ORNL/TM-2023/2922

2022 Quantum Materials Young Investigators Workshop Report

Adam Aczel
Stuart Calder

Date: April 28, 2023

OAK RIDGE NATIONAL LABORATORY
MANAGED BY UT-BATTELLE FOR THE US DEPARTMENT OF ENERGY

ORNL/TM-2023/2922

Neutron Sciences Directorate

Report from the
'2022 Quantum Materials Young Investigators Workshop'
August 18-19, 2022

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EXECUTIVE SUMMARY

The fifth edition of the workshop “Quantum Materials Young Investigators” was held August 18-19, 2022 at the Oak Ridge National Laboratory (ORNL). This workshop followed up on previous meetings that took place at ORNL starting in 2016. This important series of annual workshops, organized by Adam Aczel and Stuart Calder, ensures continuous engagement with the early career principal investigators (PIs) of the quantum materials neutron scattering community. Through a series of short scientific talks presented by the external PIs, members of the Neutron Scattering Division (NSD) learn about their scientific interests and needs. Presentations from ORNL staff members also help to inform the external PIs about the current state of ORNL’s quantum materials neutron scattering program. Topics covered include neutron scattering instruments, sample environment, neutron polarization, data reduction, visualization, and analysis, and future neutron scattering and complementary capabilities. Feedback is solicited from the external PIs in some or all of these key areas and communicated to NSD management in the form of a workshop report. This workshop series also helps to foster collaborations between NSD scientists and the research groups of the external PIs and plays an important role in attracting new neutron scattering users.

1. HISTORY AND CHARGE OF QUANTUM MATERIALS YOUNG INVESTIGATORS WORKSHOP SERIES

The Quantum Materials Young Investigator Workshop Series began in 2016 at the request of Steve Nagler, when he was the Quantum Condensed Matter Division Director. Steve thought that a yearly workshop for external early career scientists (< 10 – 15 years past their Ph.D.) would be a great way to advertise our neutron scattering capabilities to them, solicit important feedback about the user program on a wide range of topics, communicate our future plans for ORNL's neutron scattering program, and foster new collaborations between the external scientists and ORNL staff members. Adam Aczel and Stuart Calder were initially selected to organize this workshop series as co-PIs. They have now organized and ran a new workshop in this series once per year since 2016, except in 2020 and 2021 when the workshop was cancelled due to the COVID pandemic.

2. 2022 WORKSHOP PARTICIPANTS AND AGENDA

The list of participants for the 2022 workshop is presented here:

(i) External: Ben Fransden (Brigham Young University, virtual), Julia Munday (Harvard University, virtual), Kemp Plumb (Brown University), Arnab Banerjee (Purdue University), Julia Zaikina (Iowa State University), Alex Frano (University of California – San Diego), Alannah Hallas (University of British Columbia), Tai Kong (Arizona State University), Hillary Smith (Swathmore College), Mingda Li (MIT), Bill Gannon (University of Kentucky), and Nirmal Ghimire (George Mason University)

(ii) Internal: Adam Aczel (Spectroscopy), Stuart Calder (Diffraction), Travis Williams (Spectroscopy), Keith Taddei (Diffraction), Yan Wu (Diffraction), Qiang Zhang (Diffraction), Allen Scheie (Spectroscopy), Colin Sarkis (Spectroscopy), Maddy Marshall (Diffraction), Yiqing Hao (Diffraction), Jaime Fernandez-Baca (Spectroscopy), Lisa DeBeer-Schmitt (Large Scale Structures), Clarina dela Cruz (Diffraction), Matt Stone (Spectroscopy), Feng Ye (Diffraction), Doug Abernathy (Spectroscopy), Barry Winn (Spectroscopy), Valeria Lauter (Large Scale Structures), Matthias Frontzek (Diffraction), Victor Fanelli (Sample Environment and Labs), Josh Pierce (Sample Environment and Labs), Hans Christen (NSD), Jon Taylor (NSD), Ken Herwig (STS), and Mark Champion (PPU)

The fifth edition of this workshop in 2022 followed a very similar format to the previous four versions, although we did host a hybrid format for the first time with two virtual external participants. The detailed agenda is presented next:

