The Neutron Scattering Division's Diffraction Section:
Powder Diffraction Group and Single Crystal Group

Clarina dela Cruz

Group Leader and
Senior Scientist

MAGSTR 2022 October 6, 2022

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

NSD's Diffraction Section

Powder Diffraction
Group Leader
Clarina dela Cruz

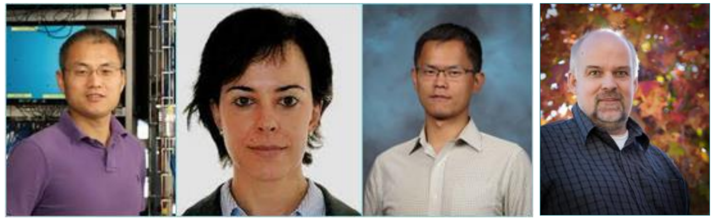
Matt Tucker
Section Head

Single Crystal Group Leader
Bryan Chakoumakos

HB2A

Stuart Calder,Keith Taddei, Clarina dela Cruz
SA: Malcolm Cochran

POWGEN

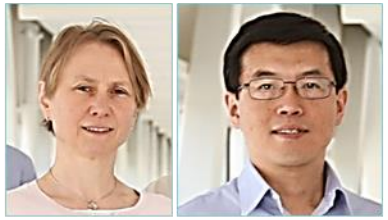


Qiang Zhang, Alicia Manjon Sanz, Cheng Li and Thomas Proffen

DEMAND

Huibo Cao, Yan Wu

TOPAZ



Christina Hoffmann, Xiaoping Wang
SA: Helen He

NOMAD

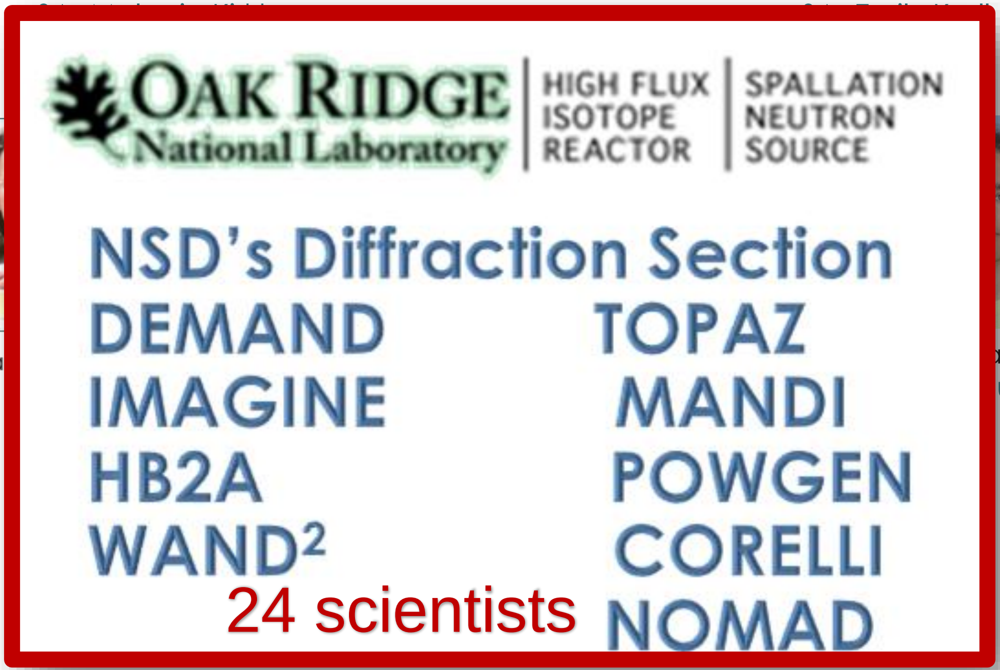
Joerg Neuefeind, Cheng LI, Jue Liu,
SA: Michelle Everett

Ma

anna Minelli
ux

IMAGINE and MANDI

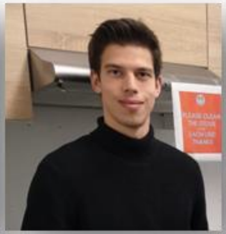
Andrey Kovalevsky, Flora Meilleur, Dean Myles
SA: Malcolm Cochran and Helen He



Yuanpeng Zhang
Computational
Instrument Scientist

Zachary Morgan
Computational
Instrument Scientist





Abbie Neill | Harvey Campos-Chaves | Ramon Zimmermans | Michael Broud | Cade Abbott

Student Interns

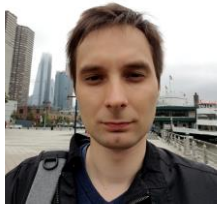
OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE

NSD's Diffraction Section

DEMAND	TOPAZ
IMAGINE	MANDI
HB2A	POWGEN
WAND²	CORELLI
	NOMAD

24 scientists

Diffraction Section

Bernadette Cladek | Maksim Eremenko | Raju Baral | VIctoria Drago

POSTODOCTORAL FELLOWS




Yiqing Hao | Kyle Ma | Maddalyn Marshall | Gaurav Vishwakarma

Kate Page
NScD and UTK-MSE

Flora Meilleur
NScD and NCSU-Biochemistry

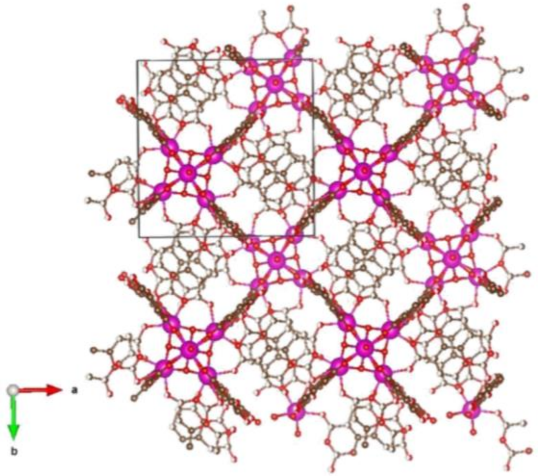
Kennedy Agyekum
UT Knoxville

Sreya Paladugu
UT Knoxville

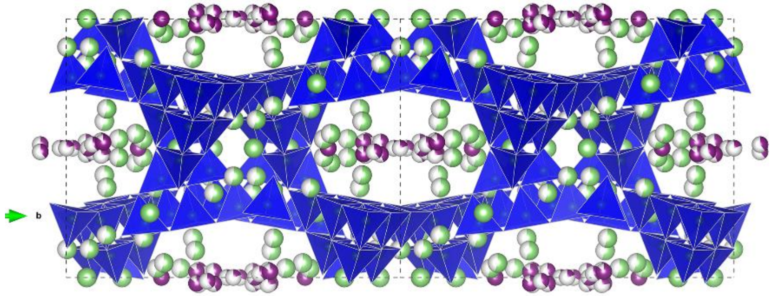
Paul Cullier
Ohio State University

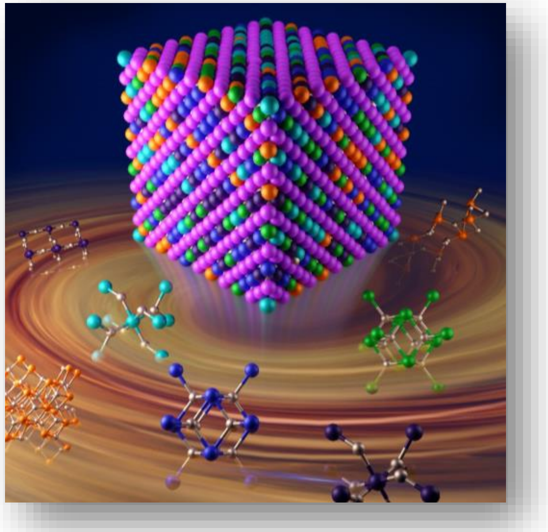
Graduate Students SCGSR Fellows

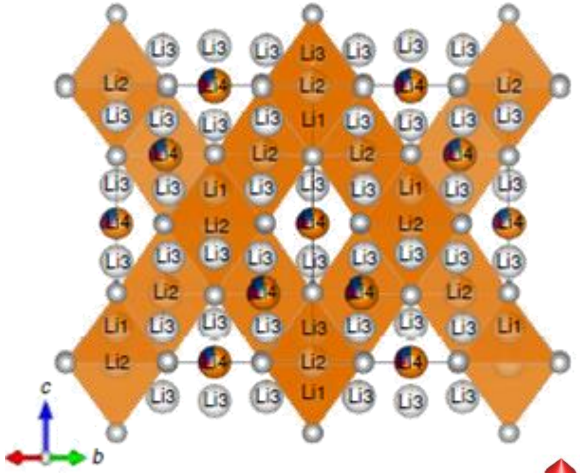
Powder Diffraction Group Mission

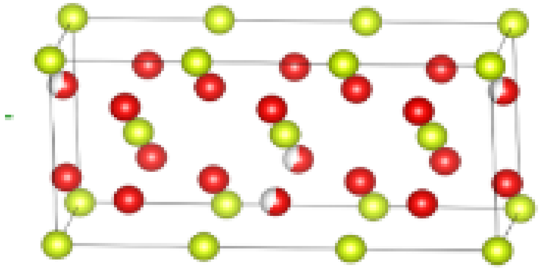


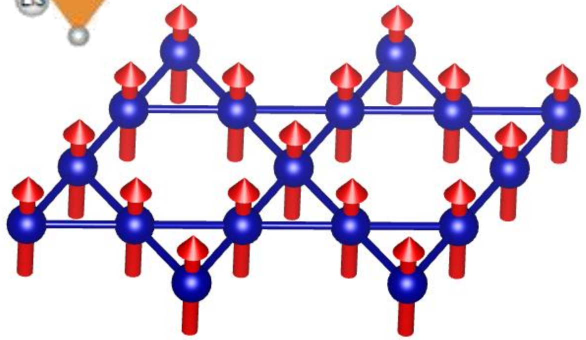
Advance NSD's Powder Diffraction Group to be the **world leader in neutron powder diffraction techniques** for materials development and discovery in energy materials, quantum matter and multifunctional materials

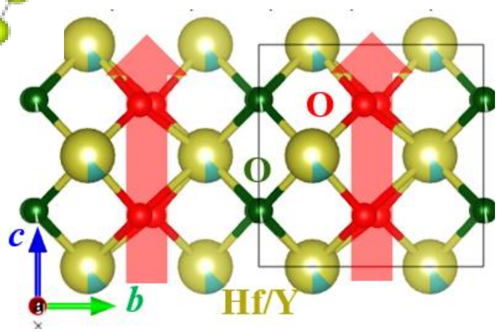


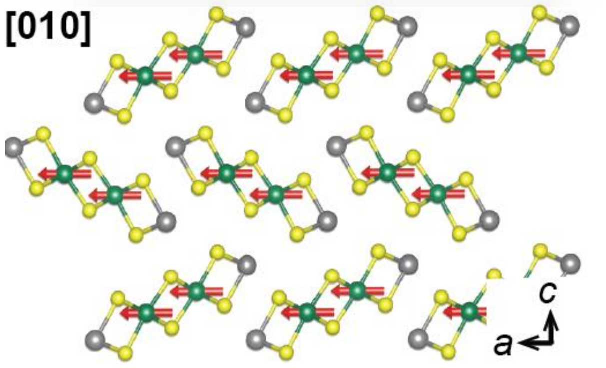




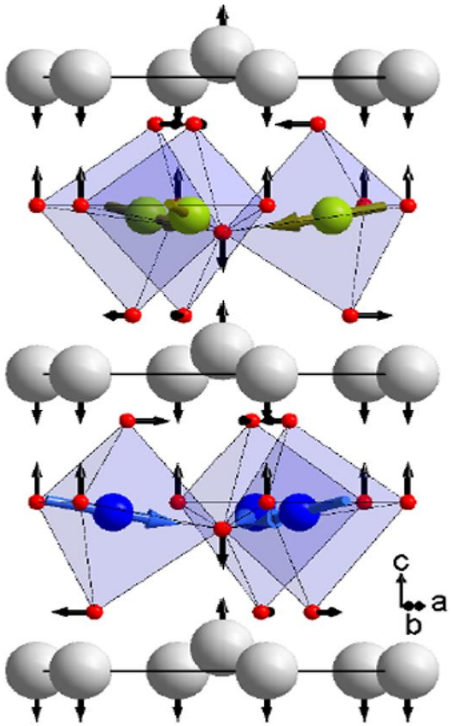




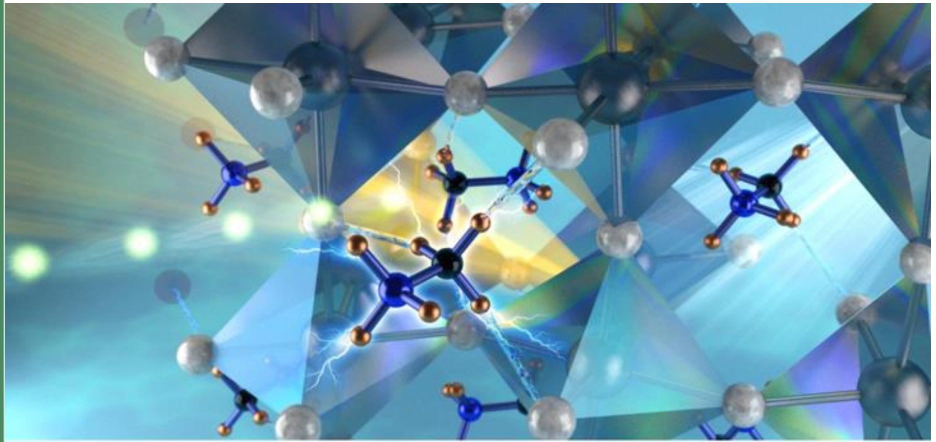


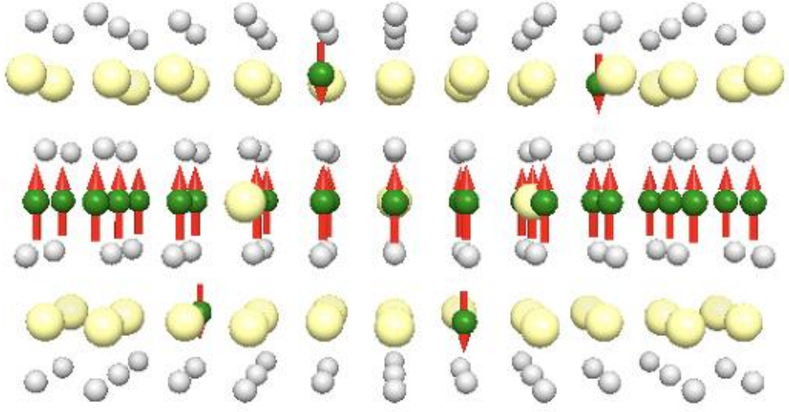


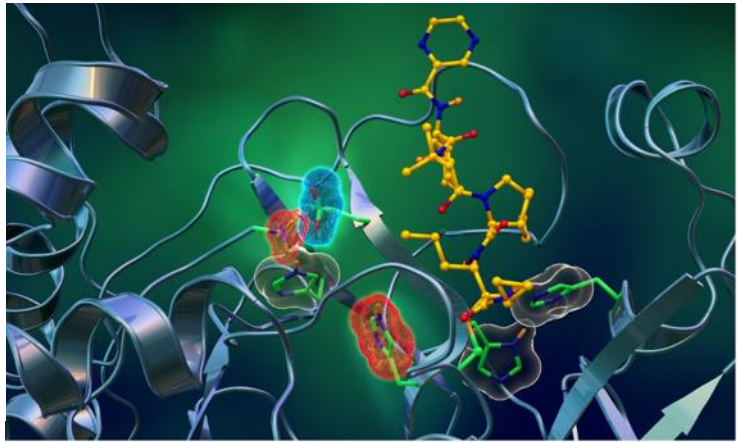
Single-Crystal Neutron Diffraction Mission



Delivering world-class neutron diffraction capabilities that enable physical, chemical, and biological studies of structure and function of materials.







Timeline in the User Program: **NSD Powder Diffraction Group**

2009

WAND 2016

2019 WAND²

HFIR

2010

2012

SNS

Single-Crystal Diffractometer Timelines at HFIR & SNS

2013 IMAGINE

FCD 2011 2019 DEMAND

WAND 2019 WAND^2

2015 CORELLI

2013 MaNDi

2011 TOPAZ

2009 SNAP

HFIR HB2A: Constant wavelength powder diffractometer with extreme sample environments and polarization

Entered fully into User Program: 2009
Average Days per an experiment: 2.5
Subscription Rate, 7-year average (Number of requested days/Number of available days): 215%

★Specially Recognized

Citation Count 20-49 (59)

Citation Count > 50 (26)

DOE Highlight (16)

Editor's Choice (8)

Journal Impact Factor >7 (49)

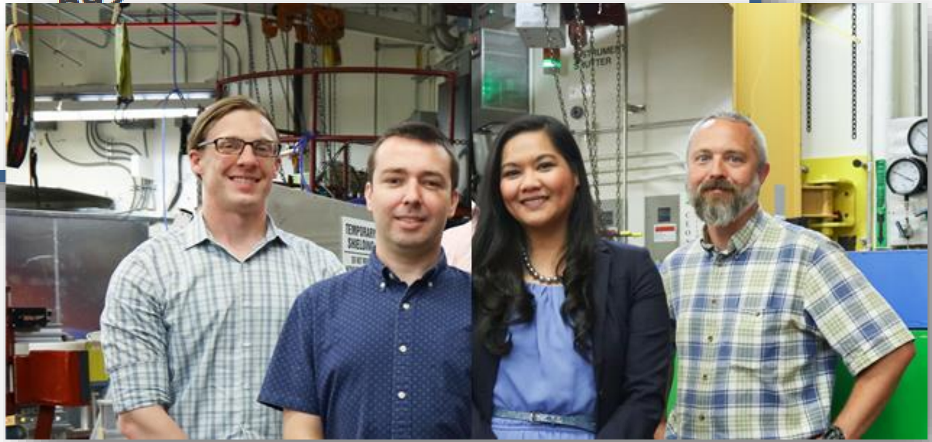
Rapid Communication (8)

Instrument Publications: **333**

Instrument H-index: **37**

Completed Experiments: **692**

Instrument Authors: **1121**

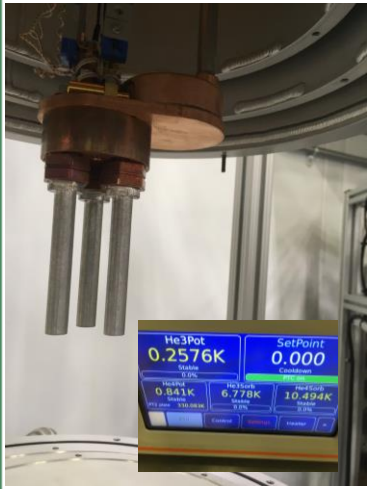


Stuart Calder (100%), IS
Clarina dela Cruz **(25%)**, IS
Keith Taddei, **(50%)**, IS
Malcolm Cochran , **SA (100%)**

HB-2A Commissioned Sample Environments

Low and ultra-low temperature and magnets

Sample changers for 0.3 – 300 K



Ultra-low temperature 10 multi-sample change to <0.3 K

1.5 K 3-sample changer cryostat with helium autofill

4-700 K CCR with 3-sample

Dilution Refrigerator (50 mK) and ^{3}He (300mK) insert options compatible with magnetic fields and pressure cells

Cryomagnets to 8 T

Pressure

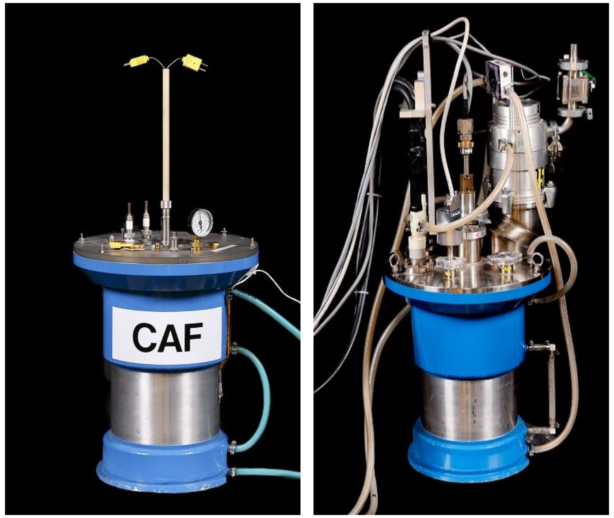
High pressure cells >2 GPa

Gas pressure to 6kbar

Electric field

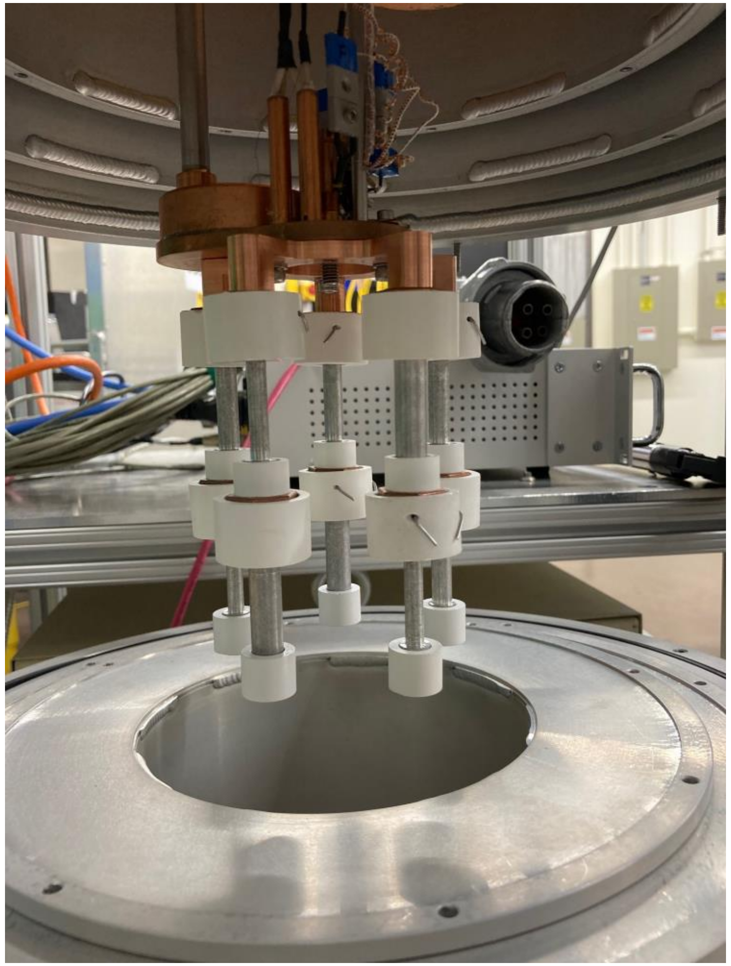
High Voltage V_{max} = 10 kV

High temperature

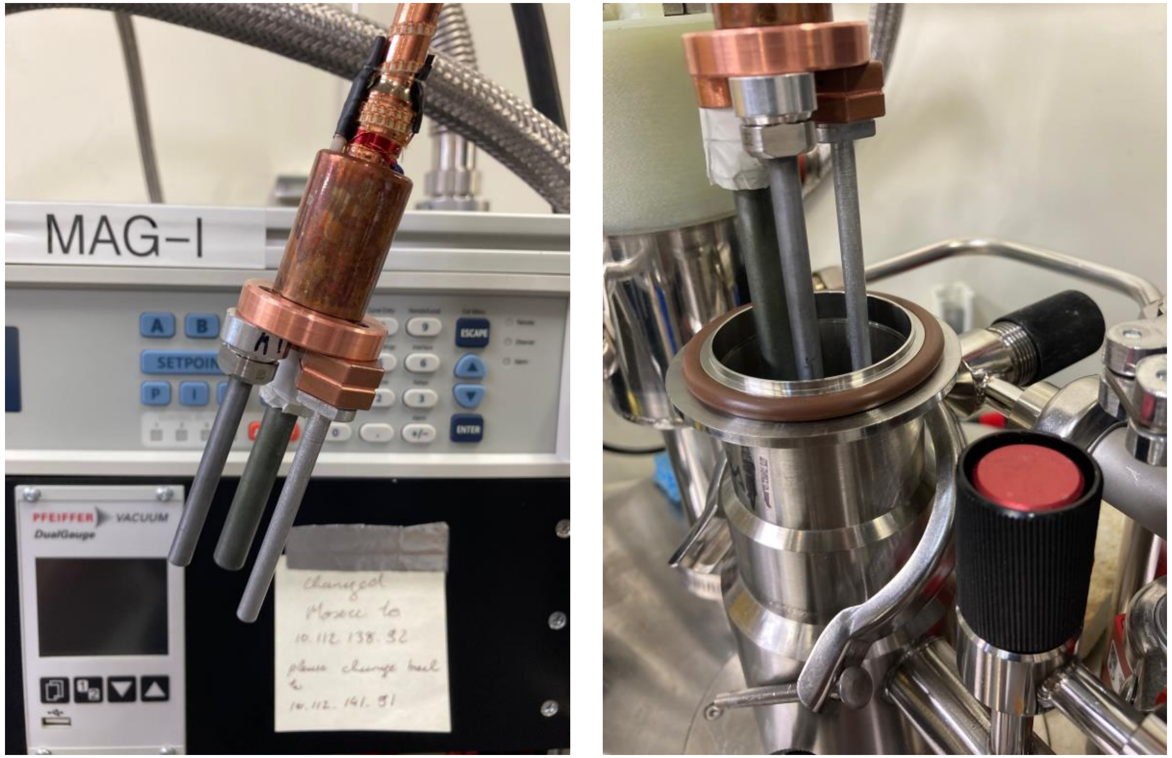


Air and vacuum furnaces to 1200 ^{o}C

HB2A and Sample Environment delivers new multiple sample changers for ^{3}He mk temperatures and the magnet



