FINAL REPORT

2022 Fundamentals of Quantum Materials School and Workshop

School: June 20-23, 2022 - at the University of Maryland, College Park
Workshop: June 24, 2022 - at The Hotel at the University of Maryland

Organizers: Johnpierre Paglione (Physics), University of Maryland
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Nick Butch, NIST Center for Neutron Research

Funding: Gordon and Betty Moore Foundation (GBMF)
National Science Foundation (NSF)
Institute for Complex Adaptive Matter (ICAM)

Narrative:
Since 2017, the University of Maryland has hosted in January the Fundamentals of Quantum Materials school and workshop. This event is dedicated specifically to the synthesis, characterization and electronic modelling of quantum materials. We continue to receive enthusiastic accolades from both the students and senior researchers who participated. The school serves current and future generations of quantum materials researchers, and has fueled the 2020 publication of the text "Fundamentals of Quantum Materials," featuring contributions from many school participants. We now provide this text to the school participants as a reference. Each year, we highlight a different subfield of quantum materials: 2018 - thin films, 2019 - materials for quantum information, and 2020 - exotic and topological superconductors, which are discussed in more detail during the lectures. The event was not held in 2021 due to the COVID pandemic and postponed to June 2022. The theme for the 2022 events was "*Magnetism in Quantum Materials*."

Structure:
This school and workshop were aimed to bring together an interdisciplinary group of researchers and students to help advance the fundamental understanding and culture behind the development, optimization and characterization of quantum materials. Because there are currently few schools in the US that focus on practical synthesis approaches in this field, our vision was to establish such a school that

will serve current and future generations of Quantum Materials scientists in the US much like the Boulder School has nurtured many successful generations of condensed matter physicists. The structure of the school includes mornings of pedagogical lectures by the nation's top practicing quantum materials scientists, with afternoons devoted to practical demonstrations in laboratories in the University of Maryland's Quantum Materials Center. The school also includes a poster session attended by senior scientists. The **FQM Workshop**, following the school event, covers current top research on quantum materials, focusing on synthesis, characterization and computational approaches to research of quantum materials such as superconductors, strongly correlated electron systems and topological materials. The lectures are recorded and available online at https://fqm.physics.umd.edu/.

Funding:
The two events were jointly sponsored by the Gordon and Betty Moore Foundation's EPiQS Program, The Institute for Complex Adaptive Matter (ICAM), the Joint Quantum Institute, the NIST Center for Neutron Research and the host (Maryland Quantum Materials Center). Funds were utilized to cover costs of hotel accommodations for all attendees and invited speakers, catering for the week's activities and two receptions (student poster session and workshop banquet), as well as the venue for the FQM workshop.

Logistics:
The school spanned 4 days, from Monday through Thursday, in the Chemistry Building and the John S. Toll Physics Building on UMD campus, with accommodations for both students and lecturers at The Hotel on Baltimore Ave, College Park, MD. The school involved two central components.

First, we brought together **14 senior researchers** with well-established reputations in materials synthesis and characterization techniques to conduct a series of one-hour lectures covering a diverse set of techniques. A wide range of topics were covered, including materials design considerations, various synthesis techniques, magnetism probes, 2D materials and electronic structure calculation tutorials.

Second, three afternoons were devoted to **practical demonstrations** of techniques at laboratories in the University of Maryland Physics and Chemistry departments. These included six modules:

1. Floating Zone/Sintering
2. Arc Melting Techniques
3. Molten Metal Flux Growth
4. Hydrothermal Synthesis
5. x-ray Diffraction Techniques
6. Sample Preparation and Transport Measurements