August 18, 2022 **Clinch River Cabin, ORNL**

Time	Event	Session Chair and Scribe
8:30–9:00 am	Morning coffee	
9:00-10:30 am	(i) Welcome: Hans Christen (9:00) (ii) Workshop Charge: Stuart Calder or Adam Aczel (9:05) (iii) Science talk: Arnab Banerjee (9:10) (iv) Powder Diffraction Suite: Clarina dela Cruz (9:30) (v) Single Crystal Diffraction Suite: Feng Ye (9:50) (vi) Diffraction Suite Discussion (10:10)	Adam Aczel, Qiang Zhang
10:30-10:45 am	Morning Break	
10:45-12:30 pm	(i) Science talks: Kemp Plumb (10:45), Julia Zaikina (11:05) (ii) Time-of-flight Spectrometers: Doug Abernathy (11:25) (iii) Triple axis spectrometers: Adam Aczel (11:45) (iv) Spectroscopy Suite Discussion (12:05) (v) Group photo (12:25)	Stuart Calder, Qiang Zhang
12:30-1:30 pm	Working Lunch: Introduction to the Quantum Materials Initiative and Possible Collaborations	Matt Stone, Clarina dela Cruz
1:30-3:30 pm	(i) Science talks: Julia Mundy (1:30), Ben Frandsen (1:50), Alex Frano (2:10) (ii) Low-T/High-B: Current Capabilities: Josh Pierce or Victor Fanelli (2:30) (iii) Low-T/High-B: Future Capabilities: Stuart Calder (2:50) (iv) Low-T/High-B Discussion (3:10)	Adam Aczel, Keith Taddei
3:30-3:45 pm	Afternoon Break	
3:45-5:30 pm	(i) Science talks: Alannah Hallas (3:45), Nirmal Ghimire (4:05) (ii) High Pressure: Yan Wu (4:25) (iii) Polarization: Barry Winn (4:45) (iv) High Pressure and Polarization Discussion (5:05)	Stuart Calder, Keith Taddei
6:00-8:00 pm	Working Dinner at the Clinch River Cabin **10 year plan for Quantum Materials and Neutrons**	Jaime Fernandez-Baca

August 19, 2022 **Clinch River Cabin, ORNL**

Time	Event	Session Chair and Scribe
8:30-9:00 AM	Morning coffee	
9:00-10:30 am	(i) Science Talks: Bill Gannon (9:00), Mingda Li (9:20) (ii) GP-SANS: Lisa DeBeer-Schmitt (9:40) (iii) Magnetism Reflectometer: Valeria Lauter (9:55) (iv) GP-SANS and Magnetism Reflectometer Discussion (10:10)	Adam Aczel, Travis Williams
10:30-10:45 am	Morning Break	
10:45-12:20 pm	(i) Science talks: Tai Kong (10:45), Hilary Smith (11:05) (ii) HBRR and HFIR SENSe: Matthias Frontzek (11:25) (iii) HFIR Upgrades Discussion (11:55)	Stuart Calder, Travis Williams
12:20-1:20 pm	Working Lunch: Data Analysis	Jon Taylor
1:20-2:45 pm	(i) PPU - Current Status and Technical Details: Mark Champion (1:20) (ii) STS - Current Status and Technical Details: Ken Herwig (1:50) (iii) PPU and STS discussion (2:20)	Adam Aczel, Yan Wu
2:45-3:00 pm	Meeting close-out	Adam Aczel / Stuart Calder
3:00-4:00 pm	Optional tours of the SNS and HFIR	Adam Aczel / Stuart Calder

3. WORKSHOP WELCOME

The Neutron Scattering Division Director Hans Christen welcomed the participants and delivered a few opening remarks at the beginning of the workshop. Adam Aczel then had the workshop participants introduce themselves and he provided some general information about the neutron scattering user program at ORNL. Adam also presented the workshop charge, which is provided in the Executive Summary of this workshop report.

4. QUANTUM MATERIALS YOUNG INVESTIGATOR SCIENCE

This workshop series plays an important role in enhancing the Neutron Scattering Division's understanding of the key science drivers and important new trends in quantum materials research. Typically, this information has been communicated to NSD staff by having the external PIs present short science talks (15-20 minutes) at these workshops. These talks may concentrate on one specific project or research area that the PI's group is interested in, or they may provide a general overview of the PI's research program. Another important goal of these talks is for the PI to communicate how his/her group uses neutron scattering as a research tool now or plans to use the technique in the future. This information helps to inform NSD's investments in ORNL's quantum materials neutron scattering program.

We had 12 external PIs present scientific talks at the 2022 workshop. Based on the scientific talks, the research expertise of the external PIs is as follows:

1. **Ben Frandsen (Brigham Young University)**: Neutron diffraction, pair-distribution function, and muon spin relaxation studies of quantum materials, including Fe-based superconductors
2. **Alex Frano (University of California – San Diego)**: Resonant x-ray scattering studies of high-temperature superconductors (e.g. cuprates) and heavy transition metal-based frustrated magnets
3. **Alannah Hallas (University of British Columbia)**: Powder and single crystal synthesis, bulk characterization, and neutron scattering studies of novel frustrated magnets, high entropy oxides, and itinerant magnets
4. **Nirmal Ghimire (George Mason University)**: Powder and single crystal synthesis, bulk characterization, and neutron diffraction studies of correlated topological materials
5. **Hillary Smith (Swathmore College)**: Neutron spectroscopy studies of lattice dynamics, spin-phonon interactions, and glass-forming liquids
6. **Julia Zaikina (Iowa State University)**: Powder and single crystal synthesis, bulk characterization, and neutron diffraction studies of novel borides, antimonides, and functional oxides and sulfides
7. **Kemp Plumb (Brown University)**: Neutron spectroscopy studies of frustrated magnets, heavy transition metal magnets, and low-dimensional magnets
8. **Mingda Li (MIT)**: Neutron scattering studies of quantum materials using machine learning
9. **Tai Kong (Arizona State University)**: Powder and single crystal synthesis, bulk characterization, and neutron diffraction studies of frustrated magnets
10. **Julia Mundy (Harvard University)**: Thin film synthesis, characterization, and neutron diffraction studies of complex oxides
11. **Bill Gannon (University of Kentucky)**: Neutron diffraction and spectroscopy studies of frustrated magnets and topological magnetic materials
12. **Arnab Banerjee (Purdue University)**: Neutron diffraction and spectroscopy studies of frustrated and low-dimensional quantum magnets, including spin liquid candidates