10 samples on the ACV, cooled down to ~300mK



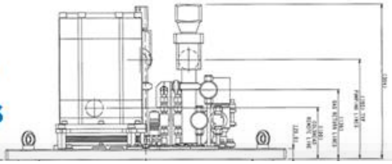
3 samples on MAG-I, down to 1.6K and 6T

Malcolm Cochran

Josh Pierce

Instrument Developments: Pushing towards the forefront with unique and challenging experiments

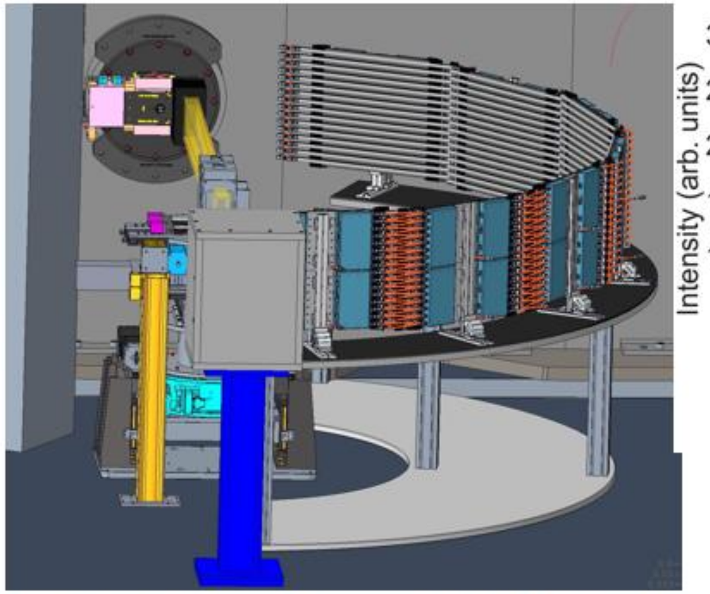
Developing multiple sample changer systems from room temperature to ultra-low temperature regimes

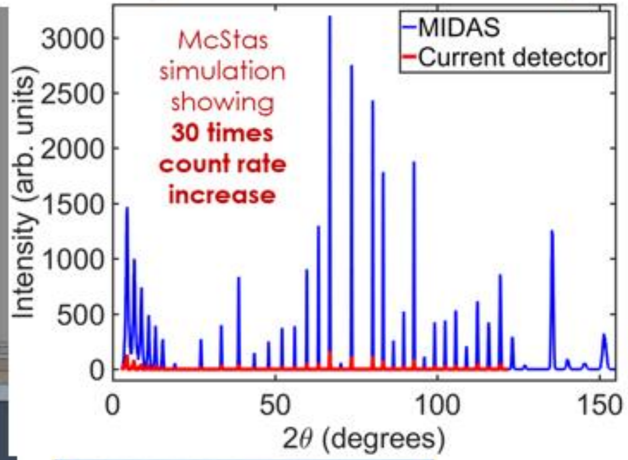


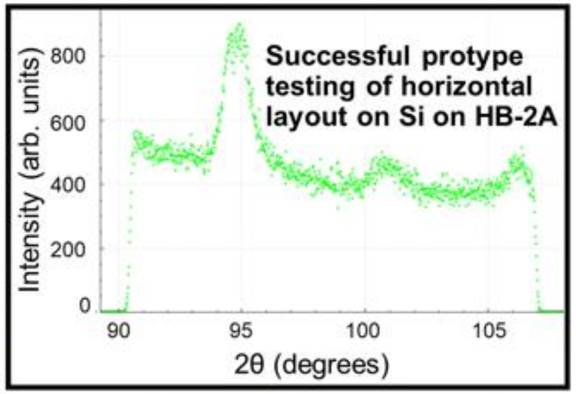
Half Polarization on HB-2A studying Ferromagnetic Heusler

Concept, Design and Prototyping development for HB2A detector upgrade continues

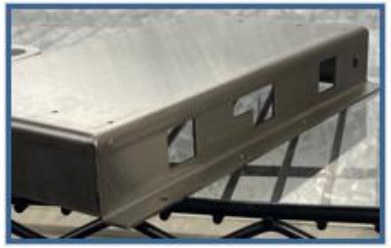
MIDAS – Modular Interdigitated Detector Array System

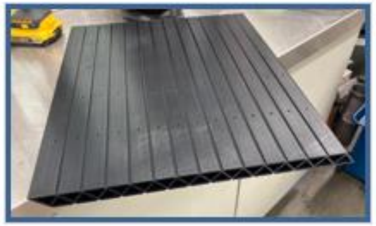




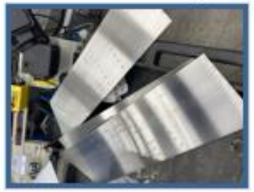


the design is based around 10 ATM Reuter-Stokes ^3He tubes inherited from IPNS





Prototype 3D printed parts for the 4 MIDAS 8-packs are with B4C epoxy



Oak Ridge National Laboratory

HFIR HB2C WAND²: US/JAPAN Wide Angle Neutron Diffractometer

Entered fully into User Program: 2016-2017 and as WAND² in 2019A
Average Days per an experiment: 4.5
Subscription Rate, 7-year average (Number of requested days/Number of available days): 117%

★Specially Recognized

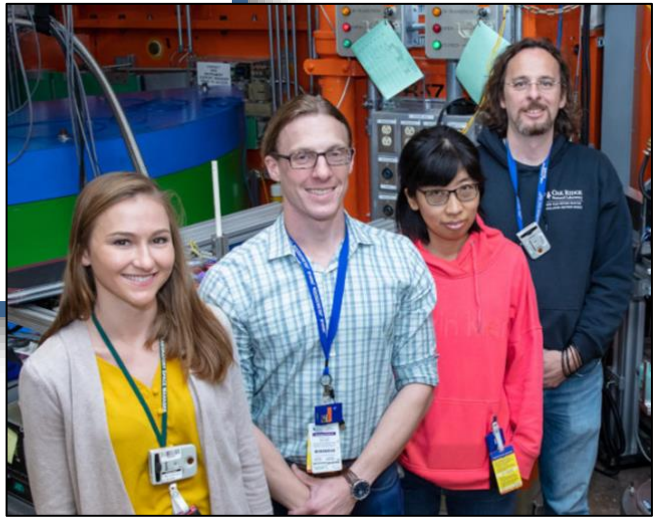
- Citation Count 20-49 (12)
- Citation Count > 50 (8)
- DOE Highlight (3)
- Editor's Choice (4)
- Journal Cover (1)
- Journal Impact Factor >7 (7)
- Rapid Communication (2)

Instrument Publications: **96**

Instrument H-index: **20**

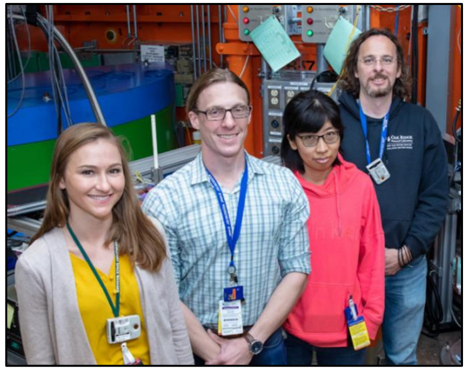
Completed Experiments: **265**

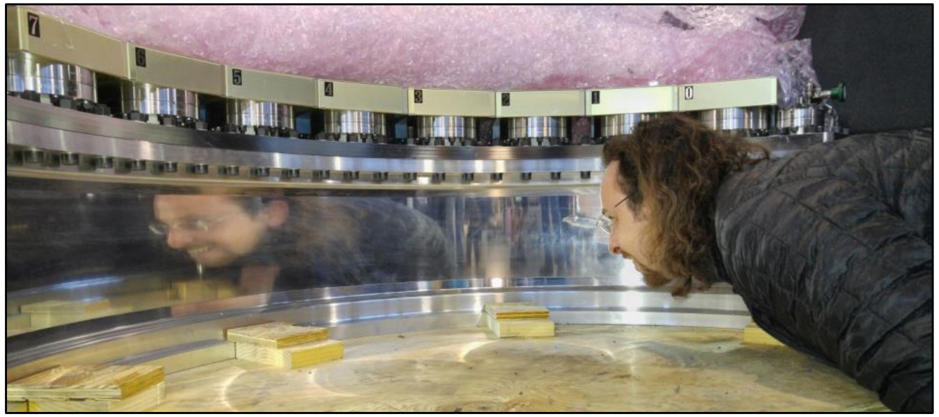
Instrument Authors: **499**



Matthias Frontzek **(50%)**, IS Yan Wu **(50%)**, IS Keith Taddei **(50%)**, IS Emily Kroll **(50%)**, SA)

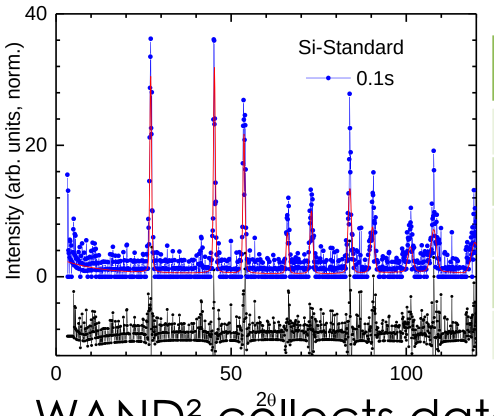
HFIR HB2C WAND²: US/JAPAN Wide Angle Neutron Diffractometer





Matthias Frontzek (100%), IS
Yan Wu **(50%)**, IS
Keith Taddei **(50%)**, IS
Emily Kroll **(50%)**, SA)

Fast Powder diffraction

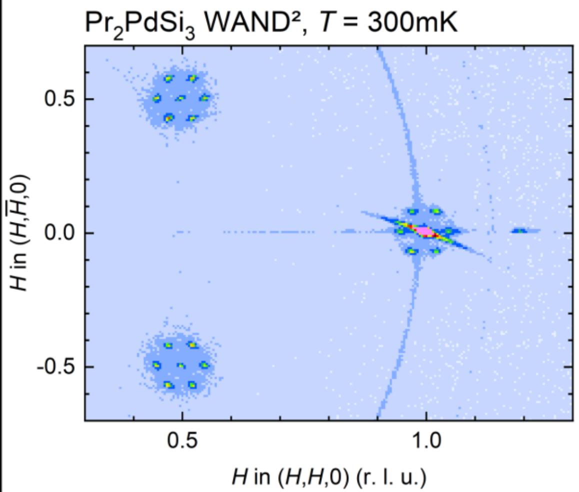


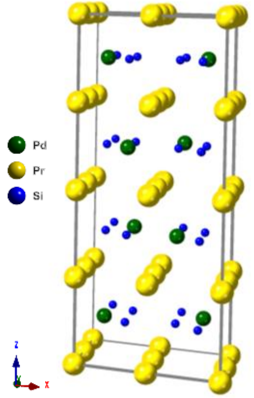
Time (s)	R_{wp}	Bragg R
600	9.02	1.35
60	9.94	1.18
10	10.8	2.52
1	29.2	11.6
0.1	58.5	34.0

WAND² collects data in Event-mode; Measurement time of seconds is sufficient for refinement, milliseconds to track changes

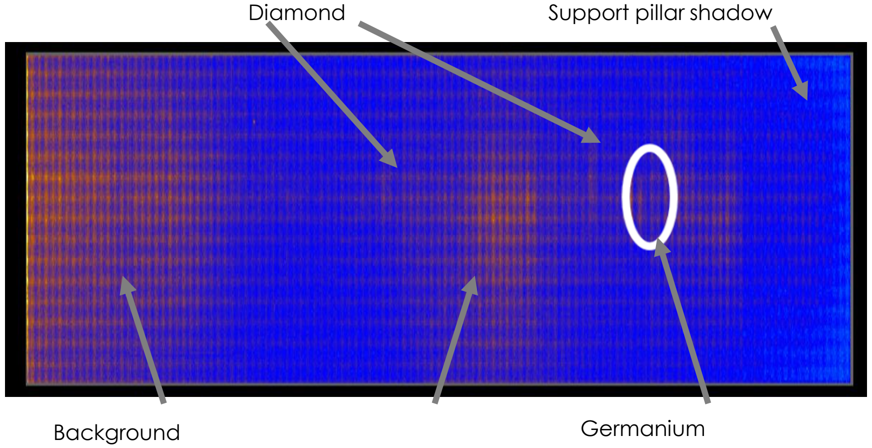
µg single crystals can be measured on WAND²

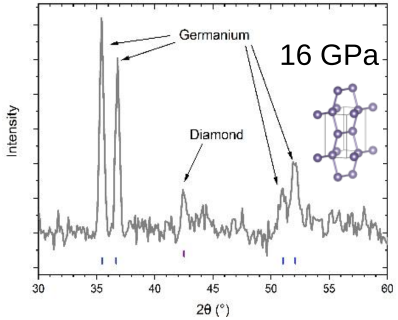
Low Background high flux single crystal diffraction





Pr_2PdSi_3 single crystal showing multiple k Skyrmion structure with k~(1/20,1/20,0)



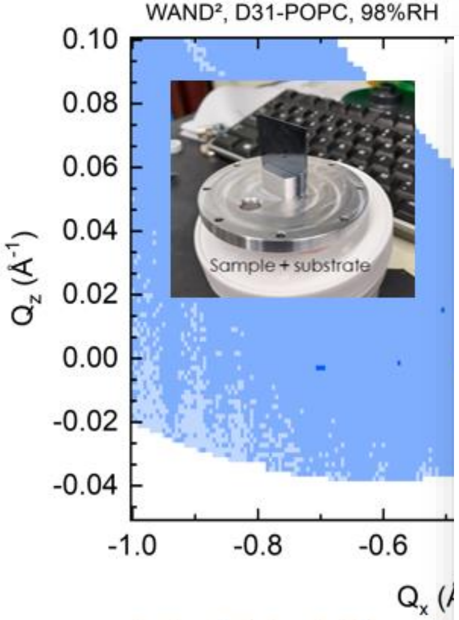


16 GPa achieved using PE – Solved long standing question in Ge phase diagram

Instrument Developments: Pushing towards the forefront with unique and challenging experiments

WAND² successfully uses humidity chamber V2.0 for implementation of insertion of LL-37 in model bilayer

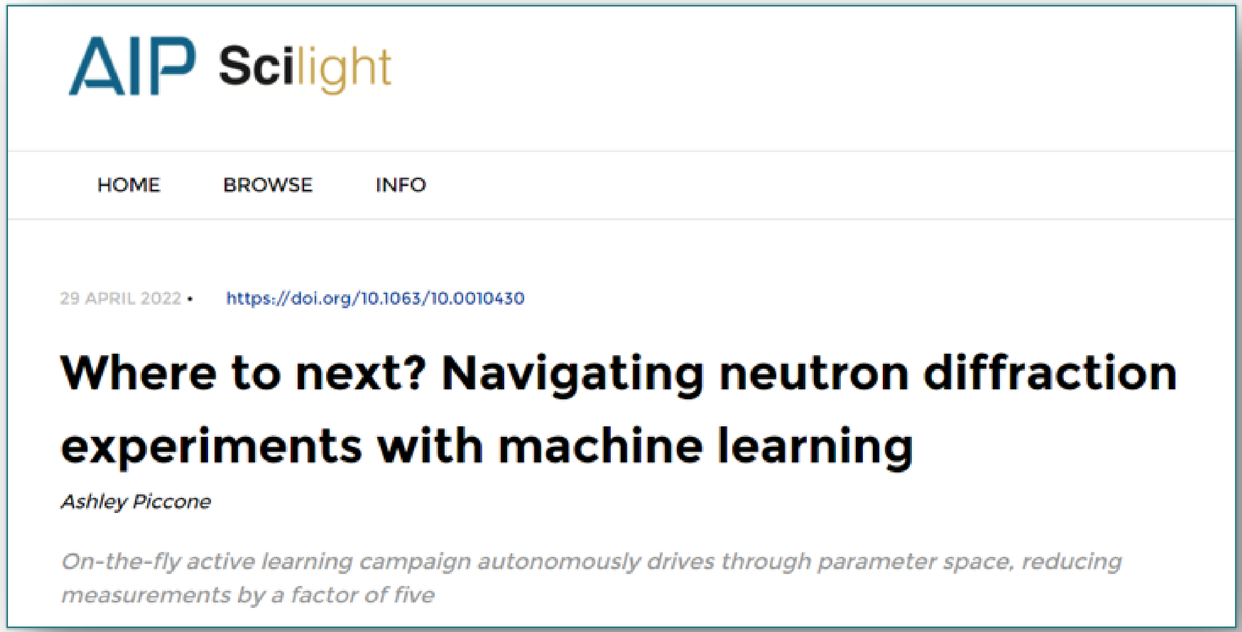
Current development of th
allows EPICS controlled ten
with easy exchange of D_2C



Contour plot of model bilayer – th

FIRST In-operando battery cell experiment on WAND²

WAND²'s work on On-the-fly Autonomous Control of Neutron Diffraction gets a nod from AIP


AIP Scilight

HOME BROWSE INFO

29 APRIL 2022 • https://doi.org/10.1063/10.0010430

Where to next? Navigating neutron diffraction experiments with machine learning

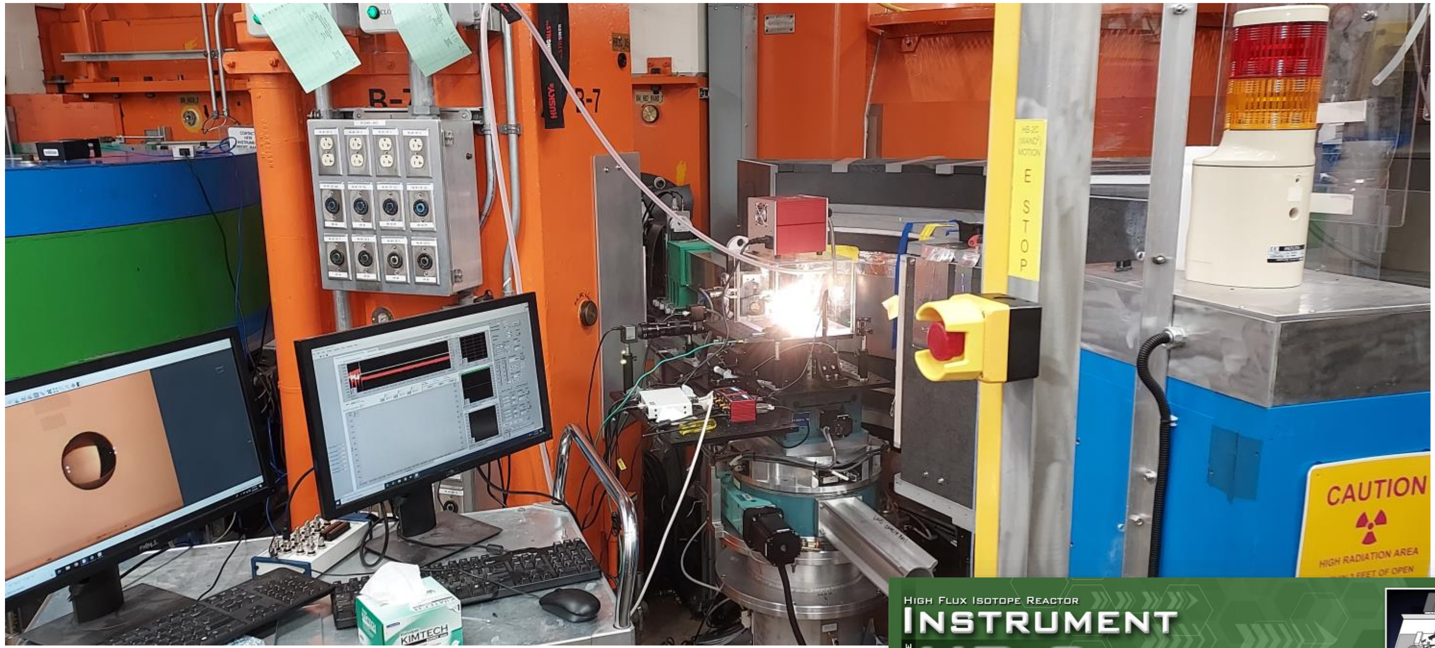
Ashley Piccone

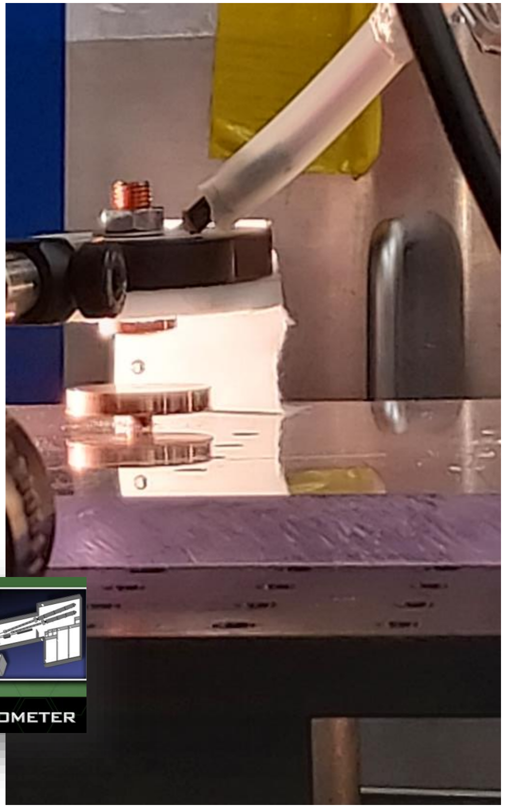
On-the-fly active learning campaign autonomously drives through parameter space, reducing measurements by a factor of five

A collaboration between NSD, NCNR and the University of Maryland Neutron used machine learning on WAND² to perform diffraction experiments measure complex magnetic ordering in a material as guided by ANDiE, the Autonomous Neutron Diffraction Explorer, which improved measurement efficiency by a factor of five.

WAND^2 successfully tests the solution electrostatic levitator

Matthias Frontzek





WAND^2 team worked with researchers from Iowa State University (Jonghyun Lee, Sai Katamreddy, Brayden Berg) to install and run the Solution Electrostatic Levitator (SEL)
The effort was complimented by thorough testing and safety discussions with HFIR support staff

ORNL Support: Dante Quirinale, Emily Kroll, Lisa Fagan, Scott Byers, John Carruth, Katie Andrews, Brandon Coday

the successful levitation of a solution droplet will enable the study of the nucleation process in the sample

SNS–POWGEN: General-purpose powder diffractometer Powder Diffractometer: crystal structure, magnetism and local structure

Entered fully into User Program: 2010
Average Days per an experiment: 2.1
Subscription Rate, 7-year average: 269%
(Number of requested days/Number of available days)

Instrument Publication Analysis

Total Publications: 670

(No. 1 instrument in ORNL)

Instrument H-Index: 60

(No. 1 instrument in ORNL)

Publication Impact: 29% publications with high impact factor

★Specially Recognized

Citation Count 20-49 (121)

Citation Count > 50 (77)

DOE Highlight (34)

Editor's Choice (7)

Journal Cover (4)

Journal Impact Factor >7 (191)

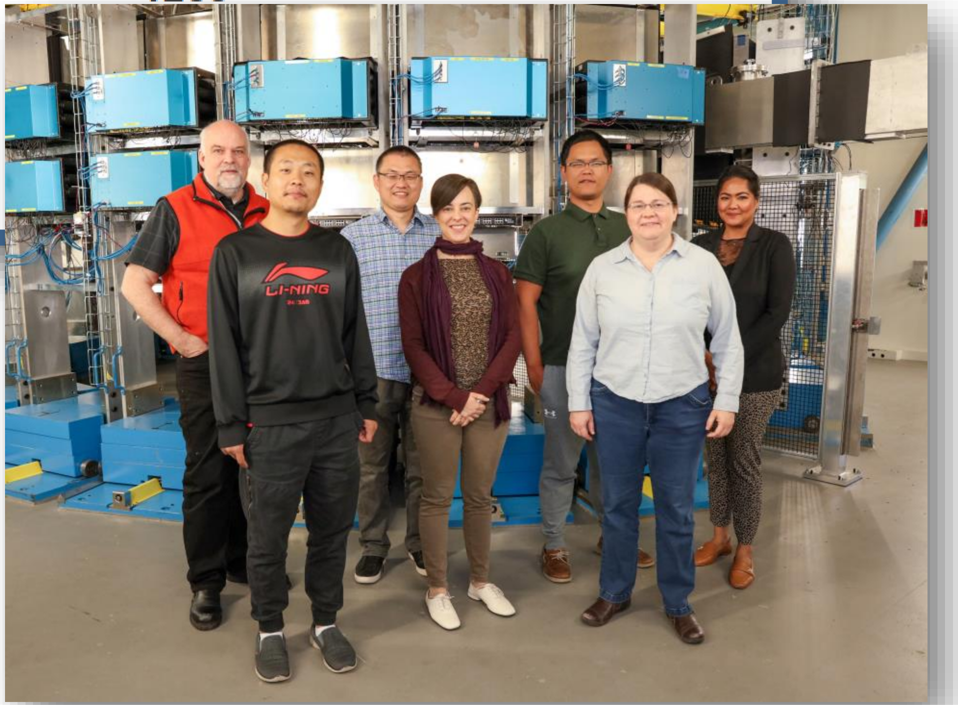
Rapid Communication (2)

Instrument Publications: **670**

Instrument H-index: **60**

Completed Experiments: **1288**

Instrument Authors: **2231**

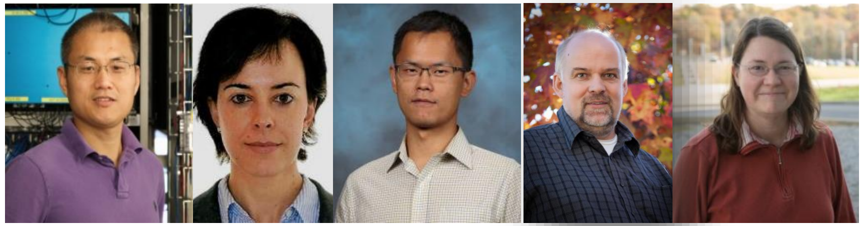


Qiang Zhang (100%), IS
Alicia Manjon-Sanz (100%), IS
Cheng Li **(50%)**, IS
Thomas Proffen **(50%)**, IS
Melanie Kirkham (100%),SA

