC is happy to see the addition of AWG capabilities to HiPER, and feel that this will have significant impact in a wide range of areas (biological, biochemical, bioinorganic, biophysical, energy materials).
- HiPER sensitivity improvements by adding a resonator, a tapered horn, and new thin layer sample holders would improve the ability of users to investigate smaller and more dilute samples.
- The 20+ year old magnet in the 14/17T transmission system, one of the workhorse instruments in EMR, is approaching its end of life. The UC is concerned that magnet failure will shut down a large fraction of the EMR user program for at least a year.
- The DNP capabilities are highly valuable to the user community, and benefit from the expertise in quasi-optical systems found in the EMR group.
- The UC is excited about the availability of the SCH magnet for EPR experiments. With the recently ordered 950 GHz source, this system will offer users unprecedented spectral resolution.
- We are pleased to see that the EMR group continues to develop new capabilities (eg FD-FT THz, 395 GHz pulsed EPR) and encourage the lab to advertise these capabilities more widely.

Other

- The UC is pleased to see that the EMR group has organized an Advanced EPR School on theory and applications. This School will train new researchers in EPR and enable them to become effective and efficient users of the EMR facilities. We hope that this initiative will be repeated regularly.

III. ICR

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1. Facility Overview

The ICR Users' Advisory Committee (UAC) continues to be extremely impressed with the progress of the ICR group. Chris Hendrickson provides outstanding leadership, and has engaged a highly talented group of scientists to lead the various activities of the ICR group. The ICR group continues to make innovative advances in instrumentation, and is currently working on implementing a higher-frequency ion trap that triples the effective magnetic field. Additional efforts over the past year have significantly improved and automated sample analysis, significantly improving the speed and efficiency of sample analysis and therefore optimal use of magnet time. These developments, along with the world-leading state-of-the-art 21T ICR system, continue to place the ICR group at the forefront of the field. This leadership position is well-recognized by the user community, as evidenced by the strong increase in the number of annual users of the facility over the past couple of years, 2015 and 2016. Amy McKenna effectively manages the external proposal process, working with potential users to develop high quality applications. The number of users has doubled since 2014 (note that the overall number of users was approximately constant from 2011-2014). The ICR group now has the second–highest number of users in the Magnet Lab. In addition to the instrumentation developments, much of the increase in external users can be directly attributable to cutting-edge innovative breakthroughs in petroleomics, environmental and biogeochemistry, nanoclusters, and intact protein analysis. These applications have been enabled by the 21T, but the ICR staff continues to make innovative sample handling developments, as well as novel software tools, that continue to facilitate novel discoveries. Overall, they have been successful in every aspect of activity expected for a user facility.

Within the ICR group, the petroleomics effort led by Ryan Rodgers continues to generate novel insights into complex mixture analysis of fuels, including a new discovery that the environmental weathering of oil leads to a massive increase in the number of chemical structures while also generating a set of toxic byproducts. These results, along with multiple successful collaborations over the past year, should lead to high profile publications for this group. Petroleomics and environmental analysis represent the largest group of users, although the user cohort for carbon cluster analysis has also increased strongly over the past two years. The carbon cluster effort led by Paul Dunk is pushing the boundaries of our understanding of cluster formation, and his enthusiasm for this fascinating chemistry is impressive. On the protein analysis side, Lissa Anderson has led the effort to provide high sequence coverage on an LC-time scale for large proteins, a technique that would be incredibly challenging on any other platform. Collaborations in the protein analysis area include antibody analysis in multiple myeloma as well as p53 proteoform analysis, two very high impact projects. Extending her outreach efforts to biologists at biology-oriented conferences will further increase the impressive user base of this group.

The ICR User Committee feels that the broad efforts of the ICR group are strong and do not recommend narrowing these efforts to focus on any particular projects. The diverse research foci within the current group provide support for a broad variety of users including astrochemistry, biology and biological chemistry, environmental chemistry, geochemistry, and petroleum characterization. In addition to supporting a wide range of users, these efforts also could enable a broader base of external funding support, which may be critical in times of limited federal funding.

2. Instrument Developments

Chad Weisbrod presented the instrumentation developments associated with the ICR user facility, which represent one of the most important facets for growth and relevance of the program. While detection at a true 21 tesla magnetic field is truly a novel and exciting platform for mass spectrometry, developing advanced instrumentation to efficiently exploit that analytical advantage completes the picture of providing differentiation from other types of competitive mass spectrometry is essential.

The pace and scope of development for the 21T project is primarily associated with enhancing or onboarding capabilities geared for analysis of large biomolecules with a specific focus on streamlining LC-based real-time approaches. The iterative progression of the dynamically harmonized cell (DHC) variant used by the magnet lab has provided a highly optimized cell in terms of detection sensitivity beyond that described in the literature and development here seems to be near frozen. This is a timely development in efficiency terms as cell modifications create the biggest drag on ICR productivity due to the need to apply lengthy bake out cycles. In addition to the physical changes associated with the cell design, the 3Ω detection scheme is showing positive progress and will further enable workflows that require high temporal resolving power which is an important differentiator to methods such as OTOF which have been shown quite efficient for LC protein studies. One highly significant result highlighted in the report was the tendency of the ICR to preserve isotopic fine structure (ISF) while adding charge density to the trap. The significance here cannot be overstated as the only competitive technology in this space cannot maintain the fidelity of this information with any level of change in the trapped charge magnitude. SWIFT isolation which was first reported over twenty years ago has shown significant improvements in efficiency at the 21T field strength which opens the door for innovative development for new MS/MS protocols for complex mixtures.