5. THE QUANTUM MATERIALS INITIATIVE IN THE NEUTRON SCIENCES DIRECTORATE

The Quantum Materials Initiative in the Neutron Sciences Directorate, currently led by Matt Stone, was founded in 2017. Since that time, the quantum materials initiative coordinator has presented a talk at each Quantum Materials Young Investigators workshop. This talk was delivered by Matt in 2022. He covered recent activities that have been organized or sponsored by the initiative, including funding proposals, workshops, and educational opportunities. He also discussed graduate student and postdoctoral fellowship opportunities in the Neutron Sciences Directorate at ORNL. The feedback from the external PIs on this talk is generally quite positive, as they are often not aware of all the educational neutron scattering and collaboration opportunities available for both themselves and their graduate students. Therefore, this talk is typically an excellent outreach platform and an effective way for the external PIs and NSD staff to begin new collaborations or enhance existing ones. This talk has generally been presented during a working lunch on the first day of the workshop to ensure that there is plenty of time for informal discussions and networking during the remainder of the workshop.

6. NEUTRON SCATTERING INSTRUMENTS FOR QUANTUM MATERIALS RESEARCH

Since one of the goals of this workshop series is to attract new quantum materials neutron scattering users to ORNL, we typically present overviews of the various instruments important for quantum materials research. We also discuss recent instrument upgrades in these talks. More specifically, the topics covered in the 2022 workshop included the following.

6.1: Powder Diffraction

This talk covered the powder diffraction suite, which includes NOMAD, POWGEN, HB-2A, and $WAND^2$. Highlights included the following topics: (1) the overwhelming success of the mail-in program at POWGEN and NOMAD, (2) implementation of a new He-3 CCR on HB-2A with a three sample changer that dramatically improves measurement efficiency down to 250 mK, (3) the addition of a half-polarized beam option to the HB-2A user program, and (4) development of gas loading capabilities at cryogenic temperatures on POWGEN.

6.2: Single Crystal Diffraction

This talk covered the single crystal diffraction suite, which includes TOPAZ, MANDI, CORELLI, DEMAND, IMAGINE, and $WAND^2$. Highlights included the following topics: (1) implementation of a significant detector upgrade at DEMAND that enables the instrument to operate in a two-axis mode that can accommodate complex sample environments, (2) the addition of a half-polarized beam option to the DEMAND user program, (3) the addition of a 14 T vertical field cryomagnet to the CORELLI user program, and (4) the addition of a cryogoniometer (base T of 5 K) to the TOPAZ user program.

6.3: Direct Geometry Spectroscopy

This talk covered the direct geometry spectroscopy suite, which includes CNCS, HYSPEC, ARCS, and SEQUOIA. Highlights included the following topics: (1) the addition of a 14 T vertical field cryomagnet to the SEQUOIA and HYSPEC user programs, (2) implementation of an elevator system at HYSPEC to facilitate quick changes between polarized and unpolarized modes, and (3) the addition of new top-loading closed cycle refrigerators to the ARCS and SEQUOIA user programs.

6.4: Triple Axis Spectroscopy

This talk covered the triple axis spectroscopy suite, which includes HB-1A, HB-1, HB-3, and CTAX. Highlights included the following topics: (1) completion of the HB-1A double-bounce monochromator system that moved the vertical beam focus to the sample position, resulting in a 3x flux gain, (2) discussion of HB-1A's ongoing backend upgrade that will improve the signal-to-noise ratio of the instrument, facilitate tilting of heavy sample environments, and enable a four-circle option, (3) implementation of Wollaston Prism technology at HB-1 for ultra-high resolution diffraction and spectroscopy, (4) implementation of a spherical neutron polarimetry capability at HB-1 to facilitate investigations of complex magnetic structures, (5) procurement of new Heusler crystals to improve HB-1's polarized monochromator and analyzer reflectivity and flipping ratio, and (6) plans to reconfigure the HFIR cold guide hall during the next Be reflector changeout in 2028 to enable the implementation of several upgrades and the construction of new world-class instruments, including a modern cold triple axis spectrometer MANTA. It is anticipated that MANTA will have an interchangeable backend with both traditional single analyzer-detector and multiplexed secondary spectrometer options.