BL-11A, General-purpose powder diffractometer Powder Diffractometer: crystal structure, magnetism and local structure

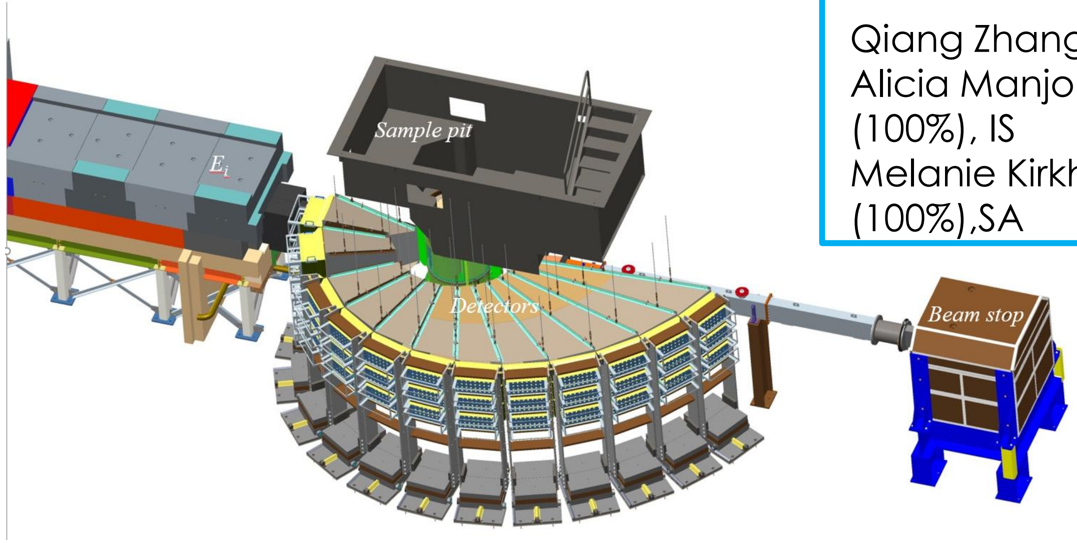
Freq (Hz)	WL center	WL min	WL max	dmin	dmax	Qmin	Qmax	Bank
60	0.533	0.15	1.066	0.075	7.50	0.82	83.45	0
60	0.800	0.27	1.333	0.134	8.00	0.76	46.88	1
60	1.500	0.97	2.033	0.485	13.00	0.48	12.95	2
60	2.665	2.13	3.198	1.070	21.00	0.30	5.87	3
60	4.797	4.26	5.33	2.140	38.00	0.17	2.94	4

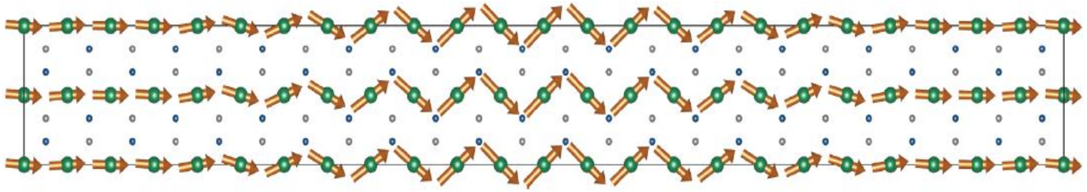
Resolution: $\Delta d/d \sim 1\text{-}25 \times 10^{-3}$



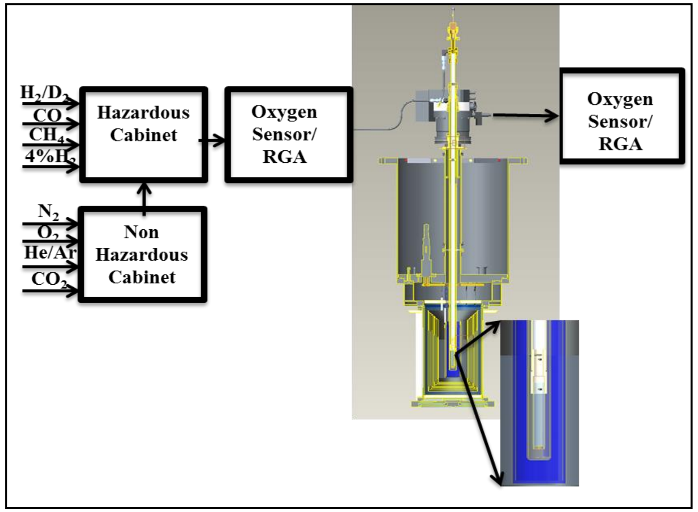
Qiang Zhang (100%), IS
Alicia Manjon-Sanz (100%), IS
Melanie Kirkham (100%),SA
Cheng Li **(50%)**, IS
Thomas Proffen **(50%)**, IS

Instrument Publication Analysis
Total Publications: 670
(No. 1 instrument in ORNL)
Instrument H-Index: 60
(No. 1 instrument in ORNL)
Publication Impact: 28% publications with high impact factor

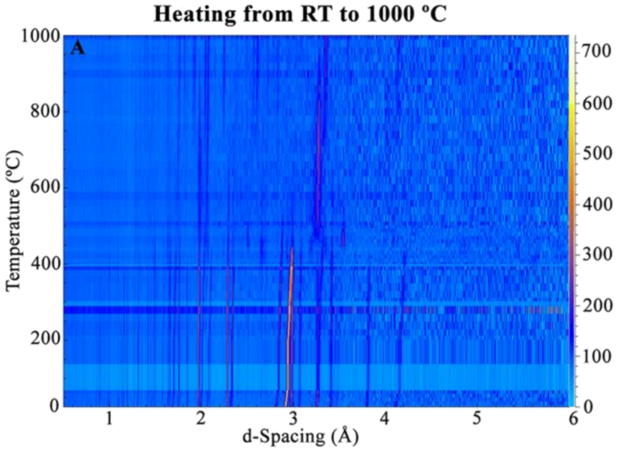




Determine the complicated magnetic structure, Physcial Review Materials 4, 044405 (2020).



gas-handling system (AGES) to enhance the synthesis science

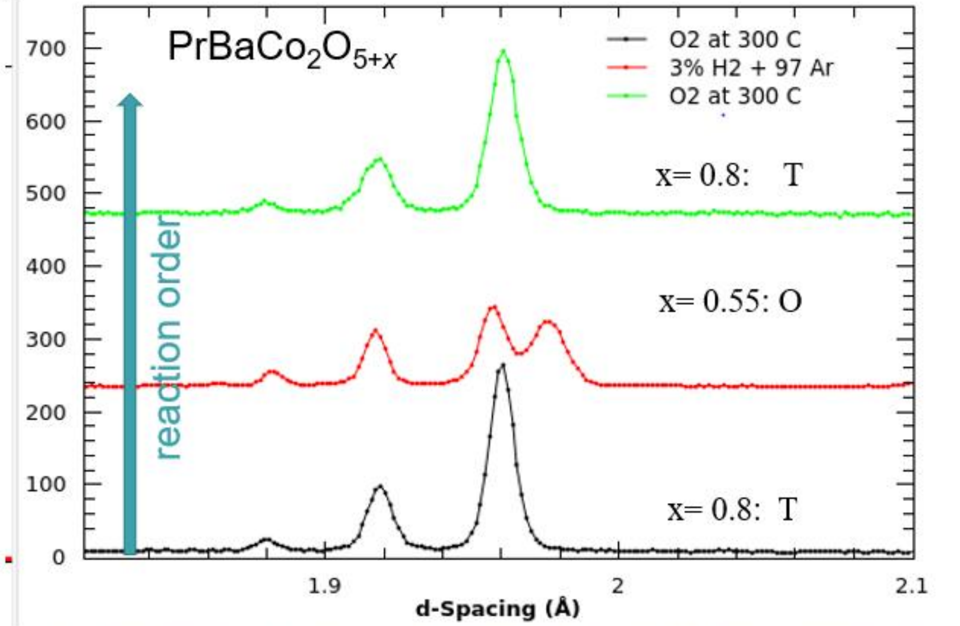


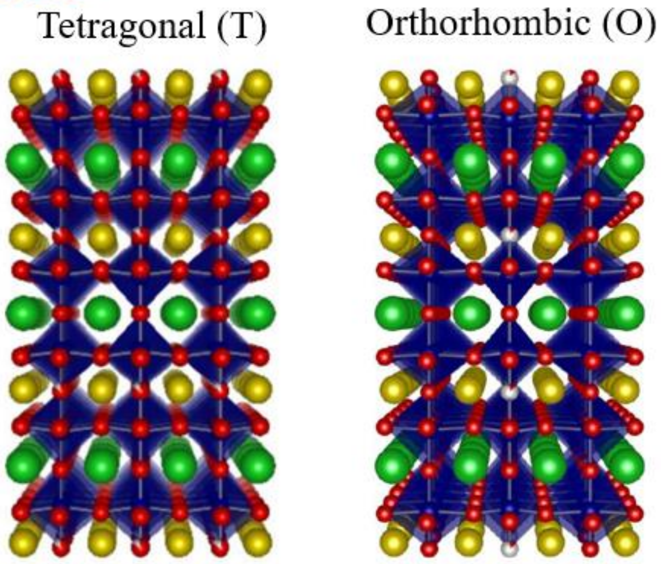
Chemistry of Materials, 2018

Instrument Developments: Pushing towards the forefront with unique and challenging experiments

POWGEN developing the capability for Gas loading at Cryogenic temperatures

Unveiling new crystal and magnetic phases by redox reaction in AGES





Switching between O_2 and 3% H_2/97% Ar, we observed a redox reaction induced Magneto-structural transition, reversible between tetragonal and orthorhombic structures

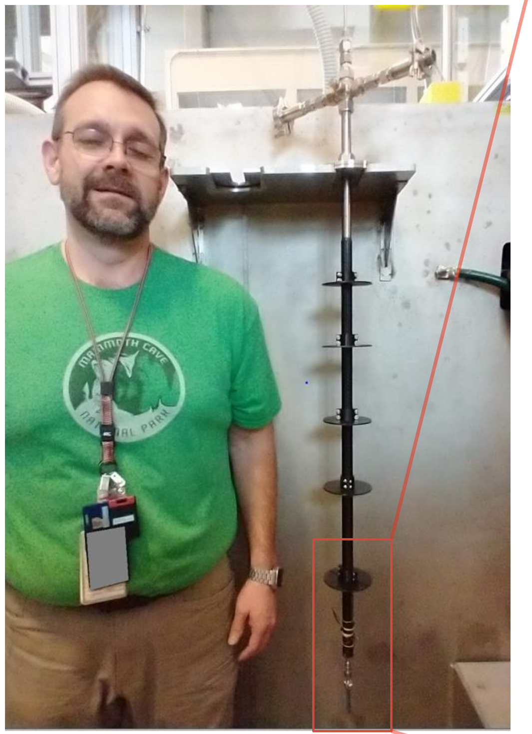
POWGEN mail-in data on novel ferroelectric material published in Nature Materials and featured in DOE highlight

Neutron Powder diffraction data on Yttrium doped Hafnium Dioxide synthesized by the Cheong measured by Qiang Zhang Group at Rutgers were using the POWGEN mail-in program

Powgen has New gas-loading stick for Janis top loading cryofurnace

- At Powgen they tested a new gas-loading stick for CCR-17, designed and built by Sample Environment Group's Matt Rucker.
- The stick uses a carbon fiber tube, instead of the standard stainless, for lighter weight and reduced thermal mass to hopefully allow for faster heating and cooling.

Melanie Kirkham
POWGEN SA



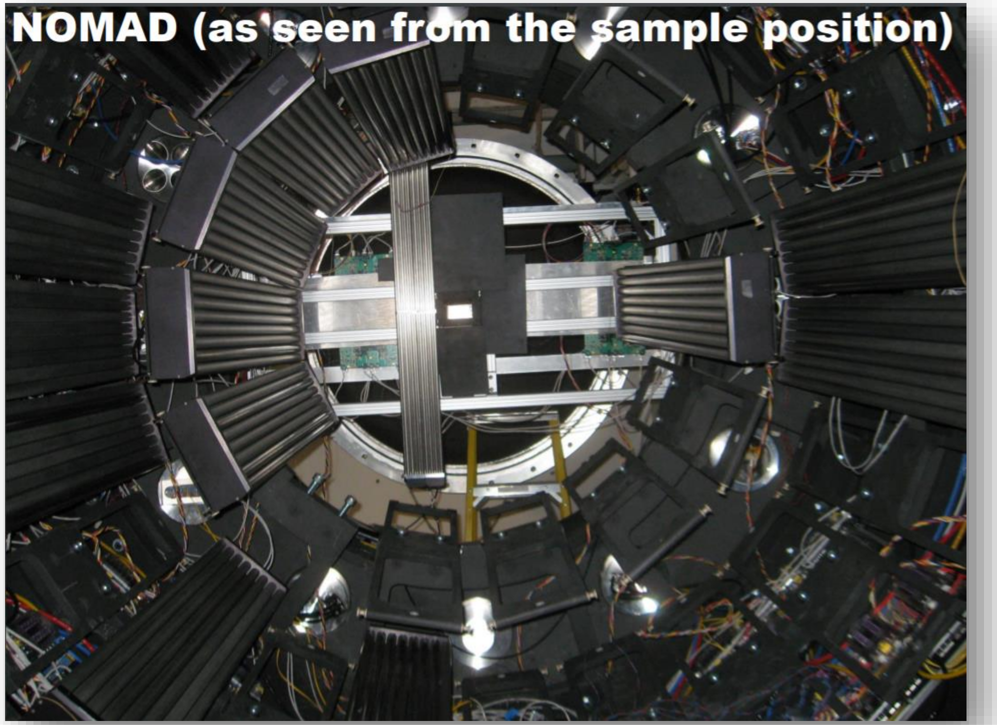
Matt Rucker
Sample Environment

SNS BL1B NOMAD: Nanoscale-Ordered Materials Diffractometer

- NOMAD is the fastest neutron diffractometer
- NOMAD is a diffractometer using a large bandwidth of neutron energies and extensive detector coverage to do structural determinations of **local order in crystalline and amorphous materials.**
- NOMAD was designed for studies of a large variety of samples ranging from **liquids, solutions, glasses, polymers and nanostructured materials to long range ordered crystals.**

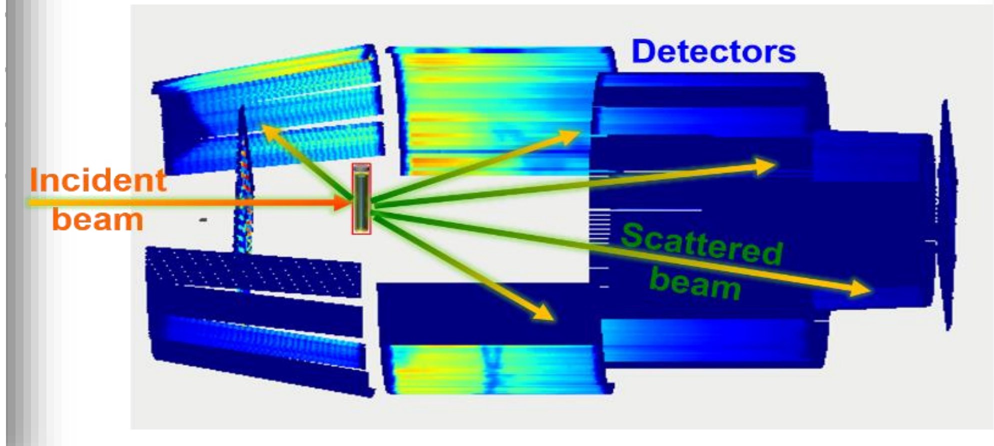
Joerg Neuefeind (100%), IS
Jue Liu (100%), IS
Cheng Li **(50%)**, IS
Michelle Everett (100%),SA

- NOMAD gives an access to:
  - high-resolution pair distribution functions (PDF)
  - small-contrast isotope substitution experiments
  - small sample sizes
  - parametric studies and in-situ diffraction.



Resolution Δd/d

Bank	$\langle 2\theta \rangle$ /degree	$\Delta d/d$ FWHM	approx. d-range /Å (60Hz*)
1	15	0.029	0.5-13
2	31	0.019	0.3-6.5
3	67	0.0137	0.3-3
4	122	0.0069	0.2-1.9
5	154	0.0036	0.2-1.5
6	7	0.039	0.5-28



SNS-NOMAD: Nanoscale-Ordered Materials Diffractometer

Entered fully into User Program: 2012
Average Days per an experiment: 2
Subscription Rate, 7-year average (Number of requested days/Number of available days): 296%

★Specially Recognized

Citation Count 20-49 (87)

Citation Count > 50 (72)

DOE Highlight (28)

Editor's Choice (2)

Journal Cover (8)

Journal Impact Factor >7 (202)

Rapid Communication (2)

Instrument Publications: **555**

Instrument H-index: **59**

Completed Experiments: **1234**

Instrument Authors: **2111**

Instrument Publication Analysis
Instrument H-Index: 59
(No. 2 instrument in ORNL)
Publication Impact: 34% publications with high impact factor

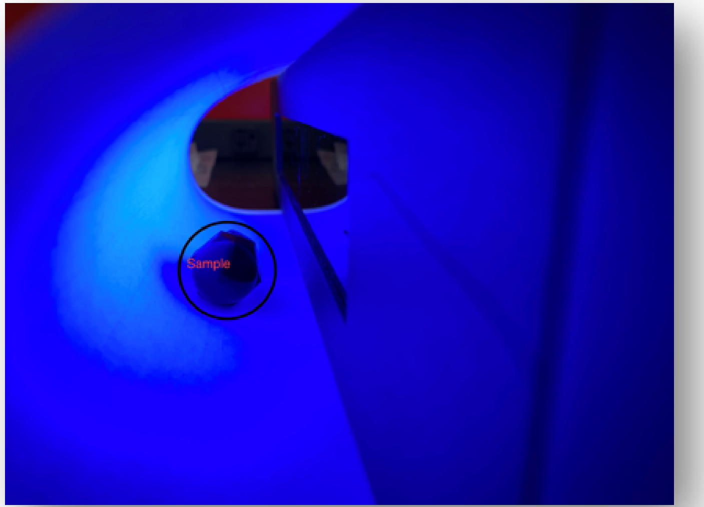
Joerg Neuefeind (100%), IS
Jue Liu (100%), IS
Cheng Li **(50%)**, IS
Matt Tucker (SH)
Michelle Everett (100%),SA

Instrument Developments: Pushing towards the forefront with unique and challenging experiments

NOMAD detector upgrade nearing completion

NOMAD Aerodynamic Levitator (NAL) is back in business!

NOMAD collaborates with MSTD and Texas A&M University to use ultraviolet radiation with NOMAD

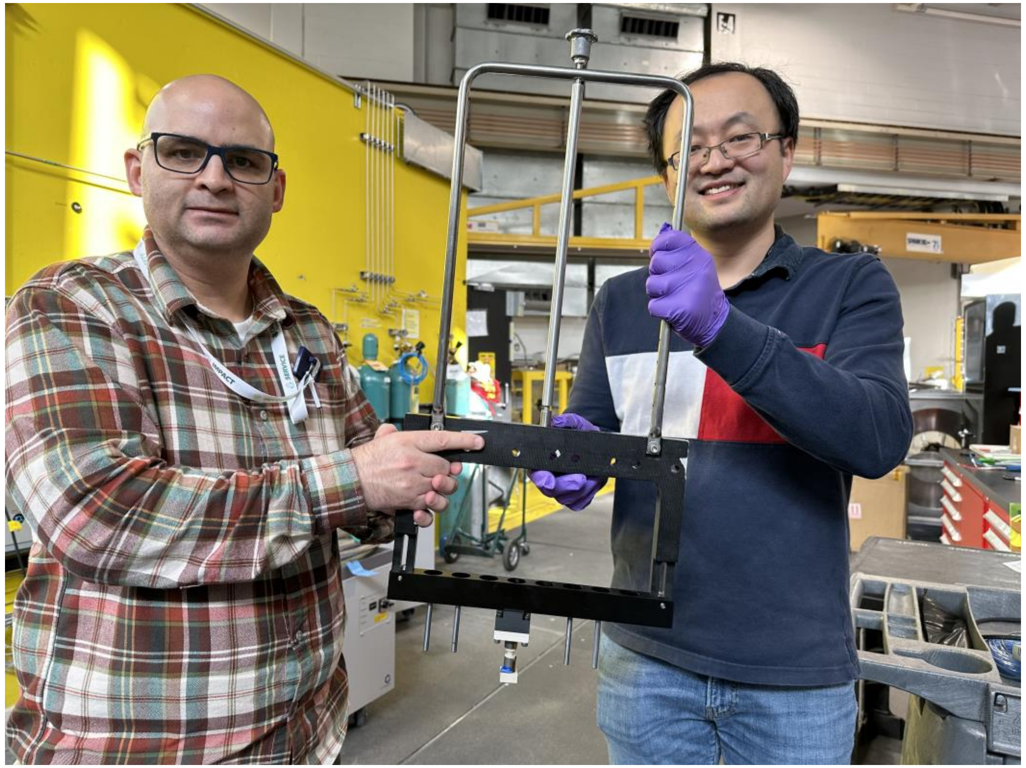


Picture shows the sample inside illuminated with the UV source, using NOMAD to measure the UV induced structural change in MOF-74-Mg

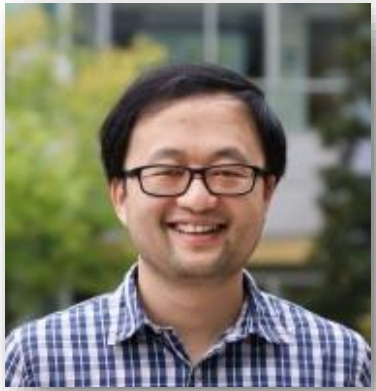
NOMAD measures hazardous molten salt materials at high temperatures

- The user team was composed of various scientists from ORNL (CSD,MSTD,NSD), MIT and UC Berkeley
- They aimed to Examine the Structure of Molten LiF-BeF_2, a highly attractive candidate molten salt that may be used as liquid fuel or as primary coolant in future Molten Salt Reactors (MSR's)

NOMAD runs FIRST *in-operando* experiment on a solid state battery



Jue used discretionary time to collaborate with ORNL-NTRC's Charl Jafta in measuring the FIRST in- operando Neutron Diffraction of Electrode Materials in All-Solid-State Li-Ion Batteries

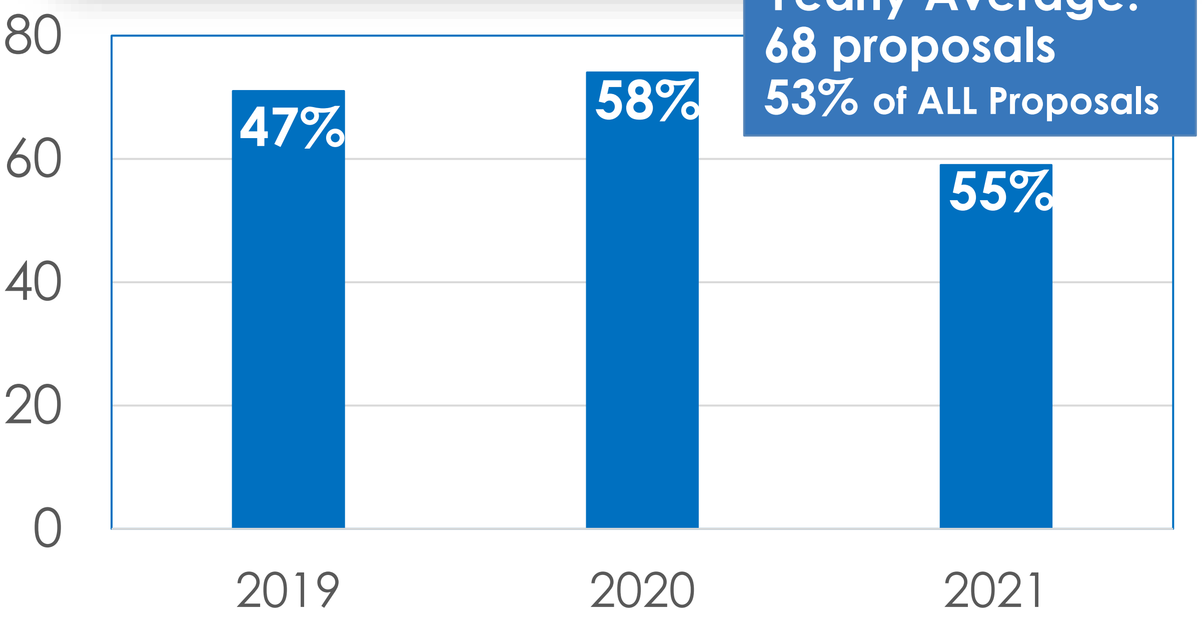


Jue Liu
(NSD)

Charl Jafta
(EEID/NTRC)