Capability for providing dissociation of intact proteins under LC conditions has been enhanced with optimization of ion counts for trap filling which needs to be modulated as a function of molecular weight. Electronic dissociation methods for highly charged proteins have also been significantly enhanced by grafting the proton transfer method developed in an associated lab to reduce the charge distribution complexity prior to applying ETD. While the aforementioned methods have been proven to significantly increase the observed sequence coverage of intact proteins, the results shown to date have been primarily model compounds.

3. Intact Protein Analysis

Lissa Anderson leads the developments and applications in intact protein analysis. These efforts capitalize on the state-of-the-art 21 tesla FTICR mass spectrometer. The Mag Lab ICR group is collaborating closely with the NRTDP, a NIH P41 resource at Northwestern University that is focused on top-down mass spectrometry/proteomics. The pipeline involves a standard 2D approach, offline GelFree electrophoresis followed by online analysis of collected fractions by LC-21T FTICR-MS/MS. Acquired data are shipped to NRTDP for analysis. (This begs a question how to accommodate other users, esp. users unfamiliar with top-down MS and we suggest bringing data analysis capabilities onsite to expand user base. [all user data will be analyzed on the NRTDP platform, but if this turns out to be a problem we will develop our own analysis platform]) 21T FTICR with front-end ETD platform provides high sequence coverage on the LC time scale and has enabled identification of over 600 human proteins (corresponding to over 3000 human proteoforms) from human colorectal cancer cell lysate (JPR 2017). In collaboration with Mayo clinic, they have also applied this technology to for the first time effectively characterize antibody overexpressed in serum of multiple myeloma patients, setting a high standard for serum antibody MS-based assay. As a part of the NRTDP collaboration, the team acquired first ever spectra of the master cell regulator, human p53. p53 family of genes and their proteins have a wide variety of functions and top-down mass spectrometry will enable us to correlate a multitude of posttranslational modifications often found on these proteins to function and phenotype. This has been an area of extensive research over the last 30+ years and provides multiple opportunities to enrich user base and/or attract new funding. Newly developed data dependent acquisition that includes an adjustable cumulative ion target (CIT), i.e. adjusting ion fill times on-the-fly to account for different molecular mass, as well the addition of PTR-PIP capability holds great promise for top-down applications. Another exciting development is the use of high-resolution ion isolation (SWIFT) in combination with in-cell UVPD for characterization of closely related proteoforms, e.g. histones. While there is still work to do in order to extend applications to larger proteins and realize the full potential of the 21T in the realm of top-down proteomics, we have seen significant progress already made. There was a lot of discussion by the committee regarding the suitability of supporting NIH funded work with the resources of the magnet lab. Overall the committee felt that this subgroup has made huge strides since hiring Lissa Anderson to direct these activities, and that this is a significant component of the ICR laboratory.

4. Petroleomics and Environmental Chemistry

Ryan Rodgers leads the activities in the area of Petroleomics and Environmental Chemistry. This group has had another great year. They accommodated a record number of users, including new principal investigators and a large number of graduate students and postdoctoral researchers. The petroleum group is expanding the analytical horizons of chemical analysis through the incorporation of pre-fractionation. These added capabilities have immediate impact for operational problems in the field, thus pushing the boundaries of fundamental chemical knowledge while simultaneously solving real-world problems. Similarly, these tools are being used to explore the mechanisms of petroleum weathering during oil spills. This foundational knowledge will inform future responses to oil spills in marine environments, particularly regarding the use of containment versus dispersant technologies. The largest growing group of users for this team are investigators interested in natural organic mixtures, most notably dissolved organic matter in different aquatic systems. Current users bring large sample sets and will require advances in chromatography and pre-fractionation protocols, similar to those developed for petroleum applications by the MagLab. The committee commends the petroleum / environmental applications group for its outreach and ability to accommodate the burgeoning user community in these fields. We anticipate another good year ahead and encourage the group to further develop advanced tools for compound characterization in these complex mixtures.

5. Nanomaterials and Clusters

Paul Dunk leads the ICR facility's efforts in the area of nanomaterials and clusters. A dedicated 9.4 tesla FTICR instrument is committed to these studies. This instrument is equipped with a Smalley-type cluster source that uses laser ablation of a graphite rod and a pulsed molecular beam for generating fullerenes and endohedral fullerene complexes. This instrument is used to address important chemical questions regarding the synthesis of fullerenes in hot plasmas. For example, research with this instrument has shown that Sc_3N endofullerenes bypass C_{60} and other states that act as traps for the growth of carbon clusters, leading to the preferential formation of $Sc_3N@C_{84}$. Interesting mixed clusters have been made by gas-phase chemistry in which boron replaces a carbon atom in fullerenes and endofullerene complexes. Endofullerene complexes with many different clusters inside the fullerene cage are targets for current studies, and FTICR will be essential for establishing the elemental composition of the products. Dr. Dunk is expanding his research activities into the area of astrochemistry, specifically carbon-cluster ions which may be responsible for important diffuse interstellar bands. The user activity for this instrument is relatively modest (7 PI's and 22 users are currently active in the program), but they have produced some high-quality publications.

6. Outreach:

Amy McKenna is doing an outstanding job of managing outreach activities, which include K-12 activities, programs for middle school and high school students, and mentorship of undergraduate students. Also, the ICR subgroup organizes a biannual meeting, the North American FTMS Conference, which attracts the participation of 100 scientists from around the world, and is an important contribution to the scientific community by the ICR group.