6.5: Small Angle Neutron Scattering

This talk focused primarily on magnetic studies using GP-SANS, but it also contained some information on non-magnetic SANS studies using the full suite of SANS instruments at ORNL. Highlights included the following topics: (1) the discussion of topical science examples including recent work on flux-line lattices in Type-II superconductors, long-period spin textures, and magnetic domains, (2) the addition of a strain cell for cryomagnets to the user program to facilitate compression or tension measurements on single crystal samples, and (3) the implementation of time-resolved SANS at ORNL.

6.6: Reflectometry

This talk discussed the magnetism reflectometer (MAG-REF) at the SNS. Highlights included the following topics: (1) a description of the instrument's unique grazing incidence neutron scattering capability for complete characterization and mesoscale control of thin film heterostructure materials, and (2) a discussion of in-operando experiments on the instrument.

7. SAMPLE ENVIRONMENT

Quantum materials studies often require low temperatures, high magnetic fields, and/or applied pressures. Therefore, 'low T/high B' and 'high pressure' sample environment support, capabilities, and developments are extremely important to ensure the continued success of a neutron scattering program in this important research area. Each workshop in this series now consists of talks in each of these sample environment focus areas. These talks provide an overview of the current capabilities and discuss active developments and future plans. We also remind the external PIs of the two relevant sample environment steering committees, who is chairing them and the charge and role of these committees in NSD. Finally, there is an extended discussion with the external PIs where we solicit their feedback on the two different sample environment focus areas.

7.1: Sample Environment Steering Committees

There are four sample environment steering committees in NSD: (i) high magnetic field, low temperature, (ii) high temperature, (iii) high pressure, and (iv) soft matter. These committees help NSD management to set priorities for acquiring new sample environment equipment in their respective areas and they work to improve operational reliability through discussion and advocation for critical spares, automation, and replacement of older equipment. These committees also stress the importance of best practices to obtain high quality data in the sample environments being used, and they solicit feedback from the user community to help ensure that the sample environment capabilities at ORNL's neutron scattering facilities are world-class. These committees provide justifications, applications for funding, prioritization of needs, and creation of specification documents to expand the equipment pool of sample environments. Finally, these committees work with potential LDRD teams at ORNL to develop and prioritize sample environment proposals.

7.2: Low Temperature, High Magnetic Fields

Most of the quantum materials neutron scattering experiments at ORNL require sample environment capabilities that are part of this focus area. The relevant sample environment steering committee is led by **Stuart Calder** and is quite active. Several new low T/high B sample environments have recently been introduced into the neutron scattering user programs at SNS or HFIR, including a 14 T vertical field cryomagnet for SEQUOIA and CORELLI at the SNS, a 6 T vertical field cryomagnet for several HFIR diffractometers and spectrometers to replace MAG-B, and a 5 T open-bore magnet for the SNS that will be used at EQ-SANS and MAG-REF. We also have an 11 T vertical field cryomagnet that will be commissioned to run on CTAX within the next year. Finally, we have recently introduced two He-3 closed cycle refrigerators into the user program for several HFIR diffraction instruments (i.e. HB-2A, $WAND^2$, and DEMAND). These are push-button systems that require limited sample environment personnel support. They are particularly beneficial for HB-2A's user program, as the instrument team has developed a three-sample changer option for this system.

Low sample environment staffing levels have been an historical concern in this area, and this topic was discussed again at the 2022 workshop. Significant improvements were noted and the decision to split up the low T/high B group into two separate groups based at HFIR and SNS was applauded. This decision ensures that the group leaders at each facility can concentrate on the individual low T/high B needs of a given source and they can provide additional operational support. It was noted that current staffing levels have almost reached an optimum level, with five FTEs (including the group leader) currently based at HFIR and four FTEs (including the group leader) working at the SNS. The diversity of the groups has also been improved, with technicians and sample environment physicists now working together on providing operational support and equipment maintenance and performing R&D activities.

Automation has also played a key role in improving the operational efficiency of user experiments that require low-temperature and/or magnet sample environments. The liquid helium autofill system (LHeAF) has been deployed across most cryostats and cryomagnets at SNS and HFIR, closed cycle refrigerator and cryostat sample changers for polycrystalline samples are now becoming more commonplace, and sample changers for polycrystalline samples that require ultra-low temperatures have either been deployed on select beamlines (i.e. He-3 CCR sample changers for HB-2A, as noted above) or they are under development (i.e. dilution fridge insert sample changer for HB-2A).

The external PIs and internal staff members expressed satisfaction with the current after-hours support model. Users with sample environment issues after hours are expected to call the instrument hall coordinator, who then calls the appropriate sample environment staff member from their call-down list. Everyone believes that this system is working quite well, and typically after-hours issues are addressed in a relatively efficient manner.