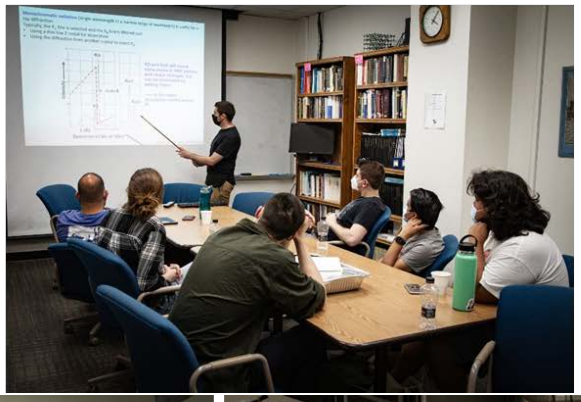
On the fourth afternoon, school participants were bussed over to Gaithersburg, MD for a tour of the **NIST Center for Neutron Scattering,** introducing them to aspects of neutron scattering routinely used in sample characterization and quantum materials research in general. Finally, the school event ended with a **poster session** attended by all participants and senior scientists, and included a diverse (and pleasingly high-quality) set of over 15 poster presentations.

The fifth day centered on a day-long workshop (Jun 24, at The Hotel), which brought together about 60 presenters and participants to discuss a variety of topics focused on the central theme **"Magnetism of Quantum Materials".** The main goal was to bring together a focused group from the physics, chemistry and materials science communities to showcase current and developing research pursuits in quantum materials research. The event was well attended and included several lively discussions about research presented during the day. The coffee breaks, lunch and dinner periods all brought together school students and invited lecturers and speakers in a very interactive atmosphere that produced very positive feedback as shown below.

Event Pictures:



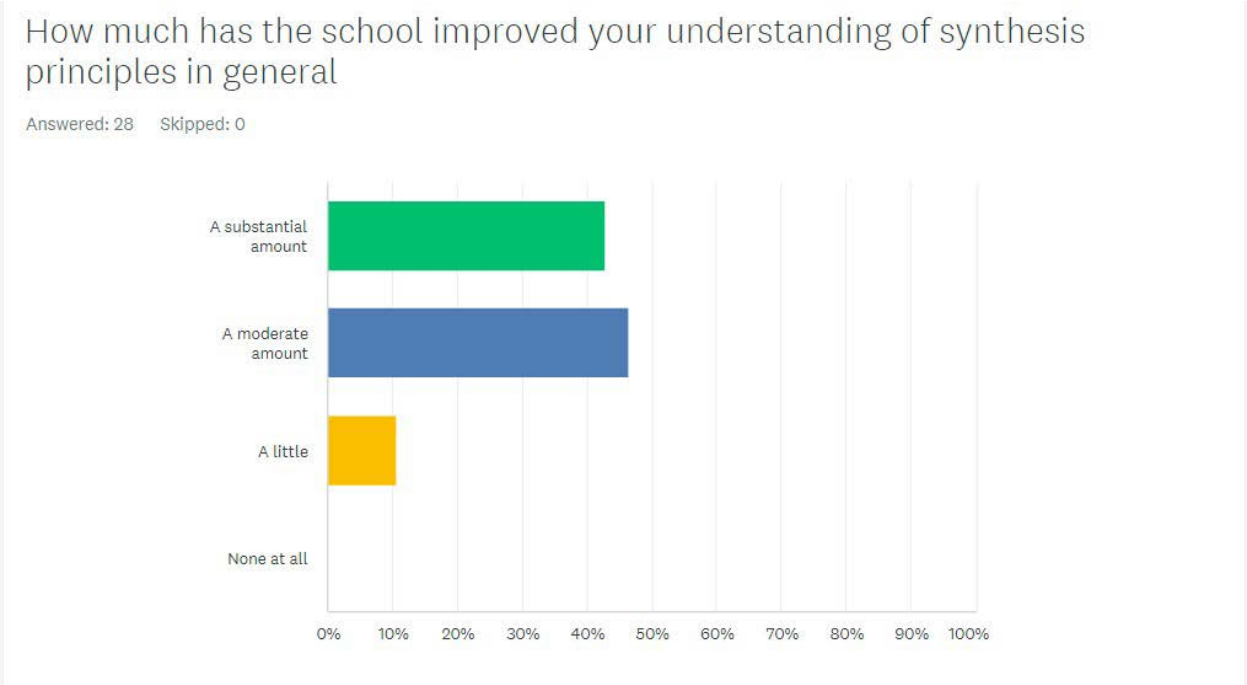
SFU

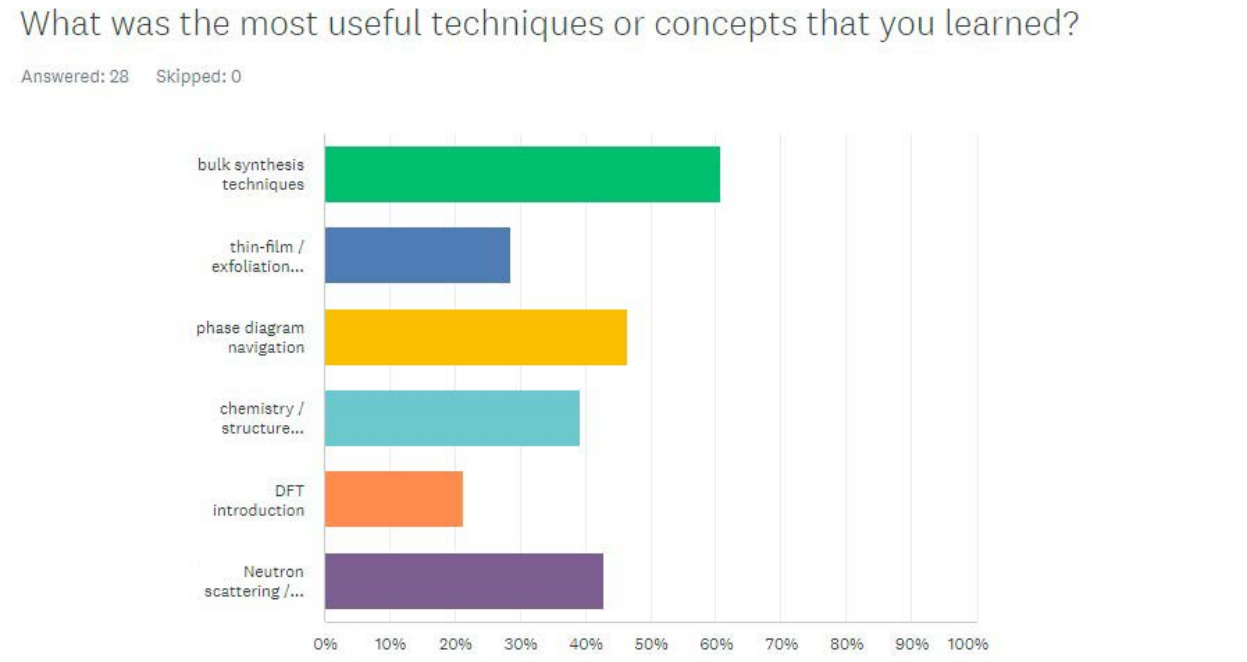






Analytics:

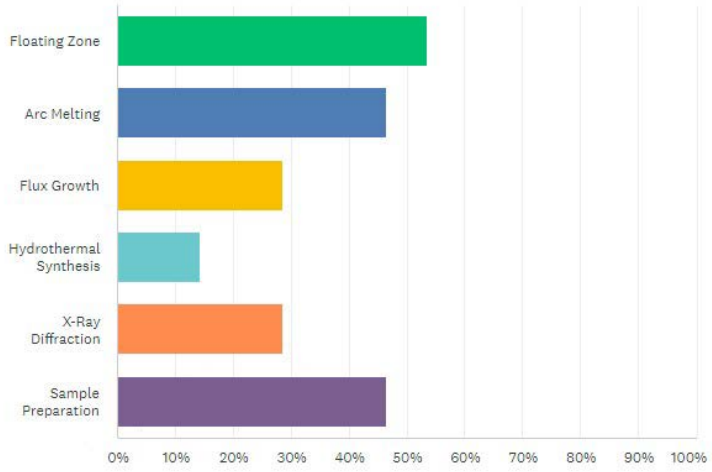
A post-event survey was conducted using SurveyMonkey, collecting data from 28 external participants on a series of questions on scope, quality, learning outcomes and general satisfaction with the school (see below for attached results). Overall, we had excellent ratings on nearly all areas:





Which practical(s) did you like the best?