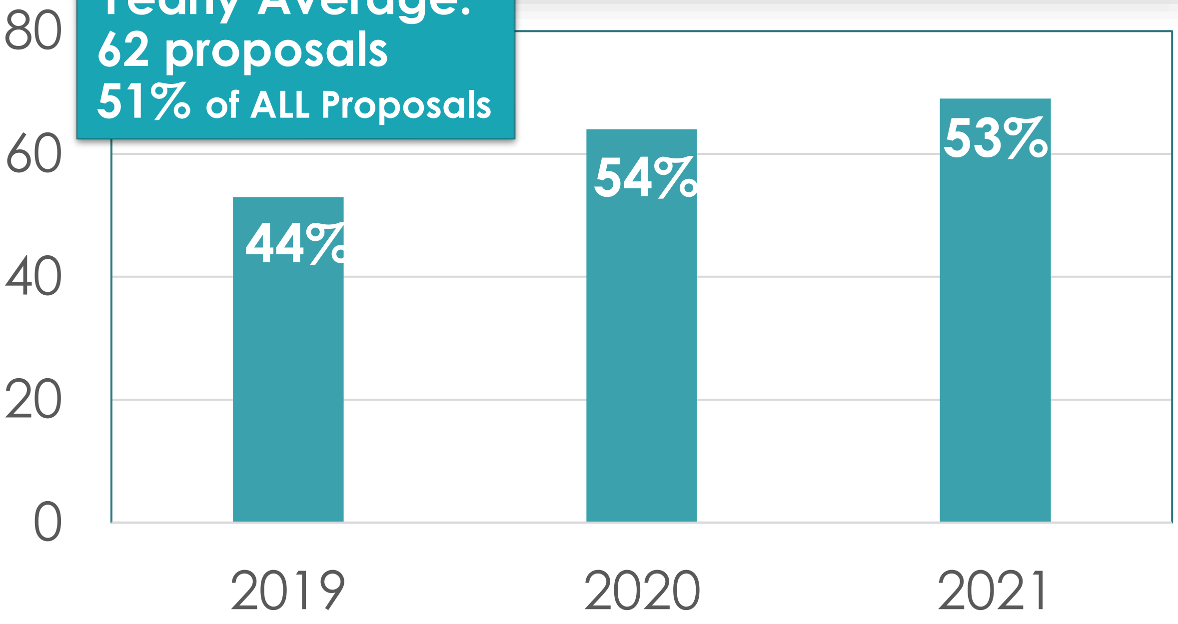
The MAIL-IN Program at POWGEN AND NOMAD

Yearly Average:
68 proposals
53% of ALL Proposals



250-350 samples per year
using the NOMAD shifter

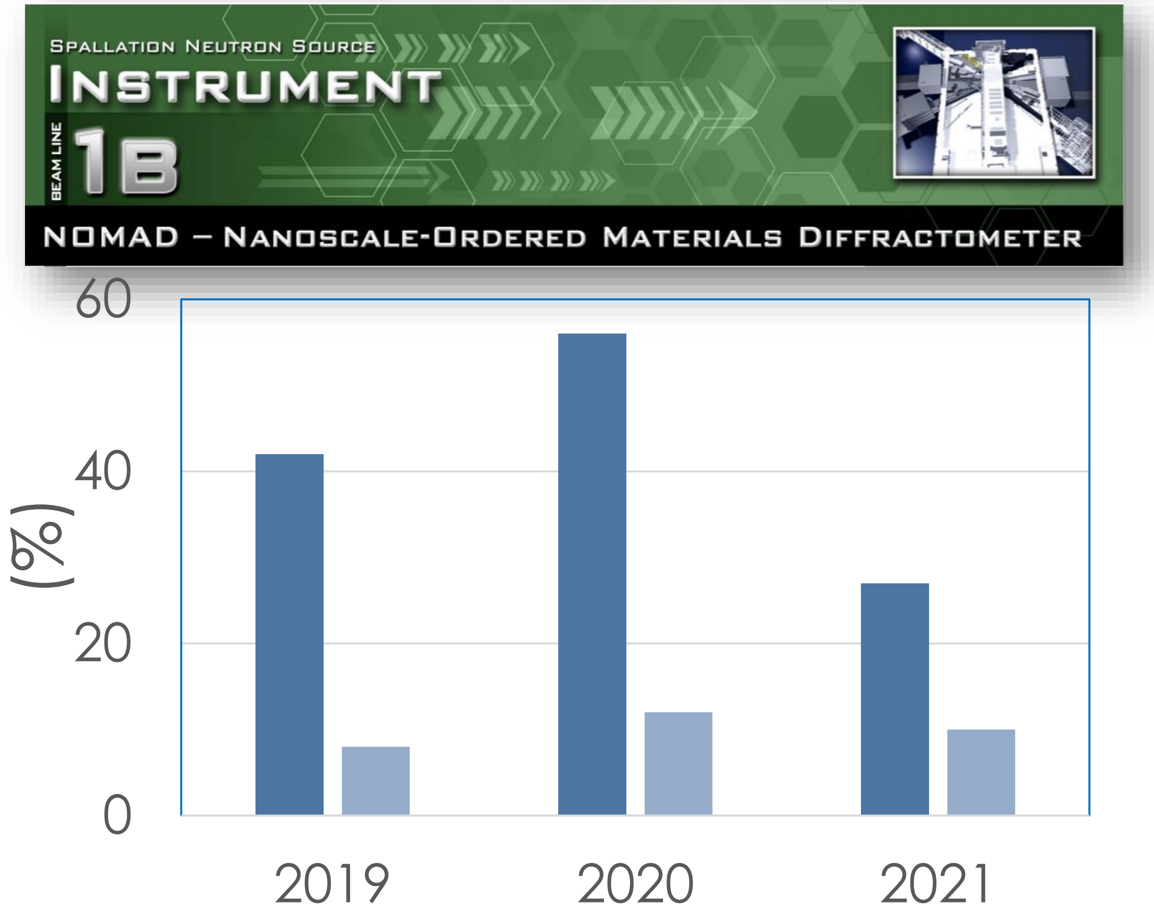
Yearly Average:
62 proposals
51% of ALL Proposals



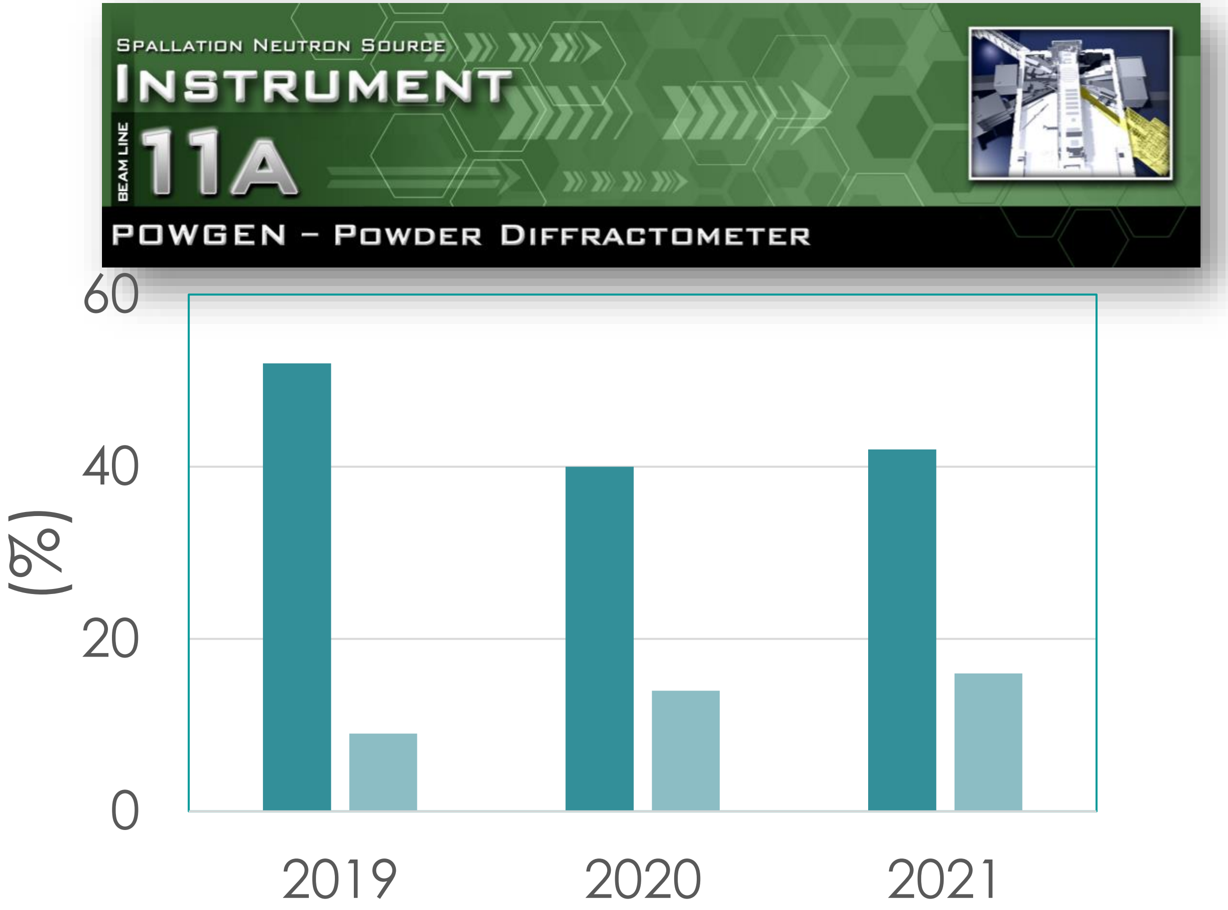
150-170 samples per year
using PAC (Powgen Auto Changer)

The MAIL-IN Program at NOMAD and POWGEN

Fraction of Papers and Beamtime for the Mail-IN Program



% of Total Publications
% of Total NOMAD Beamtime



% of Total Publications
% of Total POWGEN Beamtime

HFIR HB-3A DEMAND: a Dimensional Extreme Magnetic Neutron Diffractometer

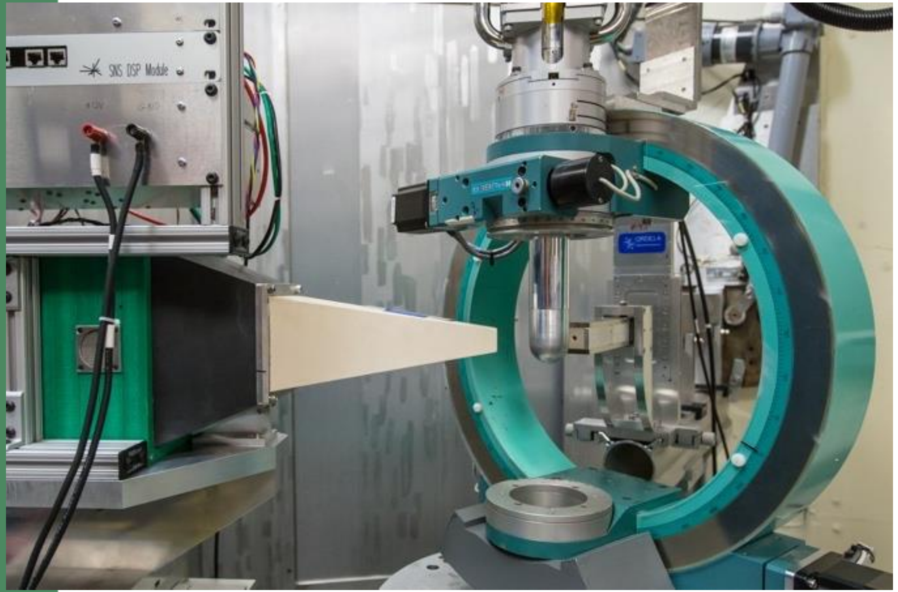
Nuclear and magnetic structures as a function of T, P, B, and E, e.g., magnetic structures, phase transitions and possible accompanied structural changes, order parameters and exploring structural phase diagrams.

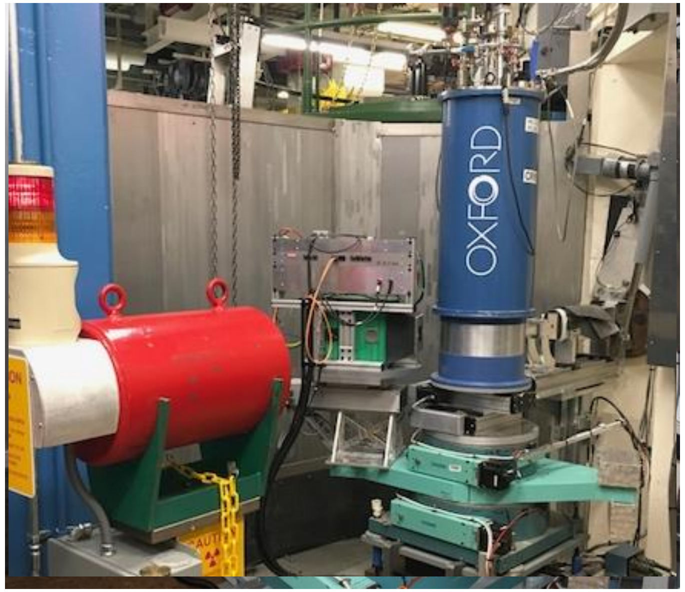
Sample Environment Upgrade

- Interchangeable 2-axis stage replaces 4-circle goniometer for extreme environment mode
- Ability to use cryostats, cryomagnets, and ultra-low temperature devices
- Single-crystal diamond anvil cell

Detector Upgrade Phase I completed

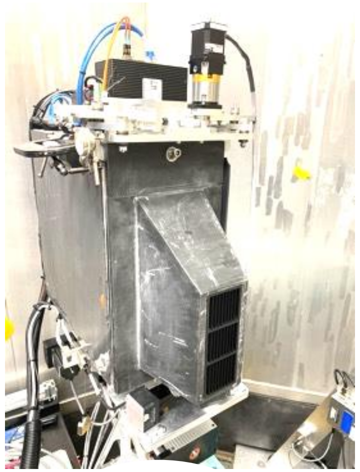
- Next generation Anger camera with Silicon photomultipliers (Magnetic-field insensitive)
- Total 348 (vertical) mm x 116 (horizontal) mm detector coverage (1536 x 512 pixels)
- Column of three modules achieves vertical angular range of 50° at 30 cm distance to the sample position
- Pixel resolution of 0.65 mm
- Allows the instrument to run in a two-axis mode with access to a large reciprocal space volume

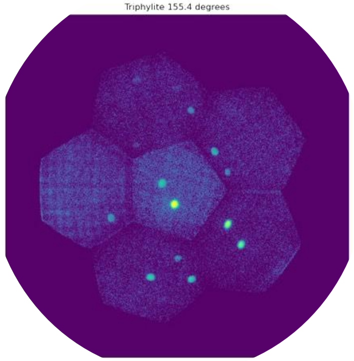




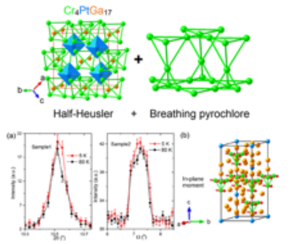

HFIR HB-3A DEMAND - What's new?

1. Oscillating collimator for complex sample environments designed, fabricated, and installed.
2. He-3 Polarizer lifting device designed, fabricated, installed, and commissioned; enables push-button switching between polarized and unpolarized mode.
3. Improved peak integration software for both 4-circle and 2-circle data collection modes.
4. Plan for post-HBRR instrument reconfiguration, extending incident beam path to reduce background and add more space for complex sample environments and polarizer.
5. 2 Huber goniometers acquired from MSTD to be used for spare parts.
6. Tested domed Anger camera prototype for the NTD Detector Group.





A Half-Heusler-Type Compound with a Breathing Pyrochlore Lattice



Ferromagnetic Cr_4PtGa_{17}: a half-Heusler-type compound with a breathing pyrochlore lattice. (a). Neutron diffraction Bragg peak (0 0 3) at 5 K and 80 K, indicating Cr_4PtGa_{17} is ferromagnetic with magnetic moments in the ab-plane (b).

Neutron data were collected at DEMAND at HFIR.

Xin Gui, Erxi Feng, Huibo Cao, Robert J. Cava, Ferromagnetic Cr_4PtGa_{17}: A Half-Heusler-Type Compound with a Breathing Pyrochlore Lattice, *Journal of the American Chemical Society* 143, 14342–14351 (2021). https://pubs.acs.org/doi/abs/10.1021/jacs.1c06667

Scientific Achievement

A new ternary intermetallic compound Cr_4PtGa_{17} was determined to be closely related to XYZ half-Heusler compounds with the formula of $(PtGa_2)(Cr_4Ga_{14})Ga$ (X = $PtGa_2$, Y = Cr_4Ga_{14}, Z = Ga).

Significance and Impact

The new material, Cr_4PtGa_{17}, the first realization of both a half-Heusler-type structure and a breathing pyrochlore lattice, offers a new way to achieve novel types of half-Heusler compounds. The compound contains a magnetic breathing pyrochlore lattice, which characteristically hosts geometrically frustrated magnetism, making Cr_4PtGa_{17} of great interest as a quantum material.

Research Details

- Single crystal growth used the self-flux method, and the crystal was characterized by single-crystal X-ray diffraction and bulk magnetic characterization.
- Single crystal neutron diffraction was used to determine the structural symmetry and finalize the ferromagnetic order at low temperature.

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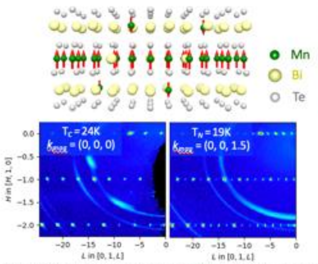
Defect Engineering of Magnetism and Topology



Depending on the details of Mn-Sb antisite defects, $MnSb_2Te_4$ crystals display either a ferrimagnetic (lower left) or an antiferromagnetic (lower right) ground state, as revealed by single-crystal neutron diffraction.

Neutron diffraction data were collected at SNS BL-9 CORELLI and BL-12 TOPAZ, and HFIR HB-3A DEMAND.

Yaohua Liu, Lin-Lin Wang, Qiang Zheng, Zengle Huang, Xiaoping Wang, Miaofang Chi, Yan Wu, Bryan C. Chakoumakos, Michael A. McGuire, Brian C. Sales, Weida Wu, Jiaqiang Yan. *Physical Review X, in press.*

Scientific Achievement

Researchers pinpoint defects' role in affecting both the magnetism and the band structure of a proximate intrinsic magnetic topological insulator compound $MnSb_2Te_4$.

Significance and Impact

This work showcases how defect engineering, which is exceptionally successful for modern semiconductor technologies, also can be critical for future quantum technologies based on magnetism and band topology, including ultra-low dissipation electronics.

Research Details

- $MnSb_2Te_4$ single crystals with different magnetic properties were fabricated with controlled growth.
- Single-crystal neutron diffraction correlated the details of structural defects and magnetism.
- Electron microscopes provided insights into the local defect structures.
- First principal calculations revealed the antisites' roles on the magnetism and band topology.

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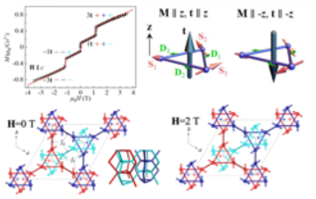
Field-tunable toroidal moment in a chiral-lattice magnet



Field-induced ferri- to ferrotoroidal transition in $BaCoSiO_4$. Top-left: Magnetization data (circles) with the field H//c and the theoretical calculations (line) from the full spin Hamiltonian. Top-right: Minimal energy configurations for three spins S_i (i = 1,2,3) on a triangle with an antiferromagnetic Heisenberg interaction and an in-plane DM interaction D_i (i = 1, 2, 3). It illustrates how a field can switch a toroidal moment t. Bottom two plots show the magnetic structures at zero field and H = 2 T and corresponding toroidal moment t (+, - represent the toroidal moment up and down).

Neutron data were collected at DEMAND at HFIR and POWGEN at SNS.

Lei Ding*, Xianghan Xu, Harald O. Jeschke, **Xiaojian Bai***, **Erxi Feng***, Admasu Solomon Alemayehu, Jaewook Kim, Feiting Huang, **Qiang Zhang**, Xiaxin Ding, Neil Harrison, Vivien Zapf, Daniel Khomskii, Igor I. Mazin, Sang-Wook Cheong, **Huibo Cao***, Field-tunable toroidal moment in a chiral-lattice magnet, *Nature Communications, in press* (2021). *supported by Cao's DOE Early Career Award.

Scientific Achievement

Toroidal moments arising from tri-spin vortex were found in a chiral lattice $BaCoSiO_4$. These moments can then interact, giving rise to ferri-toroidal order. Though controlling toroidal order is difficult, it was realized in this chiral lattice by a magnetic field and exhibits multiple toroidal and metamagnetic transitions.

Significance and Impact

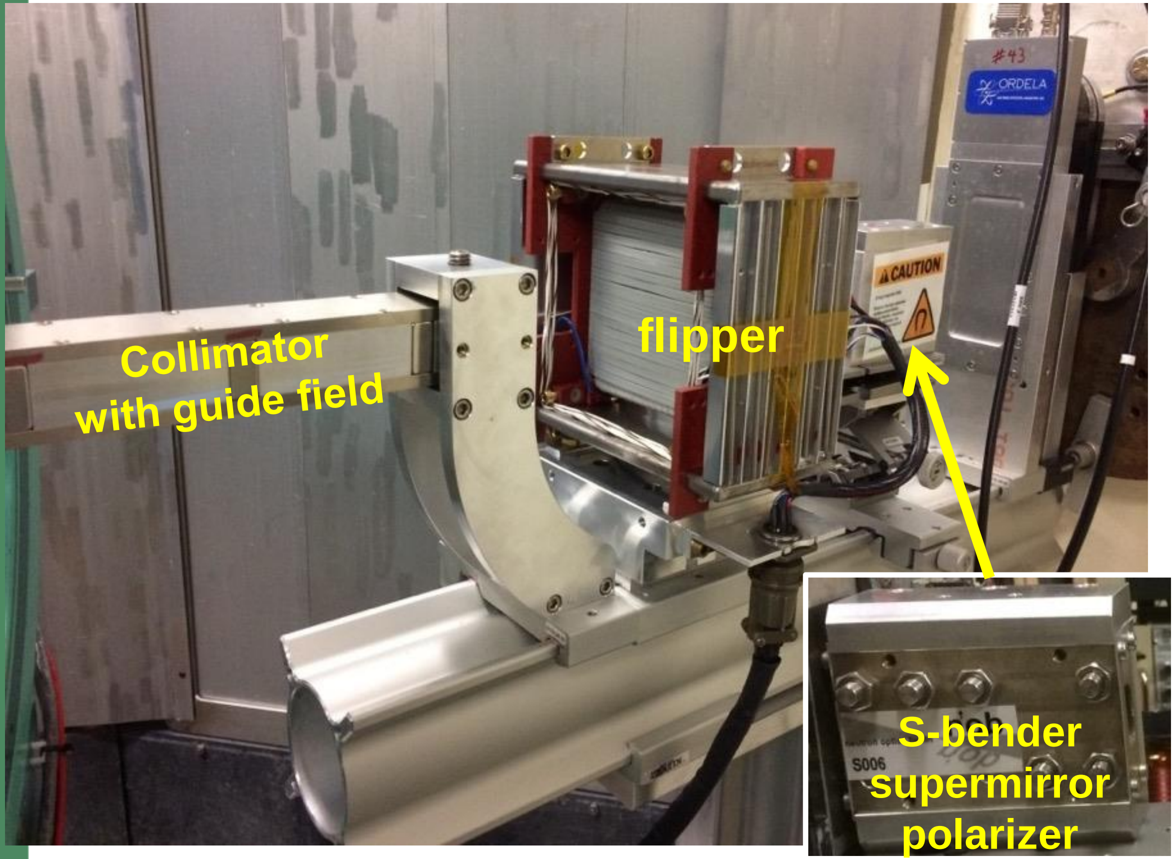
This work opens new avenues for realizing easily tunable toroidal orders. Two key ingredients are frustrated isotropic exchange couplings and antisymmetric exchange interactions driven by the crystallographic chirality.

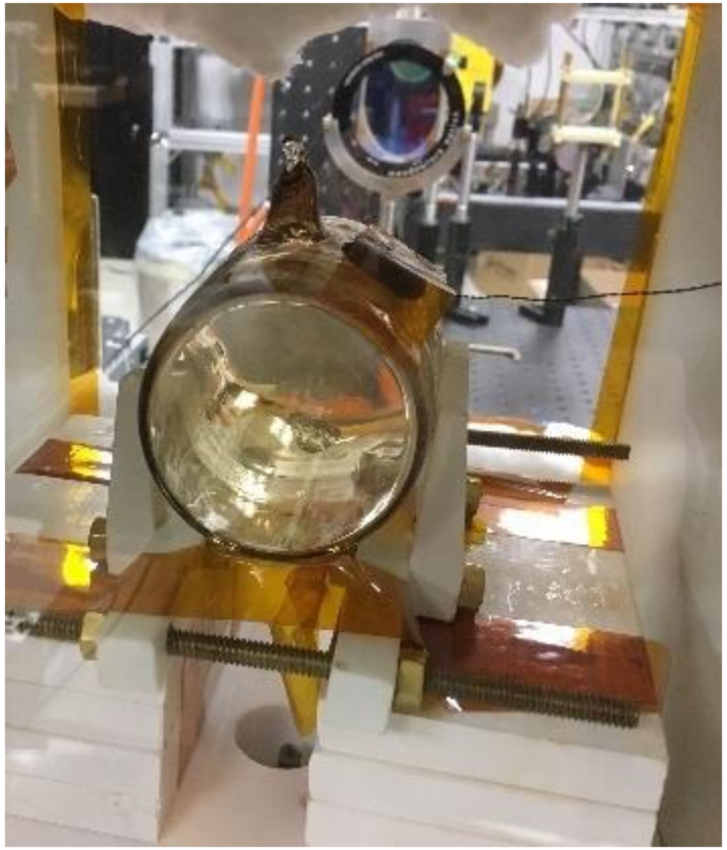
Research Details

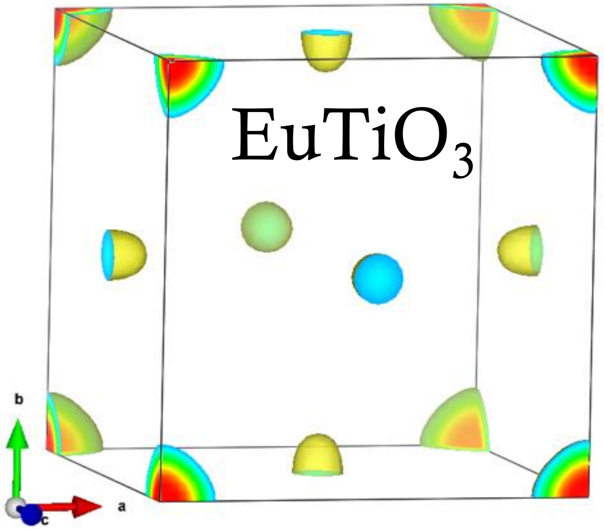
- Multi-stair metamagnetic transitions were found in a chiral lattice compound $BaCoSiO_4$.
- Neutron diffraction found a zero-field ferri-toroidal order that can be switched into a ferro-order by a magnetic-field along with multi-stair metamagnetic transitions.
- Driving mechanisms were revealed through the ab initio density functional theory calculations and theoretical modeling.