Feedback from quantum materials workshop participants:

(1) Moving to cryogen-free sample environments is a smart choice when and if it is possible.
(2) Horizontal field magnets with the small dark angles required for diffraction and spectroscopy instruments provide unique experimental capabilities that are currently not available at ORNL. For example, specific sample geometries may require horizontal fields to access the magnetic Bragg peaks or magnetic excitations of interest.
(3) Pulsed field capabilities with variable field ramp rates, pulse shapes, and maximum fields are of interest for exploring non-equilibrium physics in quantum materials.
(4) A uniaxial strain device where the user can modify the strain in-situ would be very useful for many of the diffraction instruments, and possibly for some of the spectroscopy instruments as well.
(5) Some external participants are interested in partnering with ORNL to develop specific sample environment capabilities and they would like to understand the best way to go about doing this.

7.3: High Pressure

The Neutron Scattering Division has both a High-Pressure Science Initiative led by **Bianca Haberl** and an active high-pressure sample environment steering committee led by **Yan Wu**. ORNL's user program can run neutron experiments with various types of pressure cells including different types of gas cells, SANS pressure cells, clamped piston-cylinder cells, Paris-Edinburgh cells, and diamond anvil cells (DACs). Information for commissioned pressure cells can typically be found on the beamline websites. New pressure capabilities continue to be developed and there is a plan for the collective full list to be available in an online database for the user community. For now, some essential information about each type of cell is provided below:

The gas cells are available for *in situ* pressure changes, and they usually have relatively low backgrounds and large volume sample spaces (cm^3 range). The pressure range of the gas cells are from hundreds of bars for the gas handling systems to about 0.6 GPa for the gas intensifier pressure cells. Low pressure gas handling systems are currently available at the beamlines POWGEN, NOMAD, VISION, and some other beamlines upon request. Gas intensifier pressure systems are available at most beamlines supported by the High Pressure Group. A 1 GPa gas cell is currently under development at ORNL to go with the new 1 GPa gas intensifier. The pressure limit of gas cells is restrictive for hard condensed matter investigations, but they work well to explore pressure-induced transitions and phenomena in a subset of quantum materials. Information about these capabilities can be found on the appropriate instrument websites or by contacting the high-pressure sample environment staff Mark Loguillo and Matt Rucker.

Clamp cells are the most frequently employed pressure cells for studying quantum materials at ORNL's neutron sources. They are piston-cylinder cells pressurized offline that have moderate volume sample spaces (mm^3-cm^3). They fit in most sample environments, including dilution fridge inserts. The maximum pressure of these cells typically ranges from 1.3 GPa to 2 GPa and they have minimal dark angles or none. The cell background and beam attenuation depend on the cell design. The polycrystalline background from a clamp cell usually contaminates a substantial amount of reciprocal space in both the elastic and inelastic channels that needs to be considered on a case-by-case basis. Another significant challenge with the clamp cells is that single crystal samples need to be aligned and properly cut and polished to maintain their orientation in the cell. Careful planning and loading are essential in obtaining hydrostatic pressures and completing successful experiments. Interested users should contact the relevant instrument team for specifics before they submit a clamp cell proposal.

Another pressure capability is the Paris-Edinburgh (PE) press that was first commissioned on the SNAP beamline. The maximum pressure is ~10 GPa for the single toroidal anvils (cBN) and up to ~20 GPa for the double toroidal anvils (PCD). The single toroidal anvils can also be cooled to 80 K. A major advantage of the PE cell is the (relatively) large sample volume of 31/87 mm^3 (less if used with encapsulated gaskets for liquid pressure media). This cell allows for *in situ* pressure changes and its vertical opening angle is +/- 7º for scattering experiments. It is often used for powder experiments, but it can also accommodate single crystals as well. Beyond SNAP, this cell is also being adapted to other beamlines, specifically ARCS and $WAND^2$ at HFIR. Interested users should contact instrument teams for information.

The DACs provide the highest pressures although the maximum value depends critically on the exact experiment. Important considerations are additional temperature requirements, special needs for sample preparation and experiment conditions, sample scattering power and so on. This informs the type of anvil that is used, the exact cell that is used, the smallest sample volume possible, and the maximum pressure possible. Typical guidelines are:

- Room temperature compression on high symmetry powder samples is possible to 100 GPa on SNAP. These cells allow for *in situ* pressure changes, have a scattering aperture of +/-35º and use single crystal anvils (a standard culet size would be 800 μm for a sample volume of 0.01 mm^3). Work is in process to benchmark single crystal capabilities. This cell can be gas loaded.

- Low temperature compression (T_{min} = 7 K) can be performed up to 30 GPa using the same cells on SNAP (a standard culet size would be 1.5 mm for a sample volume of 0.05 mm^3). This cell can be gas loaded.
- A clamped version of this DAC with +/- 60º has also been tested/used on the SNAP, VISION, SEQUOIA, CORELLI, DEMAND, and IMAGINE beamlines. This cell exhibits excellent temperature stability and is usually operated between 5-300 K. A DAC experiment at ultra-low temperature has recently been commissioned at SNAP. These cells can use single crystal anvils but are more typically used with polycrystalline Versimax. This allows for 3 mm culets and sample volumes of 0.9 mm^3 at pressures up to 10 GPa. These cells tend to be run exclusively with single crystal samples and liquid pressure media.