Answered: 28 Skipped: 0



Was the lecture content appropriate for the scope and level of the school:

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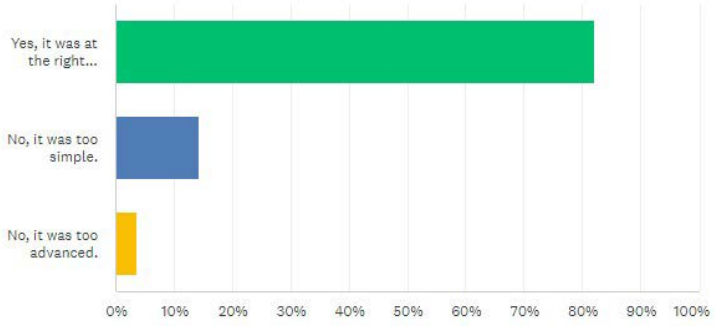
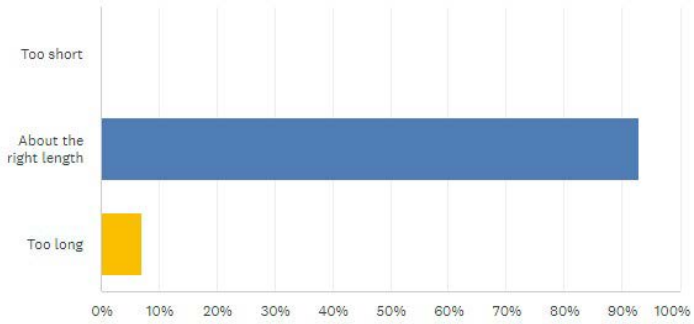
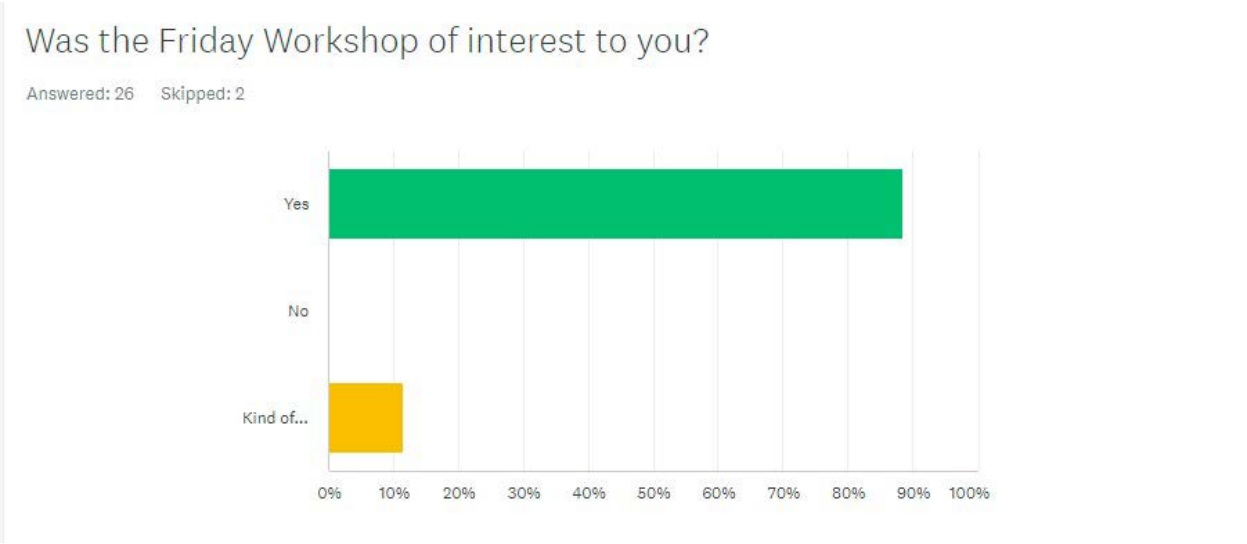
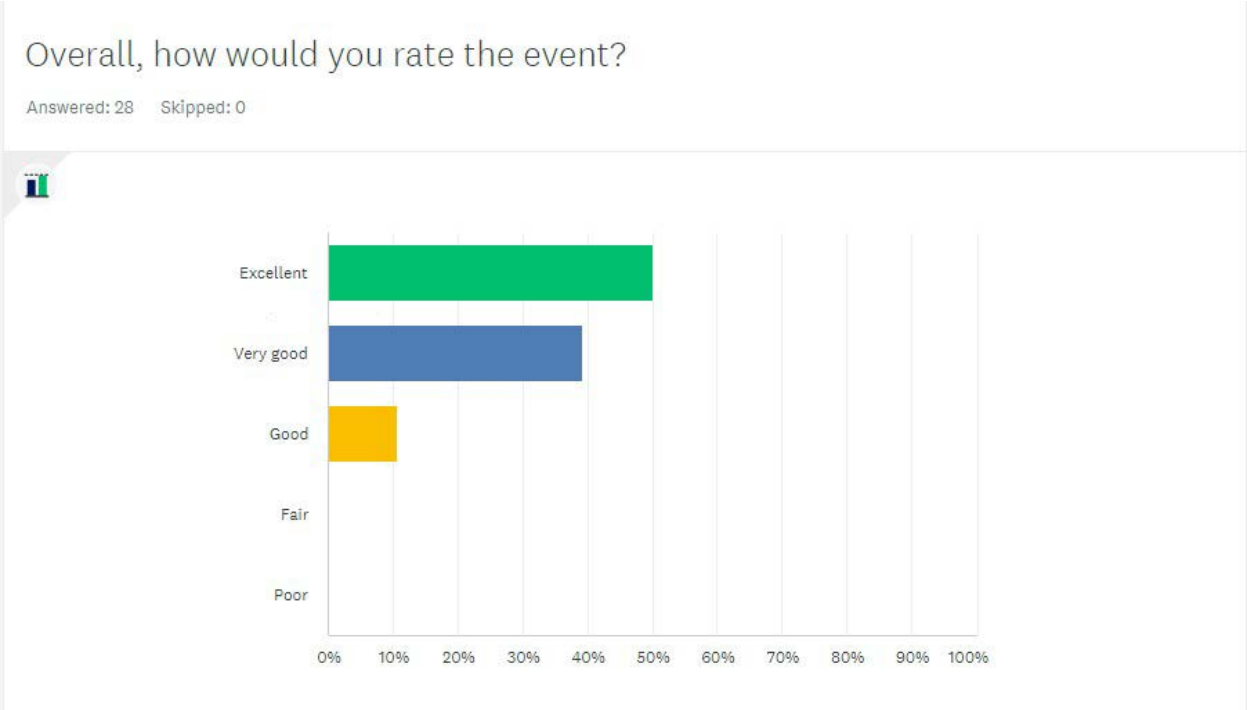


How did you find the duration of the school?

Answered: 28 Skipped: 0







The feedback from student participants was also very strong, generally highlighting the usefulness of seeing some very good examples of current research efforts to probe the materials made using techniques presented at the school.

Individual Survey Comments

What techniques or concepts were you hoping to learn at the FQM school?