U.S. DEPARTMENT OF ENERGY | Office of Science — RUTGERS — MAGLAB — OKAYAMA — GEORGE MASON UNIVERSITY — Universität zu Köln — OAK RIDGE National Laboratory — NEUTRON SCIENCES

Polarized Neutrons at HFIR HB-3A







Clockwise: S-Bender polarizer and flipper on instrument, drop-in ^3He cell, in-situ pumping ^3He cell on the beam line. The first spin density map with ^3He cell polarizer.

HFIR HB-3A DEMAND instrument – Detector Upgrade

Four-circle mode

Two-axis mode

Newly enabled extreme sample environments

Ultra-low temperature
***T* ~ 0.05 to 700 K**

High magnetic field
***H* ~ -6 to 6 T (vertical)**

New Science

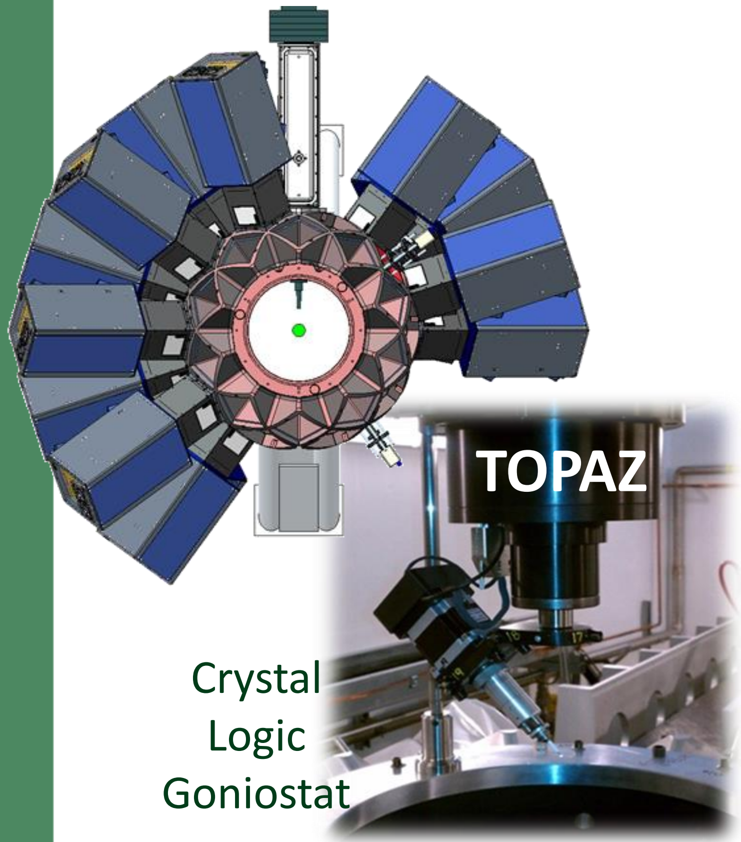
Complex magnetism & structure

New quantum materials & phenomena

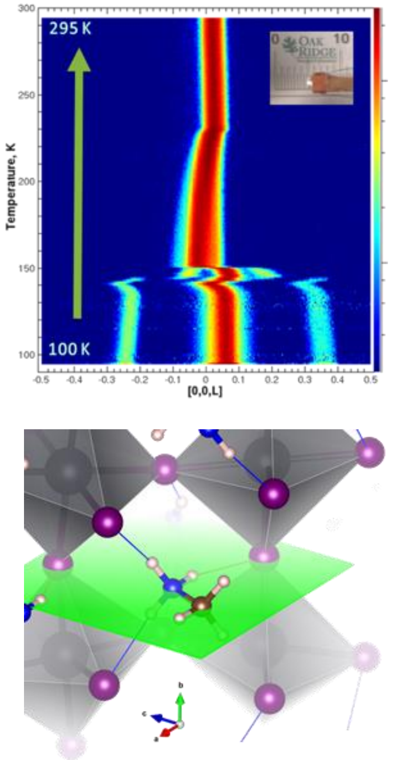
New large area detector allows out-of-plane coverage so the chi circle can be removed for the 2-axis mode making space for complex sample environments.

Cao H.B., Chakoumakos B.C., Andrews K.M., Wu Y., Riedel R.A., Hodges J.P., Zhou W., Gregory R., Haberl B., Molaison J.J., Lynn G.W., "DEMAND, a Dimensional Extreme Magnetic Neutron Diffractometer at the High Flux Isotope Reactor", *Crystals*, **9,** 5 (2019).

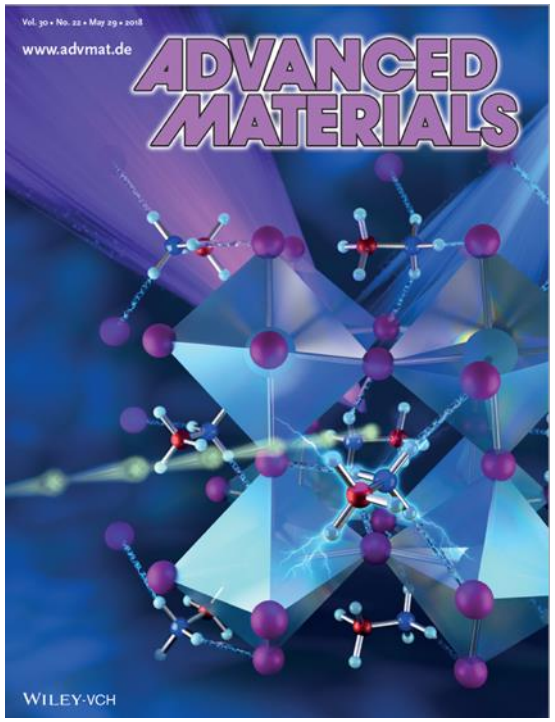
SNS BL-12 TOPAZ is a high-resolution single-crystal diffractometer. Diffraction data are recorded in event mode in 3D diffraction space together with the associated metadata for parametric studies p_i (T, E…).



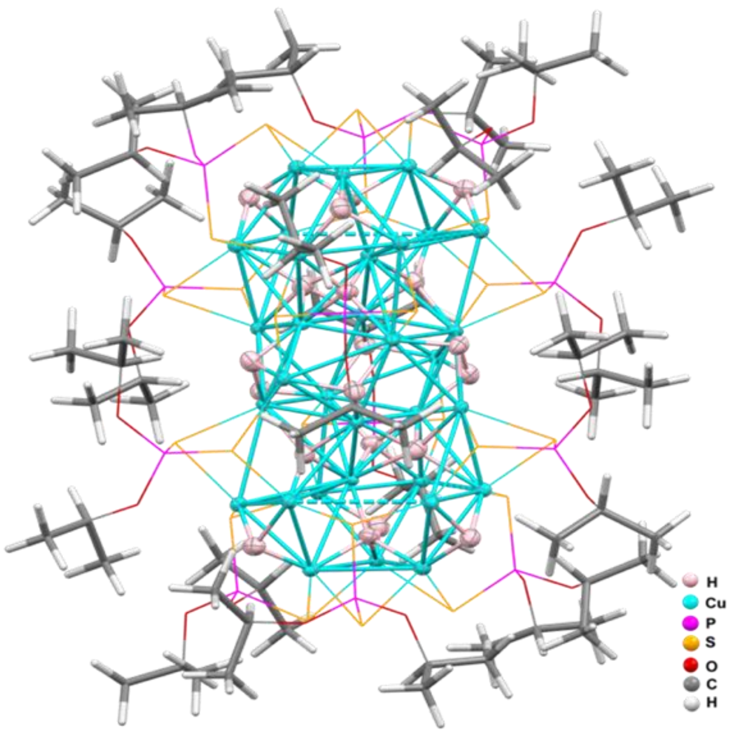
(a) Layout of TOPAZ.



(b) 4-dimensional data showing peak splitting of a hybrid organic-inorganic perovskite $MAPbBr_3$ at low temperature.



(c) Real-time T-dependent neutron diffraction and photoluminescence revealed an order-to-disorder transformation of the organic cation in $MAPbBr_3$.



(d) A record number of 20 hydrides (pink) in a polyhydrido copper nanocluster were located using data measured from a 0.45 mm^3 hydrogenated sample.

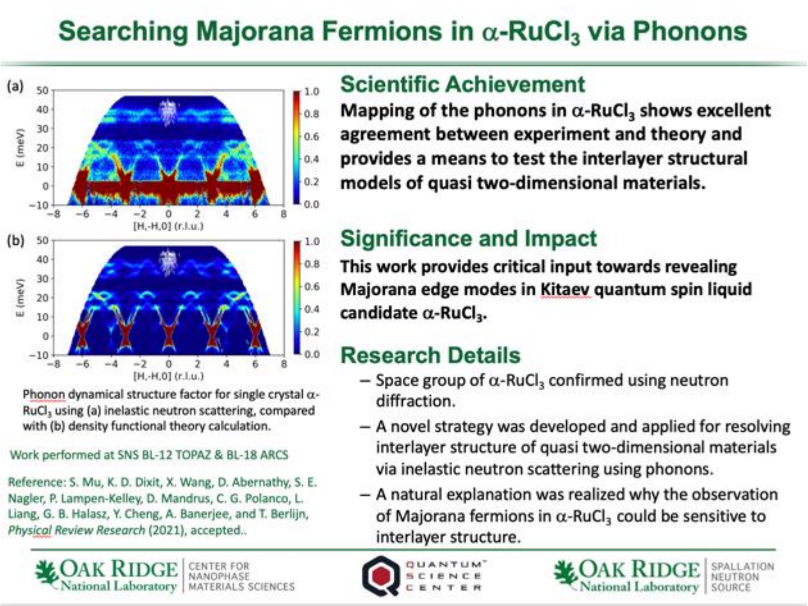
SNS BL-12 TOPAZ - What's new?

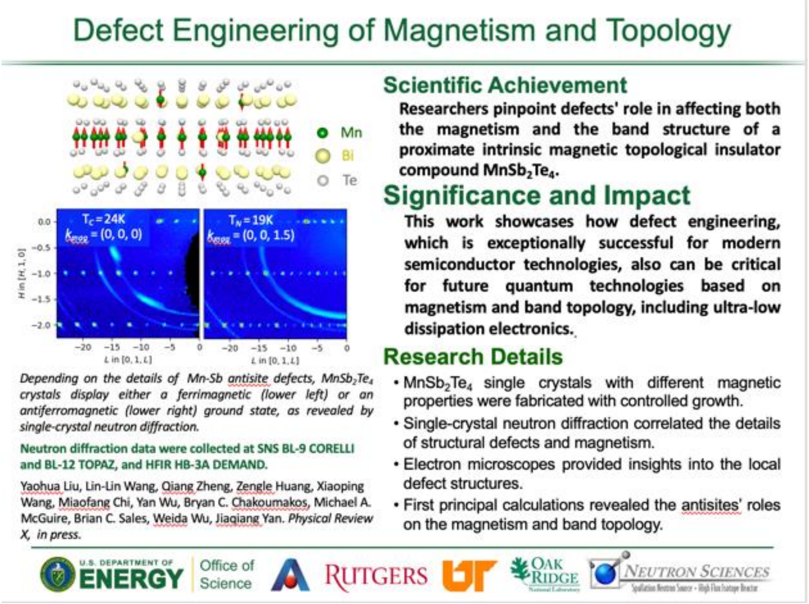
1. 5K Cryogoniometer fully commissioned and in user program.

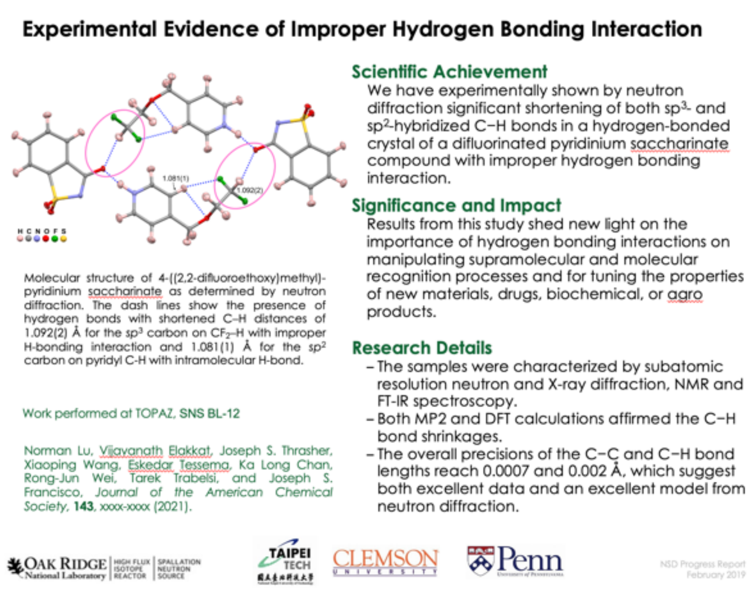
2. SBIR project with Christina Hoffmann. - Online Visualization and Data Discovery for Neutron Scattering Experiments with RadiaSoft LLC.

1. New capability showcasing applied electric current with combined low temperature and magnetic field are being led by Feng Ye and Christina Hoffmann.

2. Data integration workflow improved (Zach Morgan and Xiaoping Wang)



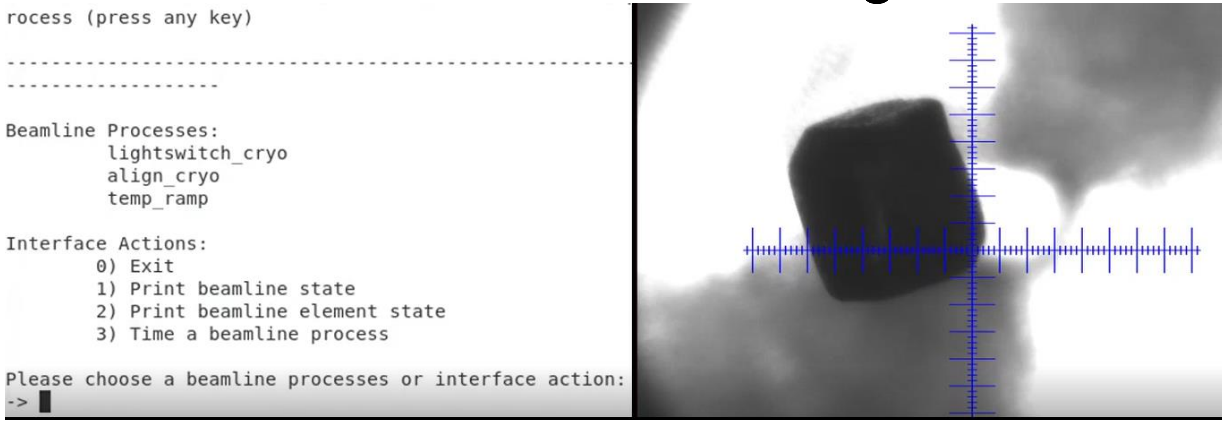




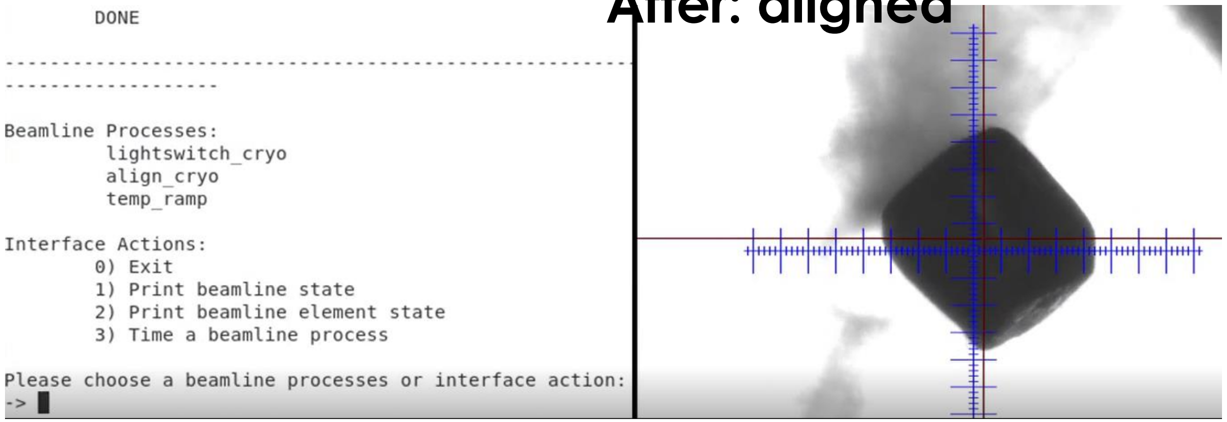
First Machine Learning Sample Auto-Alignment at ORNL Achieved

- The SBIR project for machine learning based automated sample alignment has demonstrated the first fully automated sample alignment on TOPAZ.
- Simple interface used to run the alignment.
- Bhargavi Krishna, Morgan Henderson worked with Stuart Calder, Christina Hoffman and a wider team at ORNL/Radiasoft.
- Next steps are to apply the alignment process to powder samples on HB-2A.

Before: unaligned



After: aligned



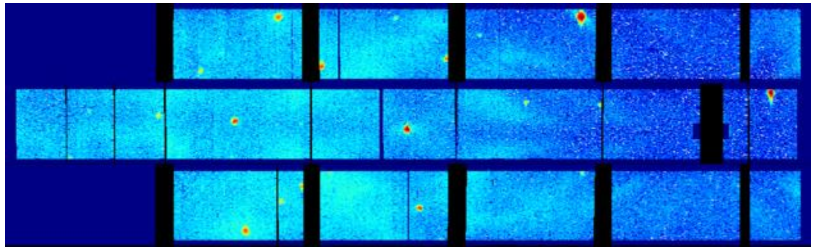
Bhargavi Krishna
DAQ, NTD

Morgan Hendersor
Radiasoft

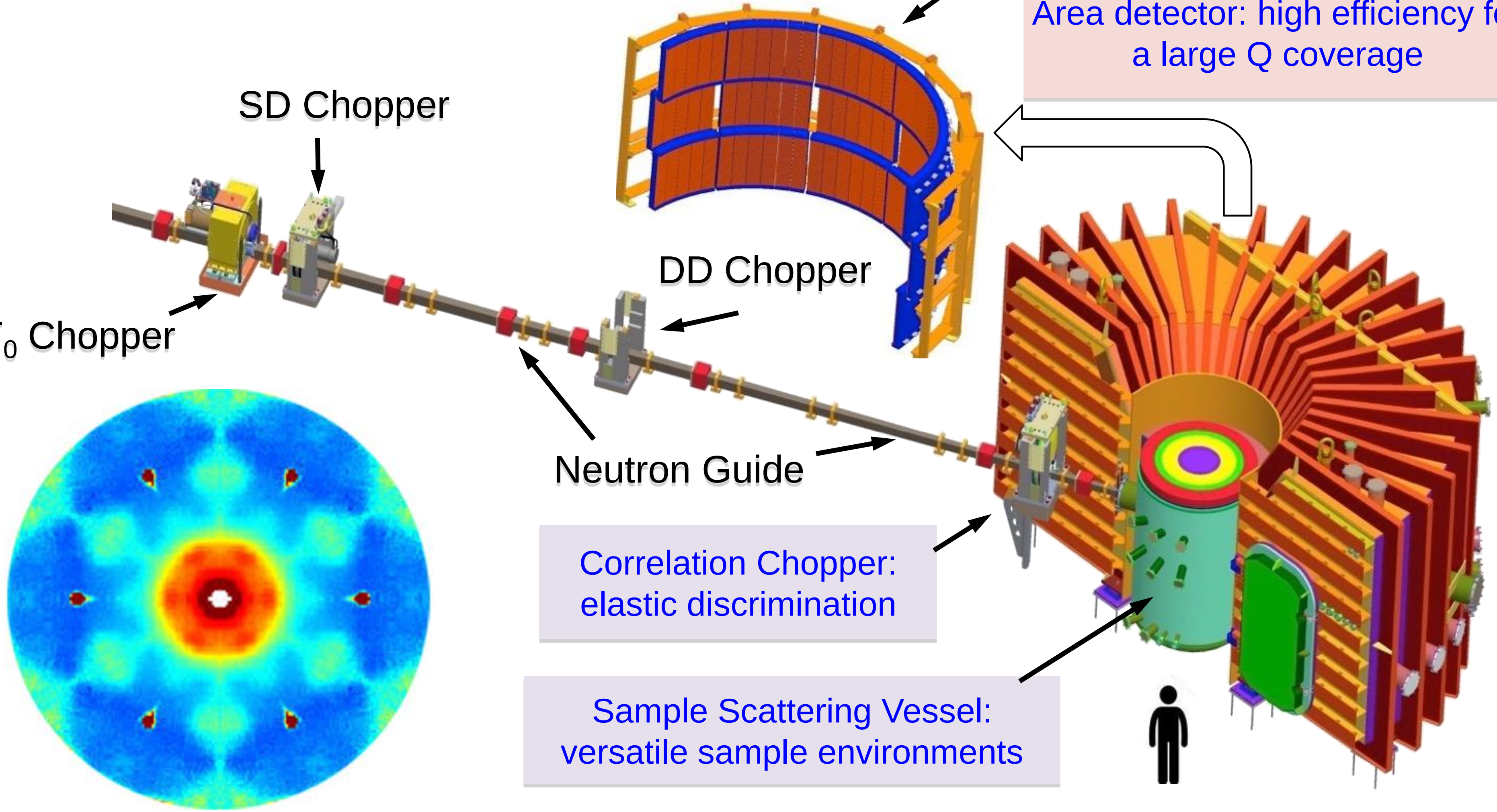
radiasoft

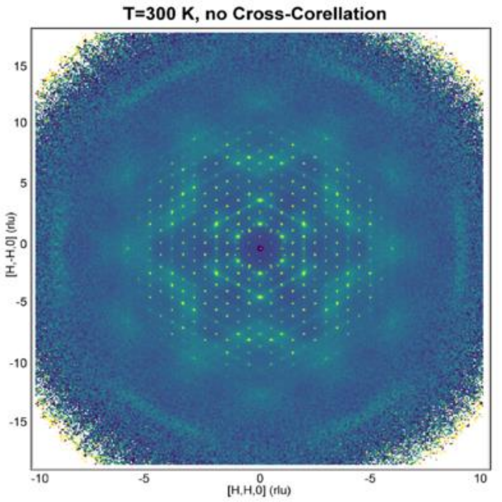
U.S. DEPARTMENT OF ENERGY | Office of SBIR/STTR Programs

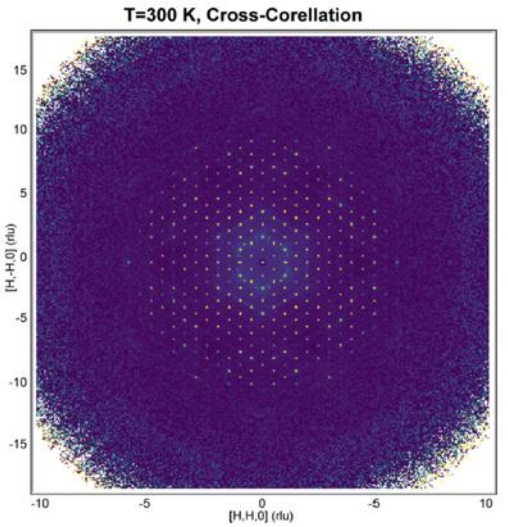
SNS BL-9 CORELLI: Single-crystal elastic diffuse scattering



Current detector coverage = 83%
vertical: +2 9° to -26°
horizontal: +147° to -19°







SNS BL-9 CORELLI - What's new?

1. Radial collimator repaired, and position improved. A second iteration of position improvement has been scheduled.

2. New bushings on sample sticks have reduced sample position wobble by an order of magnitude

3. 14 Tesla Magnet successfully tested.

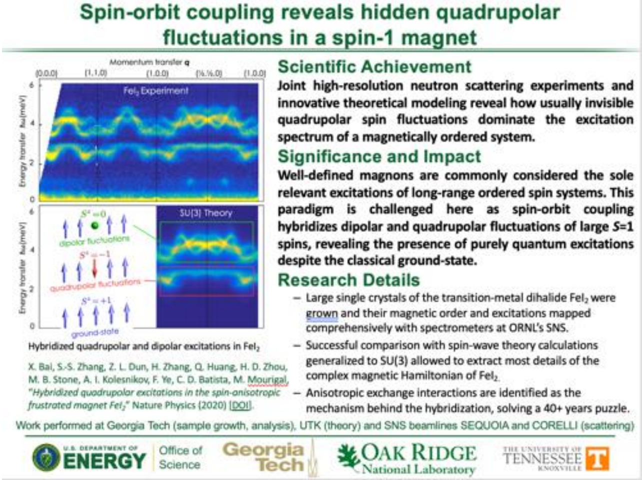
4. Improved peak integration software developed, and workflow implemented (Zach Morgan and Feng Ye).