The pressure loading process, including the choice of pressure medium needs to be carefully planned. In general, close involvement from the users is expected in the sample preparation and loading process of DACs. Interested parties should contact the SNAP team/Bianca Haberl/Yan Wu for more information about the DACs.

Finally, there are other pressure systems available including palm cubic anvil cells and uniaxial pressure systems. Palm cubic anvil cells with a maximum pressure of 8 GPa and a base temperature of 1.5 K have been run at HB-1 and $WAND^2$, in close collaboration with Prof. Uwatoko's group. Several uniaxial pressure systems are currently under commissioning and some of these capabilities should be available for the user program soon.

Feedback from quantum materials workshop participants:

(1) It was suggested that some benchmarking data of cell backgrounds be made readily available to users. Some of this information is available directly from the High Pressure Group, but it is not necessarily clear who to contact for specific requests. The sample environment website should be updated with POCs for different cell types.
(2) A complete database for ORNL's pressure cell inventory should be added to the Neutron Sciences website. Most users are not well-informed on the current high-pressure capabilities.
(3) Pressure cell experiment checklists for the different types of experiments that are performed (i.e. gas cell, clamp cell, diamond anvil cell) could be provided on the Neutron Sciences website. For example, what are the logistical issues that need to be addressed before a user arrives onsite, or after the user is onsite but before the experiment starts? How far in advance should a user arrive before a pressure experiment? What are the sample considerations? Perhaps the local experts on the High Pressure Steering Committee could work on developing these checklists.

8. NEUTRON POLARIZATION

Polarized neutron capabilities are becoming more commonplace across the instrument suite at HFIR and SNS, with four instruments at the former and three instruments at the latter routinely running polarized experiments now. Polarized neutron beams offer many advantages over their unpolarized counterparts, including the ability to isolate nuclear and magnetic scattering, solve the phase problem, explore magnetic chirality, enhance Q-resolution for diffraction, and match the instrument resolution to a dispersion curve. A polarization steering committee, led by co-chairs Barry Winn and Josh Pierce, was formed in 2022. The primary goal of this steering committee is to align the scientific needs of the Neutron Scattering Division with the Neutron Sciences Directorate development plans and to advocate for the operational resources required to support these scientific needs. This committee has already developed a summary of the current polarization capabilities across ORNL's neutron scattering instrument suite and a list of desired capabilities for the future.

At the 2022 workshop, Barry Winn presented a talk that discussed using neutron polarization for studying quantum materials. He introduced the concept of neutron polarization, he described the steering committee and its charge, he explained the types of experiments that benefit from polarized neutrons, and he went through the different polarization modes available to users at ORNL. He also advertised a polarized neutron workshop that was scheduled to take place about a month after this one.

9. FUTURE OF NEUTRON SCATTERING AT ORNL

There are several ongoing efforts to develop new neutron scattering capabilities at ORNL that will enhance the quantum materials user program. Several workshop talks provided updates on these projects.

9.1: HFIR Cold Guide Hall Re-optimization

Matthias Frontzek presented a talk that discussed ORNL's plans to re-optimize the HFIR cold guide hall during the next Be reflector change in 2028. The main highlights are as follows: (1) a new cold triple axis spectrometer, MANTA, will be built at the NB-6 position, (2) the cold guide hall building will be extended to accommodate a new cold neutron imaging and spin echo instrument, (3) the current CG-4 guide will be split into several end stations to accommodate IMAGINE, an alignment station, and the spin echo instrument. Matthias also mentioned that the long-term future of HFIR is now being actively discussed, including a possible replacement for the pressure vessel that would significantly extend the lifetime of the facility. There are additional long-term upgrade discussions taking place about building a new thermal guide hall off the HB-2 beam port.

9.2: SNS Proton Power Upgrade

Mark Champion discussed the ongoing SNS Proton Power Upgrade (PPU) project. The major deliverables are an upgraded accelerator that will provide a 2 MW pulsed neutron beam to the First Target Station and be capable of delivering a 0.8 MW pulsed neutron beam to the Second Target Station. The PPU project is expected to be completed in Jan. 2025.

9.3: Second Target Station

Ken Herwig discussed the current status and technical details of the Second Target Station. This project passed the CD-1 review phase in Nov. 2020 and it has now entered the preliminary design phase. The first eight instruments have also been approved. The quantum materials community is particularly interested in CHESS (a cold neutron chopper spectrometer), VERDI (a polarized diffractometer), and PIONEER (a single crystal diffractometer). These eight initial instruments now have an Instrument Advisory Team associated with them to provide input into the instrument design and to assist with planning for early science success.