- Synthesis Techniques
- Quantum Material electronic properties measurement setup
- This is biased from a crystal grower's point of view but, I see how others would benefit
- Anything. Further insight into sputtering or similar techniques would've been appreciated
- PLD, 2D materials exfoliation
- pitfalls and common problems

- MBE and device fabrication
- A lot of crystal growth
- I was hoping to gain a general understanding of synthesis to support my characterization skills.
- Arc melting and various other synthesis methods
- I would have benefited from more details on vapor transport growths.
- I came in with very little synthesis background - I was hoping for an overview of the techniques with some deeper information once the groundwork had been laid. That is what I got.
- I was hoping to learn more about various crystal growth techniques and was very happy with the content of the school and was very satisfied with the accomplishment of that goal.
- I had been primarily hoping to gain insight into the considerations that go into the different synthesis and experimental techniques and their limitations, which was very well addressed by the 2022 School.
- Magnetism, flux growth

What was the most useful techniques or concepts that you learned?

- Phase diagram navigation is an important topic which I wish I had more practice/time to digest.
- I have a thin film background and it was lacking in that, but that was good because I got to learn about tons of stuff I didn't know about. Not sure how others with bulk crystal backgrounds felt.
- While not exactly useful to me directly, I really enjoyed Dr. Weiwei Xie's presentation on developing intuition for finding new materials. I found the DFT talks to be a bit too technical and hard to follow. It would perhaps be better if they used an example throughout their presentation to give the subject matter some weight.
- For me, it would have been useful to have more detailed discussion of crystallography and maybe even tutorials on structure solution/refinements.
- I was excited about all the methods to grow big single crystals.

Please provide any comments about the practical training sessions, and suggest any techniques or concepts that you think should have been covered:

- Thin Film Growth Techniques like PLD, MBE
- It would be nice to opt out of practical's that students already know.
- I think the practical's were good in theory, but in practice they were hindered by a couple of things: namely, I do not think I will take any of the synthesis techniques home with me and use them (I already use arc melting and flux), as different labs already tend to have established techniques. As well, they remained pretty surface level, when I think they had the possibility to go a little deeper. Rather than learning new things from a broad range of lab techniques, it would be cool to go deep into things that I already currently use, and come away with a better understanding. For example: How does a SQUID work, and how do you maintain it? How does a VSM work? Can I play around with the inner-workings of some of them to get a really good sense of what's going on when I do a M vs H measurement? How does one setup a DFT calculation? What software do I need and what should I be looking for? Can you walk me through a pre-prepared structural solution and refinement for single crystal xray diffraction? What I like so much about the sample preparation practical is that it was exactly this sort of deep dive! Learning about the lock-in amplifier was fascinating, and a bit of knowledge that I will take with me back to my lab.
- I didn't know there were so many types of XRD techniques
- 2D materials would be a nice topic to include.
- Interactive sessions were the best which is why I liked floating zone. Some practical's like flux growth can't be interactive but not much to be done about that. Otherwise it kind of depended on who was giving the practical (I also liked XRD).
- I liked the flux growth practical because it was the most hands-on. I found all of the practical's

really informational.
- the presentation of the lock-in setup for resistance measurements was great.
- For someone with almost no prior exposure to XRD, it was very difficult for me to follow what were the differences between the different XRDs UMD owns. I got some of the more broad/obvious distinctions, but I know I missed the nuances of the science one would look at by choosing one machine over another, so from that perspective not catching the differences was disappointing.
- Super cooool!! Esp the CZ method!!!