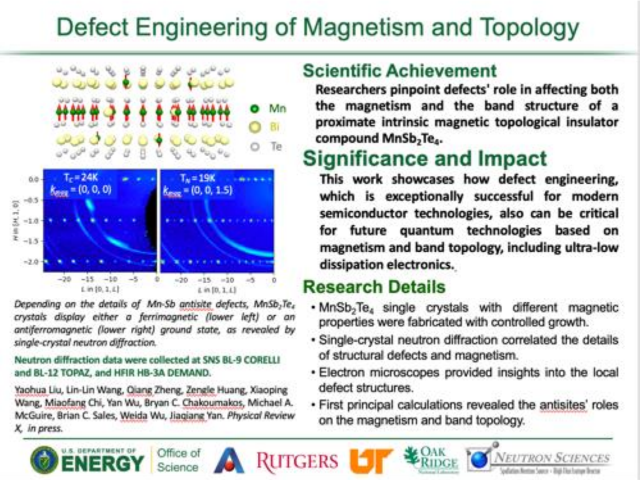
5. Improved detector calibration and wavelength dependent data reduction corrections (e.g., extinction) (Zach Morgan and Feng Ye).

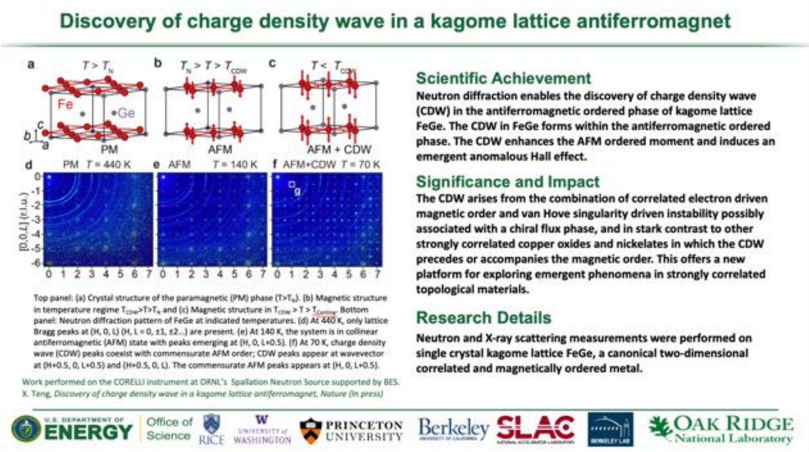
6. New CORELLI Instrument Scientist: Arianna Minelli.

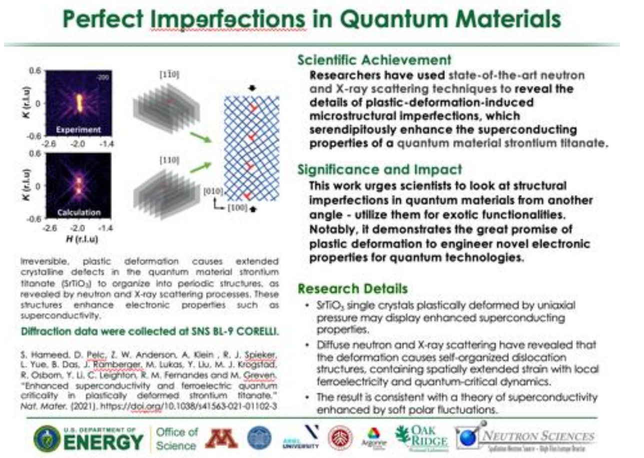
7. Led suite in publications past year.

8. First instrument paper in *Nature*.



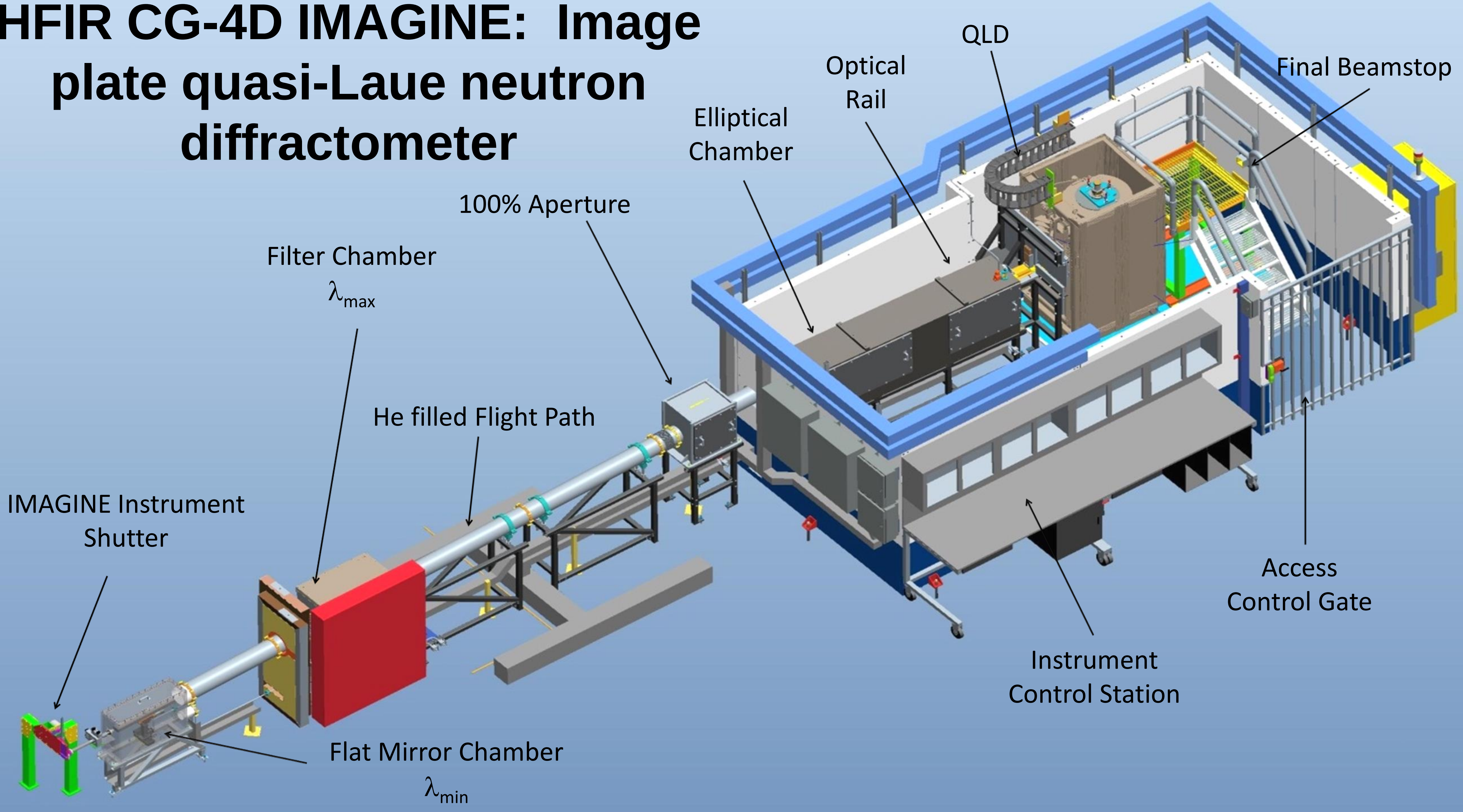




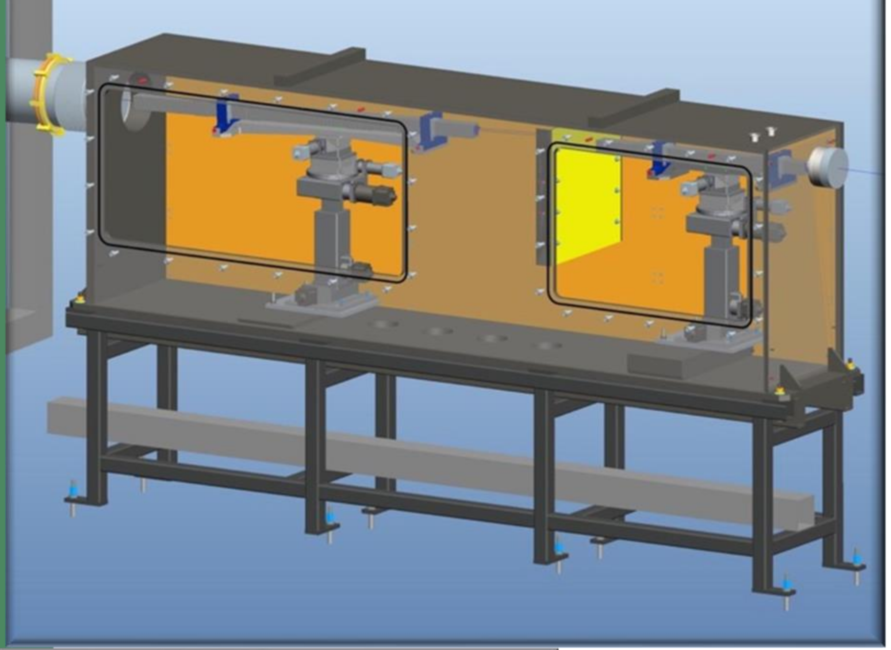


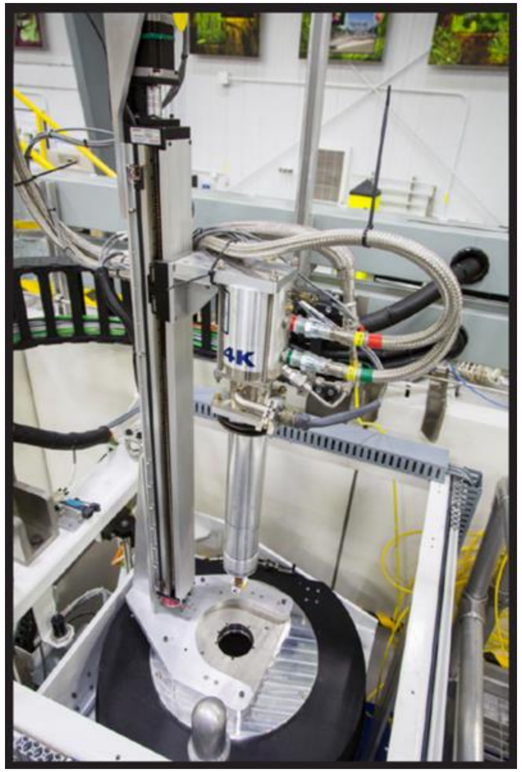
OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

HFIR CG-4D IMAGINE: Image plate quasi-Laue neutron diffractometer



HFIR CG-4D IMAGINE





Detector	Neutron image plate
Detector size	1200 x 450 mm
Pixel size	125, 250, 500 μm
Sample-to-detector distance	200 mm
Goniometer	Single Phi rotation axis

Applications

- **Macromolecular structure-function**
- **Supramolecular crystallography**
- **Materials chemistry**
- **Optimized for unit cells to 150 Å**
- **Temperature range 4 – 450 K**

Wavelength ranges:

2.0 Å - 3.0 Å	2.78 Å - 3.0 Å	3.33 Å - 4.0 Å
2.0 Å - 4.0 Å	2.78 Å - 4.0 Å	**3.33 Å - 4.5 Å**
2.0 Å - 4.5 Å	**2.78 Å - 4.5 Å**	**2.78 Å - 10 Å**

Flux: ~10^7 n s^{-1} cm^{-2}; Divergence: h0.5°, v0.6°
Beam size: 2 x 3.2 mm^2

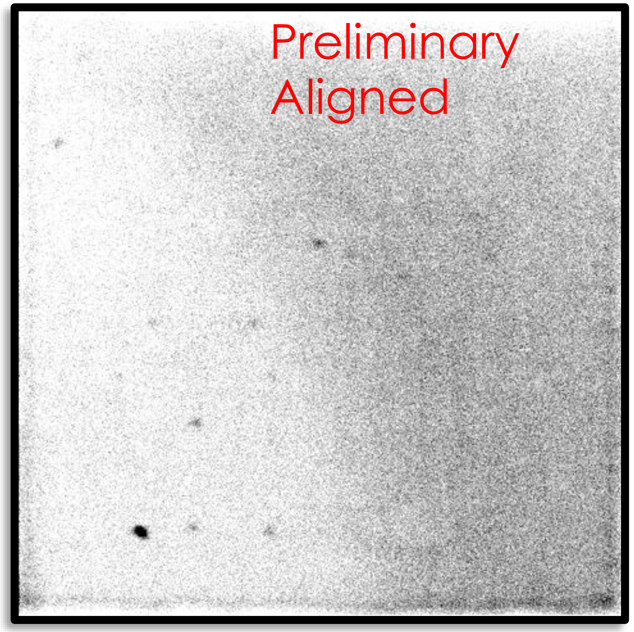
Meilleur et al., *Acta Cryst. D* **69**, 2157-2160 (2013)

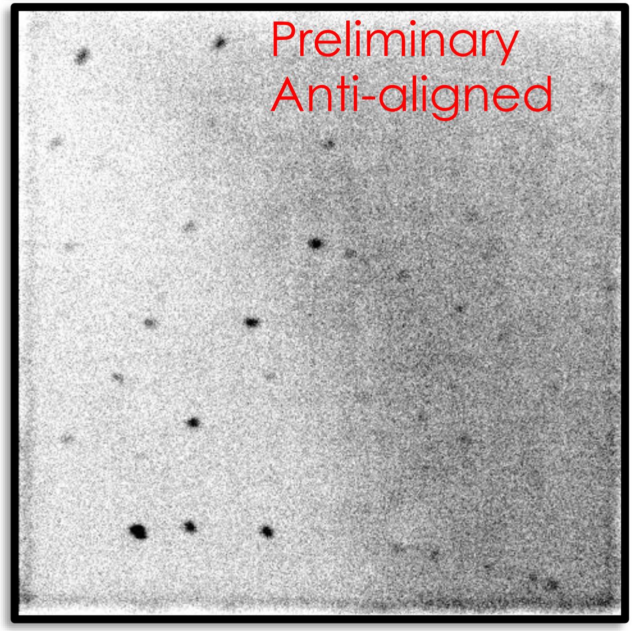
HFIR CG-4D IMAGINE - What's new?

1. Proof of concept for DNP shows progress with expected signal-to-noise gains for protein crystallography, obviating the need for deuteration.

2. Proposal for IMAGINE-X, with fully integrated DNP, real-time detectors, and modern goniometer being prepared. Need to convince management to commit to building full instrument.

3. Meanwhile, IMAGINE continues to support full protein crystallographic studies and screening of crystals for users.





Neutrons help design inhibitors of SARS-CoV-2 main protease

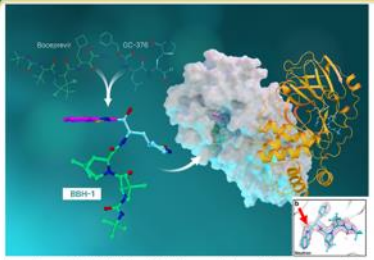


Image shows how hybrid inhibitor BBH-1 was designed from boceprevir (hepatitis C protease inhibitor) and GC-376 (SARS-CoV-1 inhibitor) and its neutron structure with SARS-CoV-2 M^{pro}. Inset shows nuclear density of BBH-1 revealing deprotonated negatively charged oxyanion (red arrow).

D.W. Kneller, H. Li, G. Phillips, K.L Weiss, Q. Zhang, M.A. Arnould, C.B. Jonsson, S. Surendranathan, J. Parvathareddy, M.P. Blakeley, L. Coates, J.M. Louis, P.V. Bonnesen, A. Kovalevsky, *Nat. Commun.* **13** 2268 (2022). DOI: 10.1038/s41467-022-29915-z.

Work performed on IMAGINE at High Flux Isotope Reactor, Center for Structural Molecular Biology, Center for Nanophase Materials Sciences, LADI-DALI at Institut Laue-Langevin, Grenoble, France.

Scientific Achievement

SARS-CoV-2 main protease (M^{pro}) enzyme is indispensable for virus replication and is an essential drug target for the design and development of small-molecule antivirals to treat COVID-19. Neutron crystallography was used to help design and characterize covalent hybrid protease inhibitors (BBH-1, BBH-2 and NBH-2) created by splicing components of known hepatitis C and SARS-CoV-1 protease inhibitors. These inhibitors demonstrated efficient inhibition of SARS-CoV-2 in cell-based assays, paving the way for further design of improved antivirals.

Significance and Impact

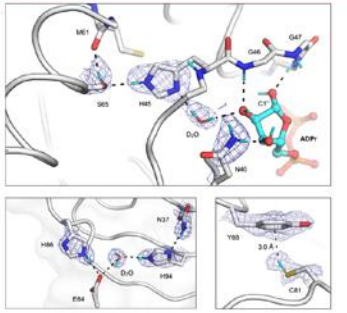
Hydrogen atoms are crucial players in drug binding, their locations determine protonation states and electric charges of ionizable residues. Knowledge of hydrogen atom positions provides unique information for drug design and was used to design potent (nanomolar) inhibitors of SARS-CoV-2 M^{pro}, map essential hydrogen bonding interactions between inhibitors and enzyme, and evaluated antiviral properties. Comparison with the FDA-approved nirmatrelvir from Pfizer indicated how inhibitor design can be further improved.

Research Details

- Neutron structure of M^{pro}/BBH-1 complex visualized critical hydrogen atoms and hydrogen bonds for the inhibitor binding; X-ray structures of M^{pro} in complexes with BBH-2, NBH-2, and nirmatrelvir were determined.
- Thermodynamics of inhibitor binding to M^{pro} evaluated by isothermal titration calorimetry.
- Antiviral properties of the inhibitors were evaluated in cell-based assays.

U.S. DEPARTMENT OF ENERGY | Office of Science

Neutrons uncover atomic details of SARS-CoV-2 macrodomain to guide design of novel antivirals



The neutron scattering length density maps at and around the Mac1 active site.

G.J. Correy, D.W. Kneller, G. Phillips, S. Pant, S. Russi, A.E. Cohen, G. Meigs, J.M. Holton, S. Gahbauer, M.C. Thompson, A. Ashworth, L. Coates, A. Kovalevsky, F. Meilleur, J.S. Fraser (2022) *Science Advances*, in press.

Work was performed at the SNS and at the HFIR

Scientific Achievement

We determined and compared the room temperature structures of the macrodomain of SARS-CoV-2 (Mac1) using neutron and X-ray diffraction to re-evaluate the catalytic mechanism of Mac1 and guide the optimization of inhibitors.

Significance and Impact

The knowledge of the protonation states of Mac1 residues that control catalytic activity and of the hydrogen bond networks that govern protein flexibility will inform the design of new Mac1 inhibitor.

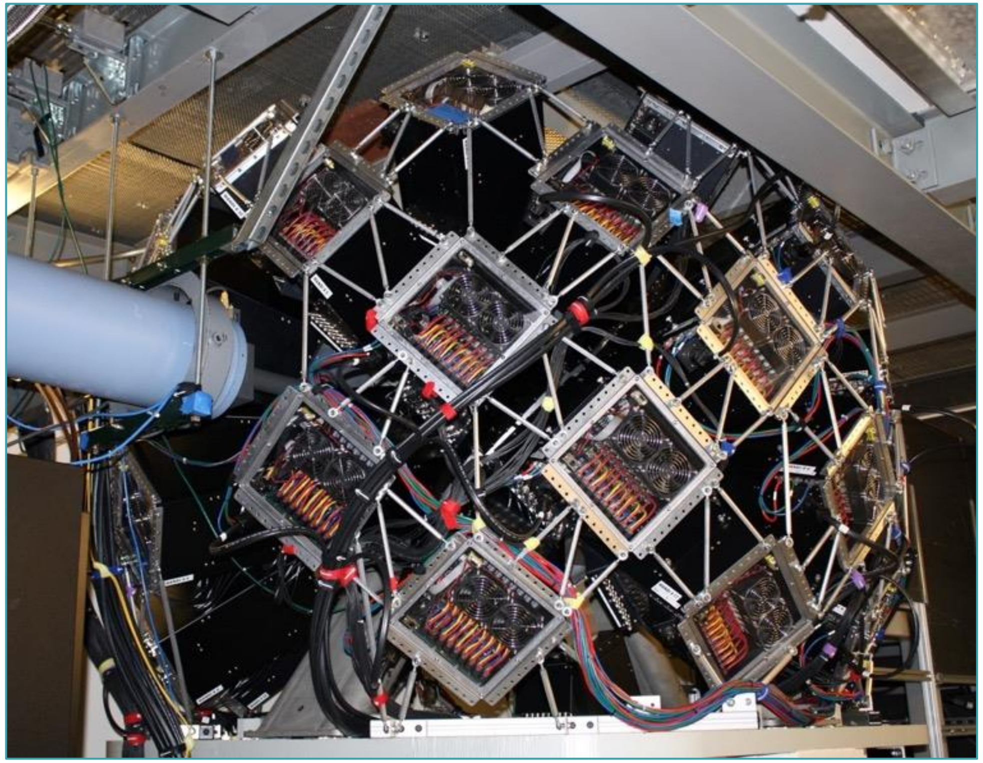
Research Details

- Neutron structures of apo Mac1 were solved in two space groups at 1.9 Å and 2.3 Å using the MaNDi and IMAGINE diffractometers.
- The neutron structure of Mac1 in complex with ADPr was solved at 2.3 Å using the IMAGINE instrument.

U.S. DEPARTMENT OF ENERGY | Office of Science

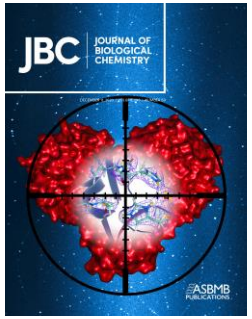
SNS BL-11B MaNDi: Macromolecular Neutron Diffractometer

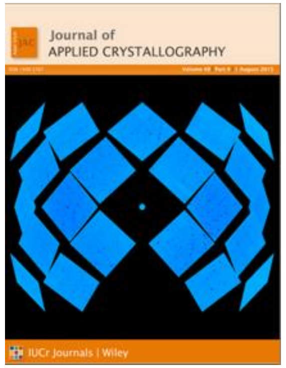
MaNDi is a unique wavelength-resolved single-crystal Time-of-Flight diffractometer, designed for flexibility and high signal-to-noise data collection. Several key instrumental parameters can be adjusted to match the parameters of the sample. These enable data collection on unit cell dimensions from 10 to 300 Å, for smaller molecules a d_{min} of 0.6 Å is achievable.

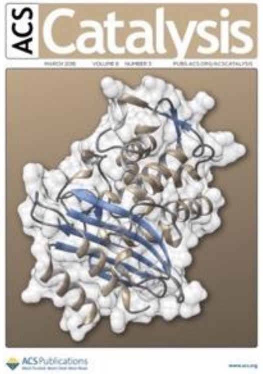


40 SNS Anger Cameras surround the sample position giving 4.1sr detector coverage

- **Beam Divergence 0.80 - 0.12°**
- **Δλ = 2.16 Å anywhere between 1-10 Å**
- **Variable Beam size 7 x 7 to 1 x 1 mm**
- **100-400K data collection available**
- **Open for user proposals since 2015**







https://neutrons.ornl.gov/mandi

SNS BL-11B MaNDi - What's new?

1. SARS-CoV-2 protein crystallography research continues to have celebrated impact.

ORNL Top 10 Science Story for 2021
https://ornl.sharepoint.com/Pages/Article.aspx?articleId=41254

COVID-19: Neutrons reveal unpredicted binding between SARS-CoV-2, hepatitis C antiviral drug (Jeremy Rumsey, March 23) Scientists have found new, unexpected behaviors when SARS-CoV-2 – the virus that causes COVID-19 – encounters drugs known as inhibitors, which bind to certain components of the virus and block its ability to reproduce. Researchers at ORNL used neutron scattering to investigate interactions between telaprevir, a drug used to treat hepatitis C viral infection, and the SARS-CoV-2 main protease, the enzyme responsible for enabling the virus to reproduce.

Andrii Y Kovalevskyi | Daniel W Kneller | Leighton Coates | Kevin L Weiss | Qiu Zhang

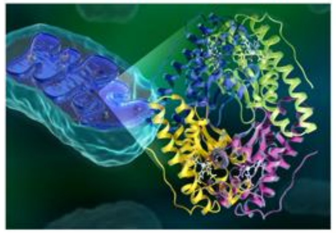
News (4)
Twitter (28)
Mendeley (20)

News (11)
Twitter (19)
Mendeley (60)

27 tweeters
6 news outlets
18 Mendeley

11 tweeters
10 news outlets
2 Wikipedia page
22 Mendeley

Inner workings of an antioxidant enzyme revealed



The mitochondria in human cells depend on manganese superoxide dismutase to keep the amount of harmful reactive oxygen molecules under control. Researchers have now obtained a complete atomic portrait of the enzyme, providing key information about the catalytic mechanism within its active site, situated between the green and blue subunits and the yellow and pink subunits. (Image Credit: ORNL/Jill Hemman)

Work performed on SNS BL-11B, MaNDi

J. Azadmanesh, W. E. Lutz, L. Coates, K.L. Weiss, G. E. O. Borgstahl, *Nature Communications* (2021). https://doi.org/10.1038/s41467-021-22290-1

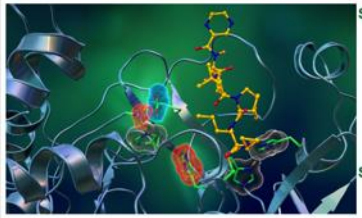
Scientific Achievement
A concerted proton and electron transfer mechanism for human manganese superoxide dismutase is identified from the direct visualization of active site protons in Mn^{3+} and Mn^{2+} redox states using neutron crystallography.

Significance and Impact
Critical understanding determined of how protons are used as tools to help an anti oxidative enzyme transfer electrons for reducing levels of reactive oxygen species in the body.