10. DATA REDUCTION, VISUALIZATION, AND ANALYSIS

There has been a great deal of turnover in this area in the last few years due to the departure of the former point-of-contact, Jay Billings, in 2020. Jon Taylor has recently been hired to replace Jay and one of his first impending tasks is to make recommendations about how to best restructure the way that neutron scattering software needs are met at ORNL. In the current model, a group of software engineers works together on software activities that are considered to have the highest priority across the neutron scattering instrument suite, with extremely limited support provided for other smaller software projects during this time. Computational instrument scientists were also hired to work in the different Neutron Scattering Division science groups. Their main tasks are to gain an understanding of the software needs of a subset of instruments, to communicate these needs to management and the software engineers, to provide software support to instrument teams and users, and to work on complementary software development. This model has produced some successes (e.g. robust SANS and diffraction data reduction capabilities), but frustration for scientists on other instruments still waiting for their data reduction needs to be met by the software engineers (e.g. instruments across the Spectroscopy Section). Jon Taylor presented a talk during the working lunch on the second day of this workshop that touched on some of this history. He also discussed future plans for data reduction, visualization, and analysis. We avoided asking the workshop participants for detailed feedback about these topics since the Neutron Scattering Division's internal plans were being revised at the time this workshop took place.

11. GENERAL PARTICIPANT FEEDBACK AND TESTIMONIALS

(1) General feedback on the workshop format or ORNL's neutron scattering user program

(i) Everybody agrees that it is appropriate for the external PIs to deliver 20-minute talks about their group's research interests at these workshops.

(ii) It would be nice if the external PIs had more time to interact with each other and build collaborations. Perhaps one option is to set aside some working group time.

(iii) In future workshops, consider discussing machine learning or supercomputing approaches to studying quantum materials. Several external PIs are interested in collaboration opportunities between their groups and the machine learning/supercomputing experts at ORNL.

(iv) Consider compiling a contact list of previous and current participants (they could opt in or out of the list). This list should include each participant's name, email, institution, and a sentence about their research activities. Sharing such a list with the relevant parties could help foster communication and collaboration between external participants and/or ORNL staff.

(v) Think about organizing a "speed networking" event towards the end of the workshop between workshop participants and instrument scientists. This event could include small working groups where instrument scientists can provide their suggestions on how a specific technique/instrument can be used to advance the understanding of quantum materials. Additionally, this could be a good time to discuss some specific/technical details of the technique or instrument.

(vi) Expanding neutron spectroscopy and diffraction mail-in programs on different instruments is invaluable for future advances in quantum materials research (especially, in the context of young investigators' research where travel funding may be limited).

(vii) Think about ways to enhance partnerships with synchrotron x-ray user facilities to facilitate simultaneous access to X-ray and neutron scattering data.

(2) Additional feedback and testimonials from specific workshop participants

(i) Mingda Li: "Thank you for organizing the wonderful meeting! I really enjoyed the meeting and meeting everyone and seeing the great research of so many colleagues.

(ii) Alex Frano: "I will think of constructive feedback to you, but overall I think the workshop was extremely interesting, informative, and inspiring me to thinking about neutron experiments."

(iii) Arnab Banerjee: "I think that the workshop was excellent and very informative, especially on the STS, Beryllium plug outage, and FTS planning details, as well as knowing a whole gamut of new research performed by the faculty in various related walks of life. The arrangement was excellent too, and the hybrid format worked well technically, except, I am not sure how long the hybrid participants hung around. Great to finally meet everyone again."

(iv) Julia Zakina: "Thank you for organizing the 2022 QMYI workshop! It was a pleasure to visit ORNL and learn about the recent developments in advanced characterization methods and the science that goes along with them. Thank you for inviting me. QMYI workshop was also a great networking experience allowing me to learn about research that is slightly outside my research area. I am looking forward to new collaborations as a result of this workshop."

(v) Bill Gannon: “Thanks for inviting me to the workshop. It was important to hear about current capabilities and those planned for the future in neutron scattering. Discussing these capabilities in specific contexts by looking at the current work of my peers was quite helpful. I would happily attend again in the future.”

(vi) Ben Frandsen: “I feel that this workshop is highly valuable for the participants. My first time participating was during the 2019 workshop, and I established multiple collaborations and friendships with other young investigators as a direct result of the workshop. I expect that I will also develop collaborations as a result of my second time participating in the workshop this year. Both workshops also taught me a lot more about the instrumentation and various capabilities at ORNL, as well as opportunities for collaboration such as the SCGSR and SULI programs. I really appreciated the accommodations that were made to allow me to participate remotely. I think the in-person component is really key to the success of the workshop by facilitating friendship and collaboration more naturally, but allowing a remote connection for a small number of participants who can't come in person was really helpful for me.”