Please provide constructive comments on how to modify/improve the lectures:
- The lectures were pretty good, in my opinion. I think maybe there could have been a couple of them that are more in the vein of: "Theoretical walkthrough of a skyrmion", or "The theoretical understanding of superconductivity". Because physics is such a mathematical science, and the range of phenomena that it attempts to explain is large, I do not have a great understanding of the stuff that I do not explicitly work on. For example, I understand, from a chemistry perspective, topological materials, but I do not really know superconductivity, and thus a lecture on BCS theory from the ground up would be really useful. I think it is almost always useful for anyone to review the theoretical foundations of the materials we work on and the properties we try to measure. Also, I think some of the lectures were a little more like research talks than lectures, and those should be saved for the workshop.
- Theoretical lectures are a bit difficult for me.
- DFT talks needed to be simplified. I spoke with other students, and this seemed to be a consensus.
- Right level but very compacted.
- Would it be possible to ask the gentleman who takes photos to not use flash in the lectures? There were several times throughout when the flash was distracting several of us from the speaker (this was something a couple folks commented on during breaks). Lovely photos, though.
- Perfect schedule! Really like the amount of talks and practical's packed into one week.

Was the Friday Workshop of interest to you?
- All talks were interesting
- This was a great time for me. As a first-year graduate student who has not been to a conference, it was very cool to meet people who do similar research and talk with them.
- I was pretty tired at this point.
- Very nice selection of talks.
- Not all applied to me but that's how talks go.
- Really good sessions. I liked the UTe2 session. It went a bit long though, my concentration died after lunch.
- I found the workshop very complimentary to the lectures!
- Having Nick Butch's talk with an overview of the current state of knowledge of UTe2 as the first presentation in the session on UTe2 was quite useful to many of us (theorist and experimentalist students alike). Having a sort of "state of the field" summary beginning a session on a particular material or set of materials like this was definitely the way to go, and something I would recommend for future iterations of the Workshop.

Overall, how would you rate the event?
- It would be better to improve food quality.
- I wish we had a channel to connect FQM participants after the event has concluded.
- Time well spent

- It would be nice to take synthesis a step further and talk about why materials are useful or how to get them to manifest the exotic "quantum" phenomena that make them interesting/useful.
- This is a wonderful summer school for me. Great lectures and practical sessions, especially the hotel. It's also excited to visit the NIST Center for Neutron Research. I really enjoyed the week in Maryland. Thanks a lot to the organizers and all the participants.
- Maybe having some structured hang out sessions at night. Most nights we would leave and be on our own and weren't sure what to do. Some nights were boring. Also helping the students have a group chat or something. Otherwise it was awesome! Maybe having more thin film growers would have been cool.
- I loved the event and I will recommend to other graduate students! I think the duration is good to not only understand the ideas and concepts, but to also gain enough comfort around the other students to network and have in depth conversations about research. I was able to meet researchers that I can collaborate with. Their methods were not even on my radar! Thanks for hosting!
- Thank you so much for accepting my application for this summer school. It was very helpful for me.

School Agenda

Monday June 20, Lecture Session I (*Chemistry Lecture Hall 1407*)		
7:30 AM	Registration and breakfast	
8:15 AM	Johnpierre Paglione	Welcome message
8:30 AM	Brian Sales	Introduction to Synthesis Techniques
9:30 AM	Halyna Hodovanets	Introduction to Binary Phase Diagrams [ZOOM]
10:30 AM	Coffee break	
11:00 AM	Julia Chan	Materials Design and Synthesis
12:00 PM	Lunch	
1:00 PM	Zak Al Bashari	Synthesis of Transition Metal Dichalcogenides
Monday Afternoon Practicals (*Quantum Materials Center*)		
2:00 PM	First Practical Session	
4:00 PM	Second Practical Session	

Tuesday June 21, Lecture session II (*Chemistry Lecture Hall 1407*)		
8:00 AM	Breakfast	
8:30 AM	Weiwei Xie	Chemistry Perspectives to Novel Intermetallics
9:30 AM	Vesna Mitrovic	Nuclear Magnetic Resonance
10:30 AM	Coffee break	
11:00 AM	Collin Broholm	Introduction to spin liquid/quantum magnet materials
12:00 PM	Lunch	
1:00 PM	Nirmal Ghimire	Growth and characterization of Kagome materials
Tuesday Afternoon Practicals (*Quantum Materials Center*)		
2:00 PM	Third Practical Session	
4:00 PM	Fourth Practical Session	