Research Details
- The complete atomic structure of Manganese Superoxide Dismutase, including its proton arrangements, was determined with neutron crystallography.
- The series of proton movements in the active site needed to enable electrons to move have been determined.
- Analysis suggests that catalysis involves two internal proton transfers between the enzyme's amino acids and two external proton transfers that originate from solvent molecules.

OAK RIDGE National Laboratory | HIGH FLUX ISOTOPE REACTOR | SPALLATION NEUTRON SOURCE — UNMC UNIVERSITY OF NEBRASKA MEDICAL CENTER

Inhibitor binding remodels active site electrostatics in SARS-CoV-2 main protease



The image shows the SARS-CoV-2 main protease bound to the hepatitis C clinical drug telaprevir (gold spheres). The colored surfaces around amino acid residues depict their electric charges determined with neutron crystallography – red for positive, blue for negative and gray for neutral charges.

Scientific Achievement
Main protease enzyme from SARS-CoV-2 that caused the deadly COVID-19 cleaves long polyprotein chains translated from the viral genome into individual proteins thereby performing a vital function for the virus replication. Main protease inhibitors can stop SARS-CoV-2 replication; thus, the enzyme is an important drug target. Neutron crystallography was used to discover that hydrogen atom locations and thus protonation states of ionizable amino acid residues in a main protease complex with hepatitis C clinical inhibitor telaprevir are modulated by the drug binding.

Significance and Impact
Hydrogen atoms are crucial players in drug binding. Protonation states of ionizable residues in a SARS-CoV-2 main protease complex with telaprevir were determined at near-physiological temperature. This study discovered that inhibitor binding modulates protonation states in the enzyme active site, completely remodeling its electrostatics. These observations emphasize the need for accurate knowledge of hydrogen atom positions and their relocation due to inhibitor binding to assist structure-based and computational drug design.

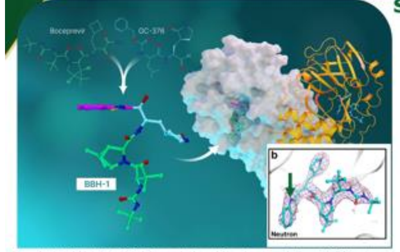
Research Details
- This study focused on main protease (3CL Mpro) enzyme from SARS-CoV-2 in complex with hepatitis C clinical drug telaprevir.
- Neutron structure of the complex was determined and room-temperature, directly visualizing protonation states in the enzyme active site cavity.

Work was performed on the MaNDi instrument at the Spallation Neutron Source, the IMAGINE instrument at the High Flux Isotope Reactor and at the Center for Structural Molecular Biology, which are DOE Office of Science User Facilities.

D.W. Kneller, G. Phillips, K.L. Weiss, Q. Zhang, L. Coates, A. Kovalevsky (2021) *J. Med. Chem.*, doi.org/10.1021/acs.jmedchem.1c00058.

U.S. DEPARTMENT OF ENERGY | Office of Science — OAK RIDGE National Laboratory

Neutrons help design inhibitors of SARS-CoV-2 main protease



How the hybrid inhibitor BBH-1 was designed from boceprevir (hepatitis C protease inhibitor) and GC-376 (SARS-CoV-1 inhibitor), and its subsequent neutron structure with SARS-CoV-2 Mpro. Inset: Nuclear density of BBH-1 reveals deprotonated negatively charged oxyanion (green arrow).

Scientific Achievement
SARS-CoV-2 main protease (Mpro) enzyme is indispensable for virus replication and, thus, is an essential drug target for the design and development of small-molecule antivirals to treat COVID-19. Neutron crystallography was used to help design and characterize covalent hybrid protease inhibitors (BBH-1, BBH-2 and NBH-2) created by splicing components of known hepatitis C and SARS-CoV-1 protease inhibitors. Neutron structure of Mpro/BBH-1 complex revealed a negatively charged oxyanion, critical hydrogen bond with the enzyme and redistribution of protonation states and electric charges in Mpro upon inhibitor binding. The three designed inhibitors demonstrate efficient inhibition of SARS-CoV-2 in cell-based assays paving the way for further design of improved antivirals.

Significance and Impact
Hydrogen atoms are crucial players in drug binding, their locations determining protonation states and thus electric charges of ionizable residues. Knowledge of hydrogen atom positions provides unique information for drug design. This study used this knowledge to design potent (nanomolar) inhibitors of SARS-CoV-2 main protease, mapped essential hydrogen bonding interactions between inhibitors and the enzyme and evaluated their antiviral properties. Comparison with the FDA-approved nirmatrelvir from Pfizer indicated how inhibitor design can be further improved.

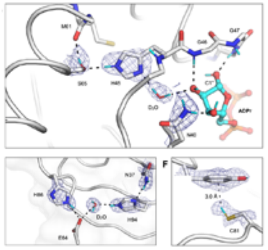
Research Details
- Three hybrid covalent Mpro inhibitors were designed–BBH-1, BBH-2, and NBH-2.
- Neutron structure of Mpro/BBH-1 complex was done at room temperature visualizing critical hydrogen atoms and hydrogen bonds for the inhibitor binding.
- Room-temperature X-ray structures of Mpro in complex with BBH-2, NBH-2 and nirmatrelvir were done.
- Thermodynamics of inhibitor binding to Mpro was evaluated by isothermal titration calorimetry.
- Antiviral properties of the inhibitors were evaluated in cell-based assays.

D.W. Kneller, H. Li, G. Phillips, K.L. Weiss, Q. Zhang, M.A. Arnould, C.B. Jonsson, S. Surendranathan, J. Parvathareddy, M.P. Blakeley, L. Coates, J.M. Louis, P.V. Bonnesen, A. Kovalevsky (2022) Covalent narlaprevir- and boceprevir-derived hybrid inhibitors of SARS-CoV-2 main protease. *Nature Communications*, 10.1038/s41467-022-29915-z.

Work was performed on the IMAGINE instrument at the High Flux Isotope Reactor, the Center for Structural Molecular Biology, the Center for Nanophase Materials Sciences, which are DOE Office of Science User Facilities, and on LADI-DALI instrument at the Institut Laue Langevin, Grenoble, France.

U.S. DEPARTMENT OF ENERGY | Office of Science — NIDDK — THE UNIVERSITY OF TENNESSEE HEALTH SCIENCE CENTER — OAK RIDGE National Laboratory

Neutrons uncover atomic details of SARS-CoV-2 macrodomain to guide design of novel antivirals



The neutron scattering length density maps at and around the Mac1 active site.

G.J. Correy, D.W. Kneller, G. Phillips, S. Pant, S. Russi, A.E. Cohen, G. Meigs, J.M. Holton, S. Gahbauer, M.C. Thompson, A. Ashworth, L. Coates, A. Kovalevsky, F. Meilleur, J.S. Fraser (2022) *Science Advances*, in press.

Work performed on SNS MaNDi and HFIR IMAGINE diffractometers.

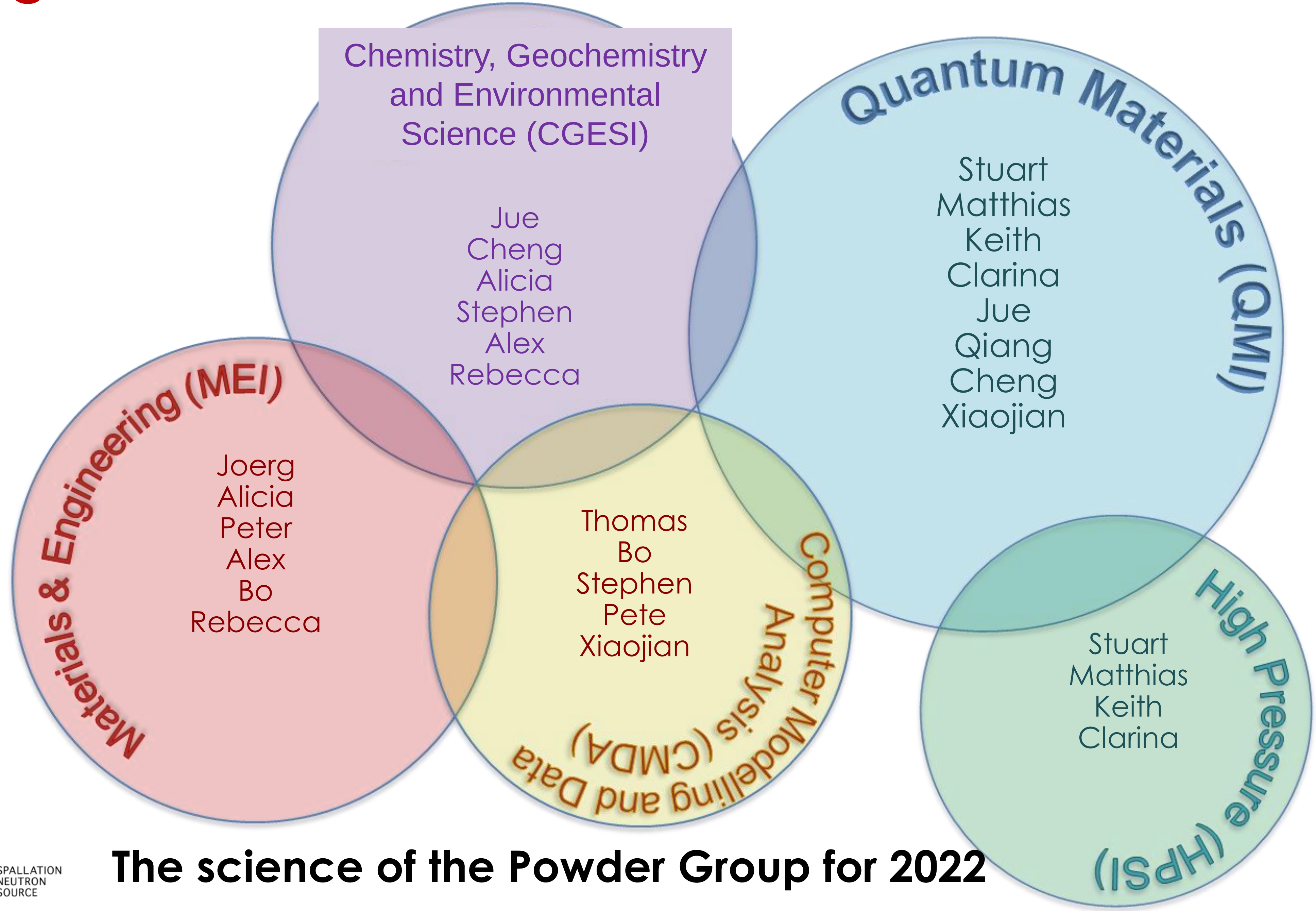
Scientific Achievement
We determined and compared the room temperature structures of the macrodomain of SARS-CoV-2 (Mac1) using neutron and X-ray diffraction to re-evaluate the catalytic mechanism of Mac1 and guide the optimization of inhibitors

Significance and Impact
The knowledge of the protonation states of Mac1 residues that control catalytic activity and of the hydrogen bond networks that govern protein flexibility inform the design of new Mac1 inhibitors.

Research Details
- Neutron structures of apo Mac1 were solved in two space groups at 1.9 Å and 2.3 Å using data from the MaNDi and IMAGINE diffractometers.
- The neutron structure of Mac1 in complex with ADPr was solved at 2.3 Å using the IMAGINE instrument at HFIR.

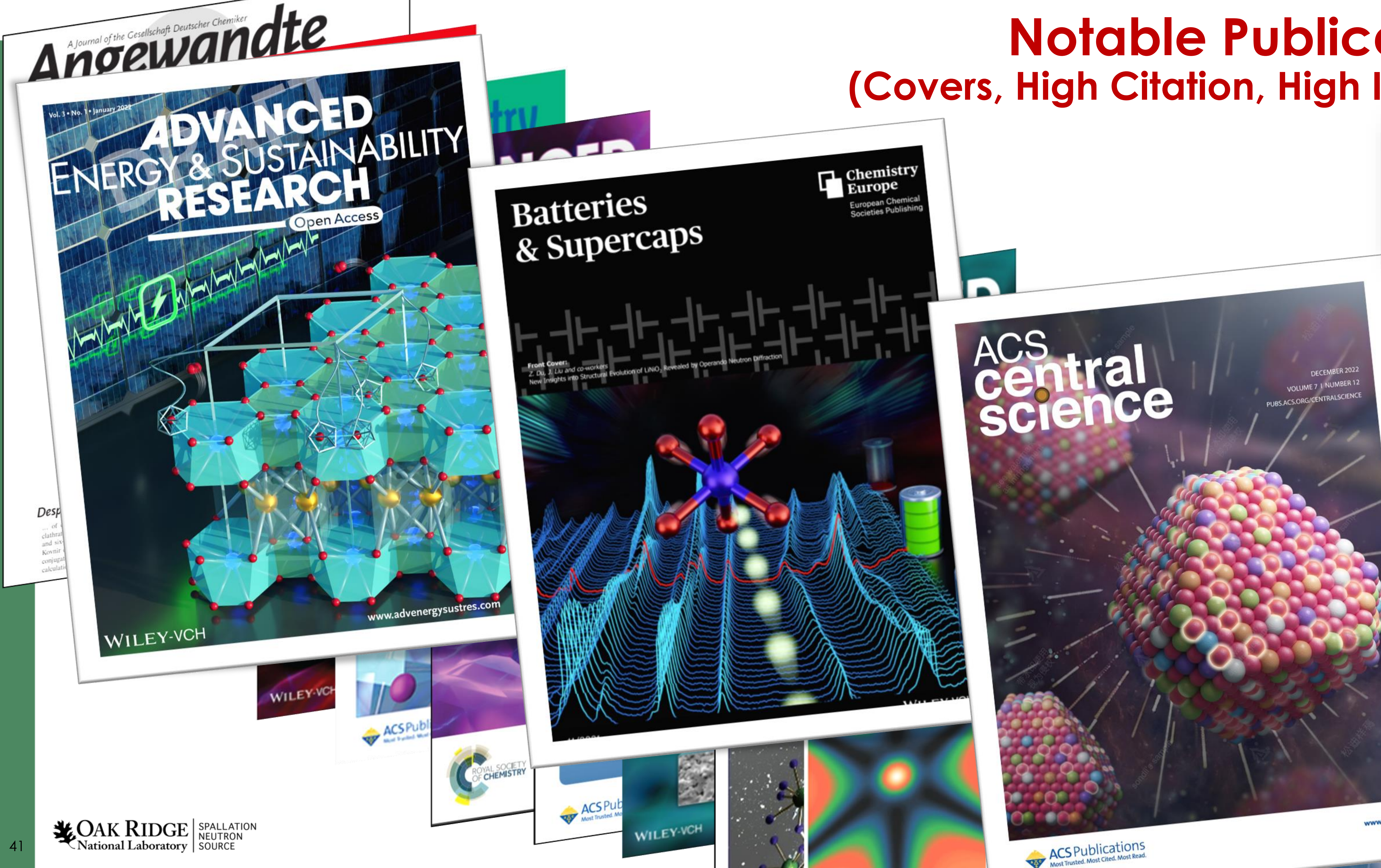
U.S. DEPARTMENT OF ENERGY | Office of Science — UCSF — SLAC NATIONAL ACCELERATOR LABORATORY — UNIVERSITY OF CALIFORNIA MERCED — OAK RIDGE National Laboratory

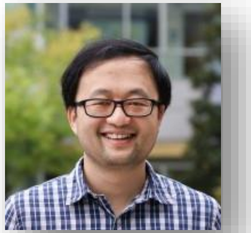
Engagement with the NSD Science Initiatives



The science of the Powder Group for 2022

Notable Publications
(Covers, High Citation, High Impact)





Jue Liu

Notable Publications
(Covers, High Citation, High Impact)

JACS — Journal of the American Chemical Society
pubs.acs.org/JACS — Article

Hidden Local Symmetry Breaking in a Kagome-Lattice Magnetic Weyl Semimetal

Qiang Zhang,* Yuanpeng Zhang,* Masaaki Matsuda, Vasile Ovidiu Garlea, Jiaqiang Yan, Michael A. McGuire, D. Alan Tennant, and Satoshi Okamoto

PHYSICAL REVIEW B **105**, L140401 (2022)

Letter

Single pair of Weyl nodes in the spin-canted structure of $EuCd_2As_2$

K. M. Taddei[1,*,†] L. Yin,[2,*] L. D. Sanjeewa,[2,‡] Y. Li,[3] J. Xing,[2] C. dela Cruz,[1] D. Phelan,[3] A. S. Sefat,[2] and D. S. Parker[2]
[1]*Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

PHYSICAL REVIEW LETTERS **127,** 117201 (2021)

Unusual Exchange Couplings and Intermediate Temperature Weyl State in $Co_3Sn_2S_2$

Qiang Zhang,[1,*] Satoshi Okamoto,[2,3,†] German D. Samolyuk,[2] Matthew B. Stone,[1] Alexander I. Kolesnikov,[1] Rui Xue,[4] Jiaqiang Yan,[2] Michael A. McGuire,[2,3] David Mandrus,[5,2,4] and D. Alan Tennant[2,6,3]

PHYSICAL REVIEW LETTERS **128,** 227201 (2022)

Spiral Spin Liquid on a Honeycomb Lattice

Shang Gao,[1,2,*] Michael A. McGuire,[2] Yaohua Liu,[1] Douglas L. Abernathy,[1] Clarina dela Cruz,[1] Matthias Frontzek,[1] Matthew B. Stone,[1] and Andrew D. Christianson[2]
[1]*Neutron Scattering Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*
[2]*Materials Science & Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

NPG Asia Materials

ARTICLE — Open Access

Toward tunable quantum transport and novel magnetic states in $Eu_{1-x}Sr_xMn_{1-z}Sb_2$ ($z < 0.05$)

Qiang Zhang[1,2], Jinyu Liu[3], Huibo Cao[1], Adam Phelan[2], David Graf[4], J. F. DiTusa[2], D. Alan Tennant[1,5,6] and Zhiqiang Mao[3,7]

CM — Chemistry of Materials
pubs.acs.org/cm — Article

Tuning Magnetic Symmetry and Properties in the Olivine Series $Li_{1-x}Fe_xMn_{1-x}PO_4$ through Selective Delithiation

Published as part of the Virtual Special Issue "John Goodenough at 100".

Timothy J. Diethrich, Stephanie Gnewuch, Kaitlyn G. Dold, Keith M. Taddei, and Efrain E. Rodriguez*

CM — Chemistry of Materials
pubs.acs.org/cm — Article

Chemical Control of Magnetism in the Kagome Metal $CoSn_{1-x}In_x$: Magnetic Order from Nonmagnetic Substitutions

Brian C. Sales,* William R. Meier, David S. Parker, Li Yin, Jiaqiang Yan, Andrew F. May, Stuart Calder, Adam A. Aczel, Qiang Zhang, Haoxiang Li, Turgut Yilmaz, Elio Vescovo, Hu Miao, Duncan H. Moseley, Raphael P. Hermann, and Michael A. McGuire*

JACS — Journal of the American Chemical Society
pubs.acs.org/JACS — Article

Chloride Reduction of Mn^{3+} in Mild Hydrothermal Synthesis of a Charge Ordered Defect Pyrochlore, $CsMn^{2+}Mn^{3+}F_6$, a Canted Antiferromagnet with a Hard Ferromagnetic Component

Vladislav V. Klepov, Kristen A. Pace, Anna A. Berseneva, Justin B. Felder, Stuart Calder, Gregory Morrison, Qiang Zhang, Melanie J. Kirkham, David S. Parker, and Hans-Conrad zur Loye*

Notable Publications
(Covers, High Citation, High Impact)

CHEMISTRY OF MATERIALS

pubs.acs.org/cm Article

Complex Structural Disorder in a Polar Orthorhombic Perovskite Observed through the Maximum Entropy Method/Rietveld Technique

Alicia María Manjón-Sanz, T. Wesley Surta, Pranab Mandal, Alex J. Corkett, Hongjun Niu, Eiji Nishibori, Masaki Takata, John Bleddyn Claridge,* and Matthew J. Rosseinsky*

CHEMISTRY OF MATERIALS

pubs.acs.org/cm Article

Lattice Disorder and Oxygen Migration Pathways in Pyrochlore and Defect-Fluorite Oxides

Frederick P. Marlton, Zhaoming Zhang, Yuanpeng Zhang, Thomas E. Proffen, Chris D. Ling, and Brendan J. Kennedy*

CHEMISTRY OF MATERIALS

pubs.acs.org/cm Article

High Dielectric Permittivity of α-$NaFeO_2$-Type Layered Nitrides

Junwei Liu,[⊥] Shenglin Lu,[⊥] Yanhui Wang, Cheng Li, Xing Ming,* and Xiaojun Kuang*

CHEMISTRY OF MATERIALS

pubs.acs.org/cm Article

Correlating Structural Disorder to Li^+ Ion Transport in $Li_{4-x}Ge_{1-x}Sb_xS_4$ $(0 \leq x \leq 0.2)$

Bianca Helm, Nicolò Minafra, Björn Wankmiller, Matthias T. Agne, Cheng Li, Anatoliy Senyshyn, Michael Ryan Hansen, and Wolfgang G. Zeier*

ELSEVIER

Journal of Power Sources
Volume 507, 30 September 2021, 230183

A high-voltage symmetric sodium ion battery using sodium vanadium pyrophosphate with superior power density and long lifespan

Jinke Li [a, 1], Rui Wang [b, 1], Wenguang Zhao [b], Xu Hou [a], Elie Paillard [c], De Ning [d], Cheng Li [e], Jun Wang [f], Yinguo Xiao [b], Martin Winter [a, f], Jie Li [a, c]

materialstoday
Volume 51, December 2021, Pages 15-26

HIGHLIGHTED PAPER Research

Structural insights into composition design of Li-rich layered cathode materials for high-energy rechargeable battery

Chong Yin [a, f, #], Zhining Wei [a, j, #], Minghao Zhang [b, #], Bao Qiu [a, f], Yuhuan Zhou [a, f], Yinguo Xiao [c], Dong Zhou [a], Liang Yun [a], Cheng Li [d], Qingwen Gu [a], Wen Wen [e], Xiao Li [a, f], Xiaohui Wen [a, f], Zhepu Shi [a, k], Lunhua He [g, h, i], Ying Shirley Meng [b], Zhaoping Liu [a, f]

Notable Publications
(Covers, High Citation, High Impact)

ADVANCED SCIENCE Open Access

Research Article | Open Access

Ferromagnetic Double Perovskite Semiconductors with Tunable Properties

Lun Jin, Danrui Ni, Xin Gui, Daniel B. Straus, Qiang Zhang, Robert J. Cava

ACS central science

http://pubs.acs.org/journal/acscii | Research Article

Defect Engineering of Ceria Nanocrystals for Enhanced Catalysis via a High-Entropy Oxide Strategy

Yifan Sun, Tao Wu, Zhenghong Bao, Jisue Moon, Zhennan Huang, Zitao Chen, Hao Chen, Meijia Li, Zhenzhen Yang, Miaofang Chi, Todd J. Toops, Zili Wu, De-en Jiang, Jue Liu,* and Sheng Dai*

ADVANCED ENERGY MATERIALS

Research Article | Full Access

Exceptional Cycling Performance Enabled by Local Structural Rearrangements in Disordered Rocksalt Cathodes

Juhyeon Ahn, Yang Ha, Rohit Satish, Raynald Giovine, Linze Li, Jue Liu, Chongmin Wang, Raphaele J. Clement, Robert Kostecki, Wanli Yang, Guoying Chen

ADVANCED MATERIALS

Research Article | Full Access

Superior High-Temperature Strength in a Supersaturated Refractory High-Entropy Alloy

Rui Feng, Bojun Feng, Michael C. Gao, Chuan Zhang, Joerg C. Neuefeind, Jonathan D. Poplawsky, Yang Ren, Ke An, Michael Widom, Peter K. Liaw

Journal of Materials Chemistry A — ROYAL SOCIETY OF CHEMISTRY

PAPER — View Article Online | View Journal | View Issue

Check for updates

Cite this: *J. Mater. Chem. A*, 2021, 9, 16982

Multi-scale investigation of heterogeneous swift heavy ion tracks in stannate pyrochlore†

Eric C. O'Quinn,[a] Cameron L. Tracy,[b] William F. Cureton,[a] Ritesh Sachan,[c] Joerg C. Neuefeind,[d] Christina Trautmann[ef] and Maik K. Lang*[a]

ELSEVIER

Acta Materialia

Volume 225, 15 February 2022, 117590

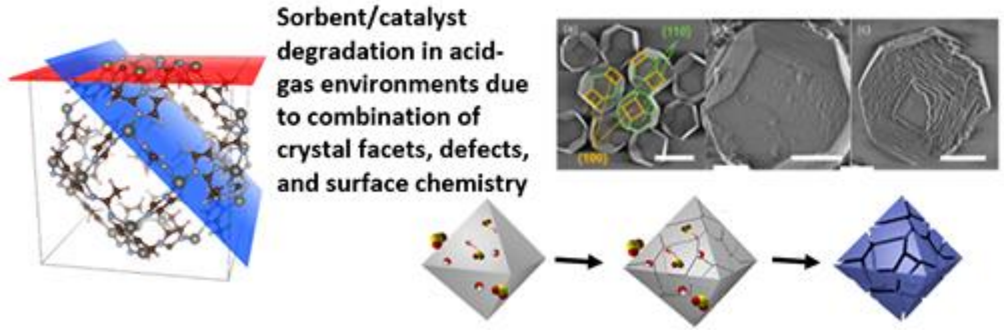
Local ordering in disordered $Nd_xZr_{1-x}O_{2-0.5x}$ pyrochlore as observed using neutron total scattering

Devon Drey[a], Eric O'Quinn[a], Sarah Finkeldei[b], Joerg Neuefeind[c], Maik Lang[a]


Sample Environments
Education and Outreach
Instrument Development
User Program
Creative Research
Software Development
Forefront Science
EuPtSi @ 1.2T, 1.5K
0.0
0.5
1.0
H in (H, H̄, 0)

FUNDING: Energy Frontier Research (EFRC)

Center for Understanding and Control of Acid Gas-induced Evolution of Materials for Energy (UNCAGE-ME)



Kate Page

Peter Metz

Bo Jiang

Stephen Purdy

Hazardous Gas Handling System (HGHS) sample environment for use for catalysis work at NOMAD

Stephen Purdy, Michelle Everett, Kate Page

FUNDING: SBIR

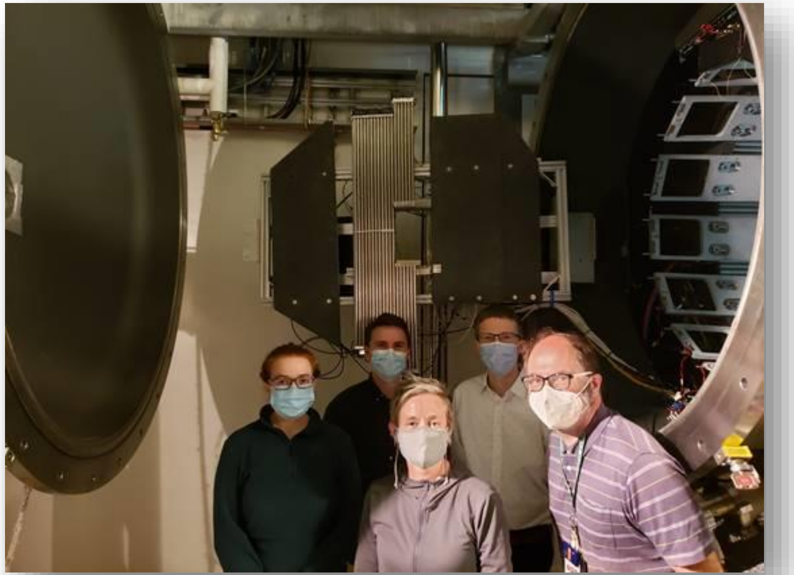
SBIR·STTR America's Seed Fund | U.S. DEPARTMENT OF ENERGY | SBIR/STTR Programs Office

SMALL BUSINESS INNOVATION RESEARCH

NOMAD welcomes SBIR collaborators from MDI,Inc in November 2021

Sarah Schlossberg and Stephen Wilke from Materials Development Incorporated (MDI) came to scope the integration of the aero-acoustic levitator. This work is part of an ongoing SBIR project.