12. QUANTUM MATERIALS YOUNG INVESTIGATORS MASTER LIST AND PAST WORKSHOP PARTICIPANTS

Table 1: Quantum Materials Young Investigators Master List and Past Workshop Participants

Name and Institution	Email Address	Years Attended
1. **Kate Ross**, Colorado State University	rosska2@rams.colostate.edu	2016
2. **Xianglin Ke**, Michigan State University	ke@pa.msu.edu	2016, 2017
3. **Deepak Singh**, University of Missouri	singhdk@missouri.edu	2016, 2018
4. **Sara Haravifard**, Duke University	haravifard@phy.duke.edu	2016, 2017, 2019
5. **Martin Mourigal**, Georgia Institute of Technology	mourigal@gatech.edu	2016, 2017
6. **Ni Ni**, University of California – Los Angeles	nini@physics.ucla.edu	2016
7. **Greg MacDougall**, University of Illinois at Urbana-Champaign	gmacdoug@illinois.edu	2016, 2017, 2018
8. **Edwin Fohtung**, New Mexico State University	efohtung@nmsu.edu	2016, 2017
9. **Christianne Beekman**, Florida State University	beekman@magnet.fsu.edu	2016, 2017, 2018
10. **Steve Bennett**, Naval Research Laboratory	steven.bennett@nrl.navy.mil	2016, 2019
11. **Corey Thompson**, Purdue University	cmthompson@purdue.edu	2018
12. **Jared Allred**, The University of Alabama	jmallred@ua.edu	2017, 2019
13. **Kemp Plumb**, Brown University	kemp_plumb@brown.edu	2017, 2018, 2022
14. **Steve May**, Drexel University	smay@coe.drexel.edu	2018
15. **Byron Freelon**, University of Houston	bkfreelon@uh.edu	2019
16. **Daniel Shoemaker**, University of Illinois at Urbana-Champaign	dpshoema@illinois.edu	2018, 2019
17. **Junjie Yang**, Central Michigan University	yang6j@cmich.edu	2018, 2019
18. **Ben Frandsen**, Brigham Young University	benfrandsen@gmail.com	2019, 2022 (virtual)
19. **Dustin Gilbert**, University of Tennessee	dagilbert@utk.edu	2019
20. **Nirmal Ghimire**, George Mason University	nghimire@gmu.edu	2019, 2022

21. **Chen Li**, University of California – Riverside	chen.li@ucr.edu	
22. **Efrain Rodriguez**, University of Maryland	efrain@umd.edu	2019
23. **Hari Nair**, University of Texas at El Paso	hnair@utep.edu	2019
24. **Weiwei Xie**, Louisiana State University	weiweix@lsu.edu	2019
25. **Arnab Banerjee**, Purdue University (Jan. 2020)	banerjeea@ornl.gov	2019, 2022
26. **Julia Zaikina**, Iowa State University	yzaikina@iastate.edu	2022
27. **Alex Frano**, University of California – San Diego	afrano@physics.ucsd.edu	2022
28. **Joe Checkelsky**, Massachusetts Institute of Technology	checkelsky@mit.edu	
29. **Ryan Baumbach**, Florida State University	baumbach@magnet.fsu.edu	2018
30. **Valentin Taufour**, University of California - Davis	vtaufour@ucdavis.edu	2018
31. **Chetan Dhital**, Kennesaw State University	cdhital@kennesaw.edu	2018
32. **Alannah Hallas**, University of British Columbia	alannah.hallas@gmail.com	2022
33. **Bill Gannon**, University of Kentucky	wgannon@uky.edu	2022
34. **Ming Yi**, Rice University	mingyi@rice.edu	
35. **Stephen Wilson**, University of California – Santa Barbara	stephendwilson@engineering.ucsb.edu	2016, 2017
36. **Jamie Neilson**, Colorado State University	james.neilson@colostate.edu	2017
37. **Marc Janoschek**, Paul Scherrer Institute	marc.janoschek@psi.ch	2017
38. **Olivier Delaire**, Duke University	olivier.delaire@duke.edu	2018
39. **Gavin Hester**, Brock University	ghester@BrockU.ca	
40. **Mingda Li**, Massachusetts Institute of Technology	mingda@mit.edu	2022
41. **Tai Kong**, University of Arizona	tkong@arizona.edu	2022
42. **Julia Mundy**, Harvard University	mundy@fas.harvard.edu	2022 (virtual)
43. **Hillary Smith**, Swathmore College	hsmith3@swarthmore.edu	2022
44. **Ryan Need**, University of Florida	rneed@ufl.edu	

45. **Min Gyu Kim**, University of Wisconsin – Milwaukee	mgkim@uwm.edu	
46. **Thao Tran**, Clemson University	thao@clemson.edu	
47. **Matthew Krogstad**, Argonne National Lab	krogstad@anl.gov	
48. **Xiaojian Bai**, Louisiana State University	xbai@lsu.edu	
49. **Allen Scheie**, Los Alamos National Laboratory	scheie@lanl.gov	
50. **Rebecca Dally**, National Institute of Standards and Technology	rebecca.dally@nist.gov	
51. **Jon Gaudet**, National Institute of Standards and Technology	jonathon.gaudet@nist.gov	
52. **Pat Clancy**, McMaster University	clancyp@mcmaster.ca	