Wednesday June 22, Lecture Session III (*Chemistry Lecture Hall 1407*)		
8:00 AM	Breakfast	
8:30 AM	Jeff Lynn	Introduction to Neutron Scattering
9:30 AM	David Mandrus	Van der Waals Materials and Exfoliation
10:30 AM	Coffee break	
11:00 AM	Brandon Wilfong	Hydrothermal Growth Techniques
12:00 PM	Lunch	
1:00 PM	DISCUSSION: Careers in Quantum Materials Research	
Wednesday Afternoon Practicals (*Quantum Materials Center*)		
2:00 PM	Fifth Practical Session	
4:00 PM	Sixth Practical Session	

Thursday June 23, Lecture Session IV (*Chemistry Lecture Hall 1407*)		
8:00 AM	Breakfast	
8:30 AM	Fazel Tafti	TUTORIAL: Density Functional Theory Techniques
9:30 AM	Andriy Nevidomskyy	Frustration in Classical and Quantum Magnets
10:30 AM	Coffee Break	
11:00 AM	Igor Mazin	Magnetic interactions in DFT
12:00 PM	Lunch	
1:00 PM	[POSTER SETUP: *Physical Sciences Complex Lobby*]	
1:30 PM	**Tour of NIST Center for Neutron Research**	
5:00 PM	**Poster Session and Banquet (*Physical Sciences Complex Lobby*)**	

Workshop Agenda - "Magnetism in Quantum Materials"

Friday June 24, "The Hotel" at the University of Maryland – 7777 Baltimore Ave, College Park, MD		
7:00 AM	Registration and breakfast (Foyer B)*	
8:15 AM	Johnpierre Paglione, UMD	*Welcome Message*
Session I:	***Novel Quantum Phases (Salon E)****	
8:30 AM	Ludi Miao, Cornell	*Controlling Berry Curvature and magnetic anisotropy in $Sr_{1-x}Ca_xRuO_3$*
9:00 AM	Andriy Nevidomskyy, Rice	*Sleuthing Out Quantum Spin Liquids in Cerium Spin Ices*
9:30 AM	Patrick Vora, GMU	*Excitons in $TiSe_2$-$MoSe_2$ Heterostructures*
10:00 AM	COFFEE BREAK (Foyer B)*	
Session II:	***Superconductivity and Magnetism in UTe2 (Salon E)****	
10:30 AM	Nick Butch, UMD	*Symmetry of Magnetic Correlations in UTe_2*
11:00 AM	Florian Theuss, Cornell	*Resonant Ultrasound Spectroscopy*
11:30 AM	Steve Anlage, UMD	*UTe_2 Electrodynamics*
12:00 PM	LUNCH (Salon F)*	
Session III:	***Kagome Systems (Salon E)****	
1:30 PM	Madalynn Marshall, UTK	*Charge Density Wave in Kagome Lattice Intermetallic ScV_6Sn_6*
2:00 PM	Nirmal Ghimire, GMU	*Anomalous Hall Effect in Kagome Magnets RMn_6Sn_6*
2:30 PM	Brian Sales, ORNL	*Flat-Band Itinerant Antiferromagnetism in Kagome Metal $CoSn_{1-x}In_x$*
3:00 PM	COFFEE BREAK (Foyer B)*	
Session IV:	***Novel Magnetic Excitations and Textures (Salon E)****	
3:30 PM	Collin Broholm, JHU	*Magnetic Excitations and Interactions in Honeycomb AF $BaCo_2(AsO_4)_2$*
4:00 PM	Igor Mazin, GMU	*"Altermagnetism"*
4:30 PM	Jeff Lynn, NIST	*Incommensurate Spin Textures in the Topological $EuGa_2Al_2$ System*
6:00 PM	COCKTAIL HOUR (Foyer B)*	
7:00 PM	DINNER BANQUET (Salon F)*	