MDI Instruments for Innovation®



Joerg Neuefeind

Michelle Everette

Dante Quirinale

FUNDING: SBIR

SBIR·STTR America's Seed Fund | U.S. DEPARTMENT OF ENERGY | SBIR/STTR Programs Office

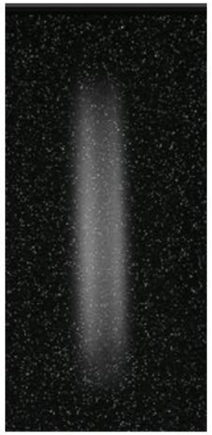
SMALL BUSINESS INNOVATION RESEARCH

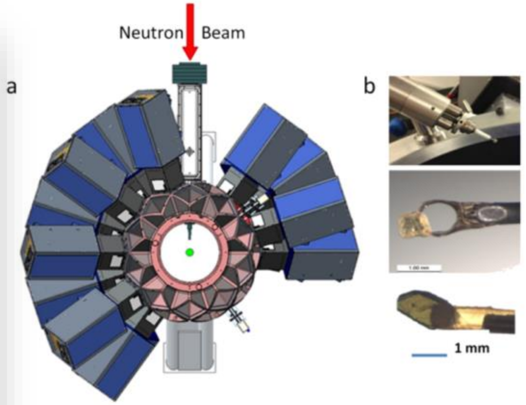
- Develop a suite of machine learning based tools that can be used to automate sample alignment in a wide range of experiments using image data and other metadata about the experiment.
- Tools will be accessible in a browser-based GUI and Python-based libraries.
- Users will have access to pre-trained examples that have been validated and tested on experimental setups.

"AI Based Stabilization of Sample Environments"

Jonathan Edelen & Stuart Calder, PI

Stuart Calder





OAK RIDGE National Laboratory | SPALLATION NEUTRON SOURCE

AWARDS and Fellowships

Thomas Proffen

- Fellow of American Crystallographic Association (2018)
- Fellow Neutron Scattering Society of America (2019)
- Fellow of the American Association for the Advancement of Science (2021)

Clarina dela Cruz

- Young Scientist Prize, International Union of Physics and Applied Physics, Commission on the Structure and Dynamics of Condensed Matter (2014)
- Early Career Research Award, UT-Battelle Awards Night (2014)

Keith Taddei

- 2015 ACA Margaret Etter Presentation Award in the category of Neutron Scattering
- 2016 NIU Dissertation Completion Fellowship

Katherine Page (UTK)

- Presidential Early Career Award for Scientists and Engineers PECASE (2019)
- Neutron Scattering Society of America Exceptional Service Award (2018)
- DOE Office of Science Early Career Research Program Award (2015)

The Powder Diffraction Group’s Professional Memberships

APS
AMERICAN PHYSICAL SOCIETY

NEUTRON SCATTERING SOCIETY OF AMERICA
NSSA

ACA
AMERICAN CRYSTALLOGRAPHIC ASSOCIATION

ACS
Chemistry for Life®

MRS
MATERIALS RESEARCH SOCIETY®

Komitee Forschung mit Neutronen

AAAS

Swiss Society for Crystallography

TMS
The Minerals, Metals & Materials Society

DPG

P D S

ASM INTERNATIONAL

IUCr

Leadership and Service in Professional Societies

Alicia Manjon-Sanz

- Chair Elect - Neutron Special Interest Group (SIG) Elect 2021
- SIG Chair 2022 for the American Crystallographic Association (ACA)
- Co-chair for WiNS

Yuanpeng Zhang

Topic editor for *Materials* journal

Clarina dela Cruz

- Vice Chair , GMAG American Physical Society
- Argonne Photon Source Diffraction Beamline Review Committee
- Session Chair for APS, ACA, ACS and MAGNA
- NSD Quantum Materials Science Initiative Coordinator
- Co-Chair ORNL's Big Science Questions

Thomas Proffen

- Co-Chair of Research Data Alliance IG Research data needs of the Photon and Neutron Science community
- Commissioning Editor for Instrumentation and Materials for IUCr
- Co-editor for Journal of Applied Crystallography
- Member of editorial board of Zeitschrift fur Kristallographie.
- Member of the IUCr commissions on Neutron Scattering and Crystallographic Computing
- Program Committee member for IUCr 2020 congress

Leadership and Service in Professional Societies

Matthias Frontzek

- US-Japan Cooperative Program on Neutron Scattering
- J-PARC Science Review Committee
- Chair, NSD High Temperature Steering Committee
- NScD Instrument selection process committee
- NSD User experience metrics

Keith Taddei

- Executive committee member (Secretary) of ORPA 2017-2018
- ORPA Research Committee Vice-Chair 2017-208
- Session Chair APS March Meeting

Kate Page

- NSLS-II High Energy Diffraction Proposal Review Panel,
- Session Chair ACA and International Union of Crystallography (IUCr)
- Consultant Member, International Union of Crystallography Commission on Powder Diffraction

Stuart Calder

- Chair of the APS Inelastic x-ray scattering Proposal review Panel (IXS-PRP).
- SIG chair for Powder diffraction at ACA
- Session organizer for Pittsburgh Diffraction Conference, ACA and APS
- Organizing committee for GMAG APS

Leadership in Professional Societies

Executive Committee, International Union of Crystallography
IUCr contact to the American Crystallographic Association (ACA)

Thomas Proffen

Associate Member of the IUPAP C9 Commission on Magnetism

IUPAP International Union of Pure and Applied Physics

GMAG Chair Elect 2022-2023
GMAG Program Chair, March Meeting 2023

APS physics GMAG MAGNETISM

Topical Group on Magnetism and its Applications

Clarina dela Cruz

Leadership in Professional Societies

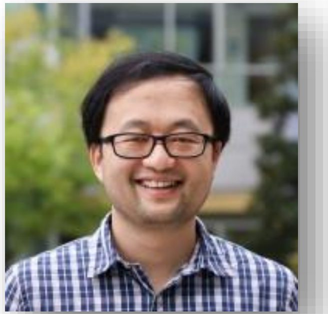
Alicia Manjon-Sanz

Keith Taddei

NEUTRONS
SCIENTIFIC INTEREST GROUP

CHAIR 2022: Alicia Manjon Sanz
CHAIR-ELECT 2022/CHAIR 2023: Keith Taddei
PAST CHAIR: Benjamin Frandsen

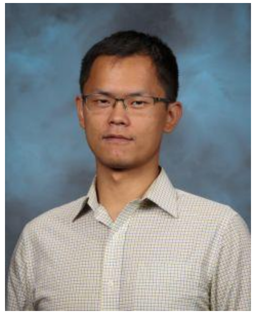
aca The Structural Science Society



Jue Liu

MATERIALS
SCIENTIFIC INTEREST GROUP

CHAIR 2022: Rebecca McAuliffe
CHAIR-ELECT 2022/CHAIR 2023: Jue Liu
PAST CHAIR: Vicky Doan-Nguyen



Cheng Li

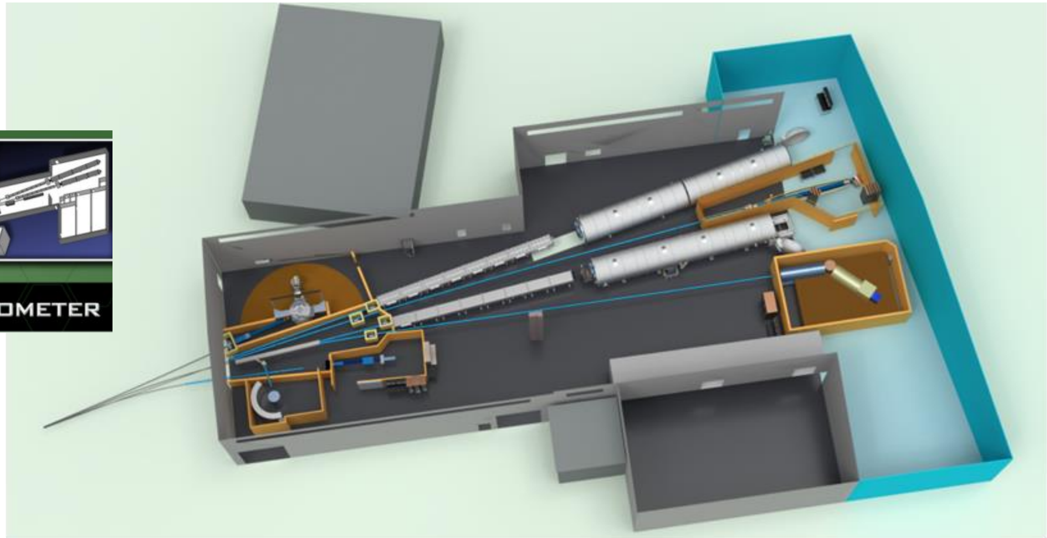
POWDER
SCIENTIFIC INTEREST GROUP

CHAIR 2022: Jared M. Allred
CHAIR-ELECT 2022/CHAIR 2023: Wenqian Xu
PAST CHAIR: Cheng Li

Matthias takes on Lead Scientist role for the HFIR Beryllium Reflector Replacement (HBRR) Project

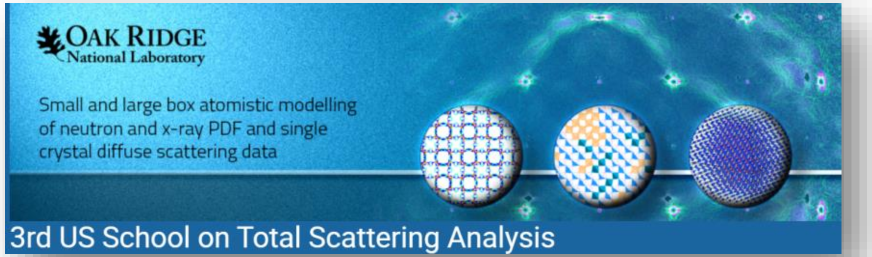
Matthias Frontzek

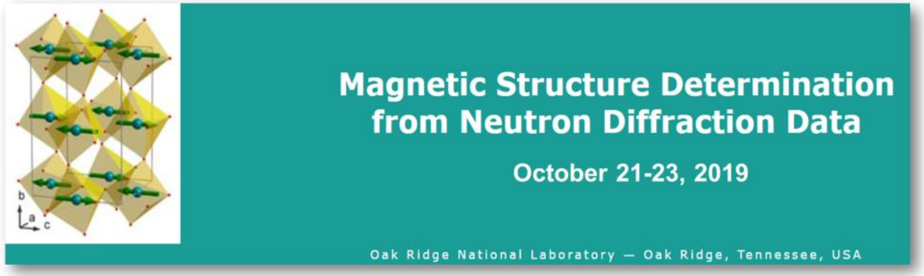
Matthias will assumed the role of Lead Scientist for the HFIR HBRR projecton Dec 6, 2021, splitting his time between this new position and as one of the Instrument Scientists for WAND^2



HFIR Beryllium Reflector Replacement and Cold Guide Hall Extension

Workshops and Schools Organized





2020-2021 Virtual Workshops and School

Neutrons and Complementary Techniques for Quantum Materials

18-21 August 2020
Virtually
US/Eastern timezone

OAK RIDGE National Laboratory

NEUTRON SCIENCES

Magnetic Structure Determination from Neutron Diffraction Data

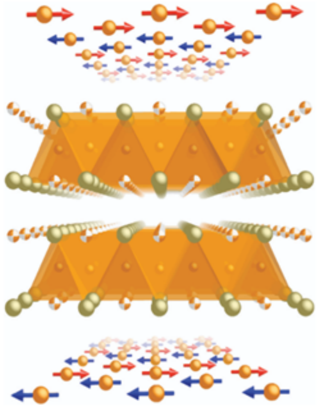
28 September 2020 to 2 October 2020
Teams
US/Eastern timezone

2021 School on Representational Analysis and Magnetic Structures (RAMS)

University of Maryland College Park, USA

November 8-12

Learn how to solve your magnetic structure with neutron diffraction data. This week-long school will feature experts in magnetic symmetry from the U.S. and around the world. Various approaches will als be taught including representational analysis, magnetic space groups, and magnetic super space groups. This year due to the ongoing pandemic, we will host the school entirely online.



US MUON WORKSHOP 2021

A road map for a future Muon Facility

A VIRTUAL WORKSHOP

February 1-2, 2021

Co-sponsored by the Department of Energy, Basic Energy Sciences, and the National Science Foundation

MRS

2021-2022 Workshops and School

2021 Joint Nanoscience and Neutron Scattering User Meeting August 9-12, 2021

"Workshop 5: Materials Synthesis Science and Opportunities Aided by in-situ Scattering Tools",
"Workshop S4: Quantum Materials Multiple Length Scales",

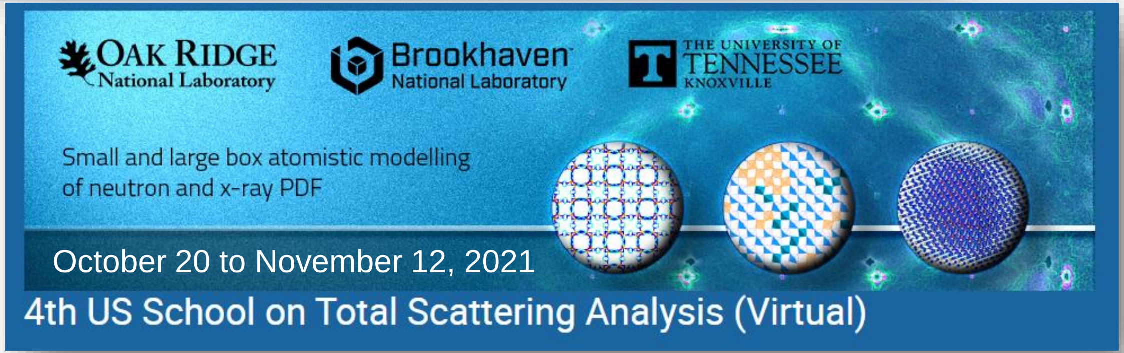
US-Japan Cooperative Program on Neutron Scattering

39th Joint Meeting of the DOE-ISSP and DOE-JAEA Steering Committees

Remote **August 2-3, 2021**

Oak Ridge National Laboratory

Oak Ridge, Tennessee 37831, USA



Rigaku

Mentoring

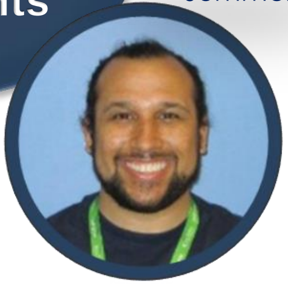
Undergrad Higher Education Research Experience

High School Research Experience

Undergraduate and High School Students

Alex Greenhalgh
Summer 2021

Caleb Cho
Summer 2022



Jackson Wesley
Summer 2022

U.S. DEPARTMENT OF ENERGY | Office of Science

Office of Science Graduate Student Research (SCGSR) Program

Danielle Yahne (2021)
Colorado State Univ
Mentor: **Stuart Calder**

Paul Cuillier (2022)
Ohio State University
Mentor: **Yuanpeng Zhang**

Sreya Paladugu (2022)
UT–Knoxville
Mentor **Cheng Li**

Powder Diffraction Group: The Postdoctoral Fellows

Peter Metz	Stephen Purdy	Bo Jiang	Xiaojian Bai	Po-Hsiu Alex Chien	Amanda Huon	Rebecca McAuliffe	Bernadette Cladek

Informal mentoring of Grad students
Thesis Committees

Graduate Students

Graduate Higher Education Research Experience

Advanced Short Term Research Opportunity

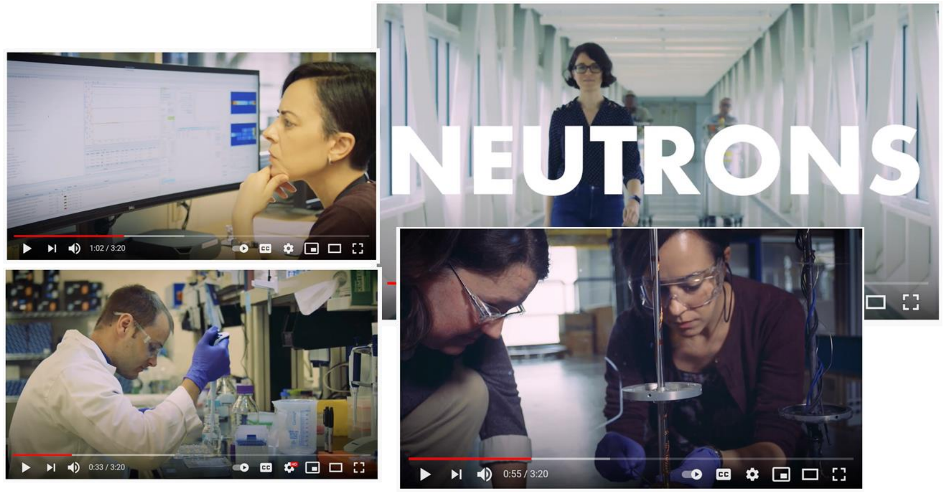
GEM Fellowship

DOE Graduate Student Research Fellow

POWDER GROUP Spreading the Word on Neutrons, Science and More

POWGEN team hosted a visit from staffers of Sen. Blackburn and Sen. Haggerty's

The new SNS video features our very own Daniel, Gabriela, Melanie and Alicia.



Clarina Dela Cruz (l) describes the Spallation Neutron Source's instruments to Sec. Granholm.

Clarina attended the virtual APS Leadership Meeting as Vice-Chair of the GMAG Unit

Alicia, Matthias, Melanie and Michelle hosted NSF REUs undergrads from Georgia Institute of Technology

POWDER GROUP Reaches Out!

Alicia Manjon-Sanz

APAC
Asian Pacific
American Committee

Community Conscience

ORNL Community Engagement Newsletter

OAK RIDGE National Laboratory

community@ornl.gov @ORNLCommunity #ORNLGives September 2021

ORNL scientist Thomas Proffen and Laboratory Director Thomas Zacharia field questions from a camp participant during a fireside chat at SAGE summer camp.

Clarina dela Cruz

Thomas Proffen

Team UT-Batelle

POWDER GROUP Reaches Out!

Thomas leads first ORNL Science Accelerating Girls' Engagement (SAGE) Summer Camp

SAGE is an initiative across multiple laboratories and **Thomas Proffen** is the PI for ORNL.

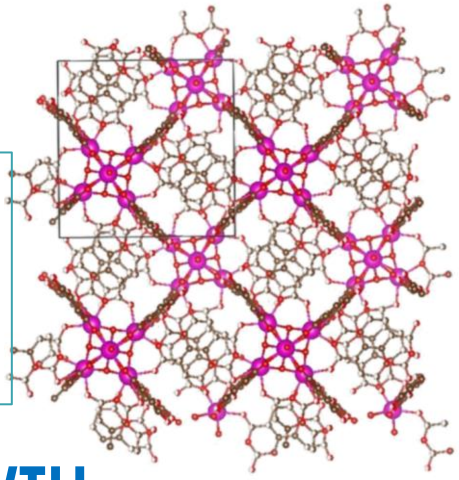
Thomas Proffen

Kate Page

Michelle Everett

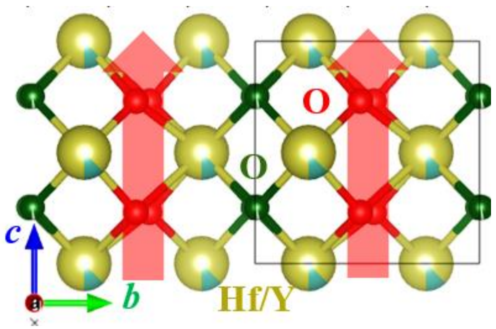
Kate Page gave a talk on structure and materials science
Michelle Everett gave a tour of SNS

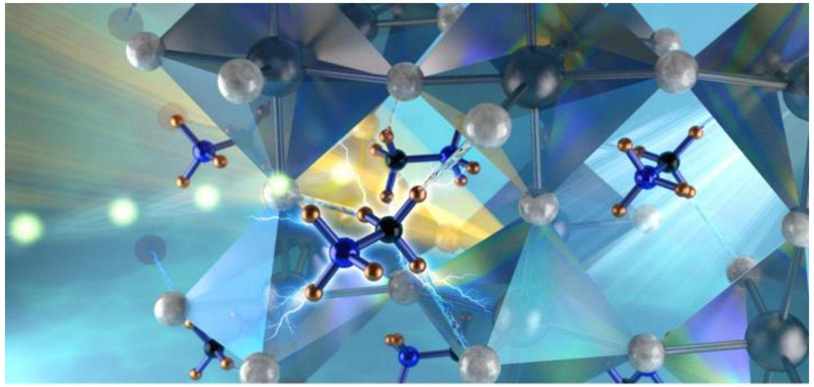
Diffraction Section Vision Statement

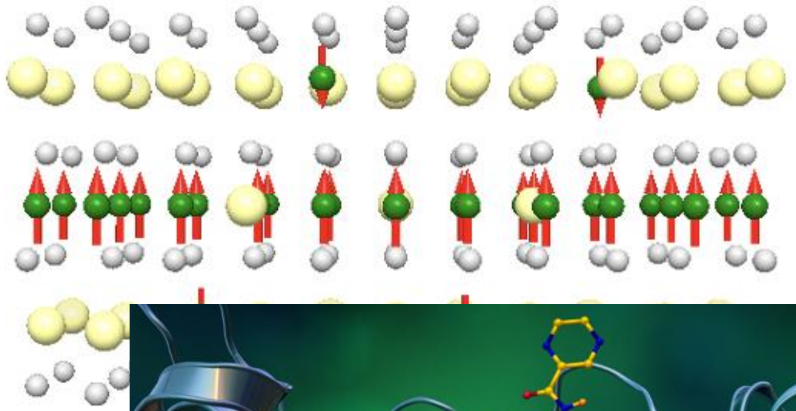


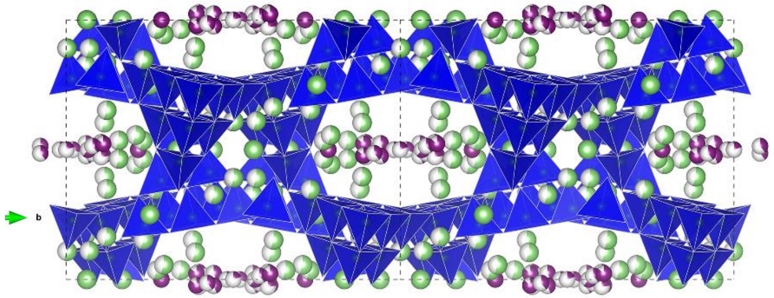
Grow across three neutron sources (HFIR, SNS, STS) world-class diffraction capabilities that enable physical, chemical, and biological studies of structure and function of materials.

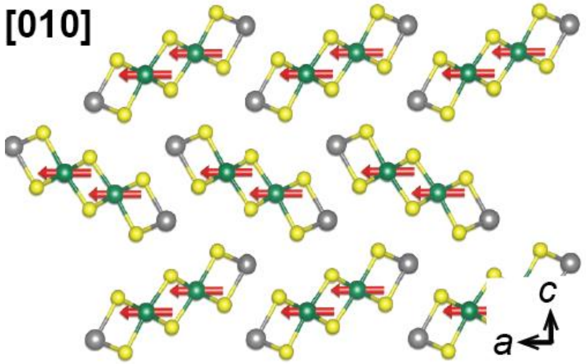
SAFETY • SCIENTIFIC EXCELLENCE • DIVERSITY • CAREER GROWTH

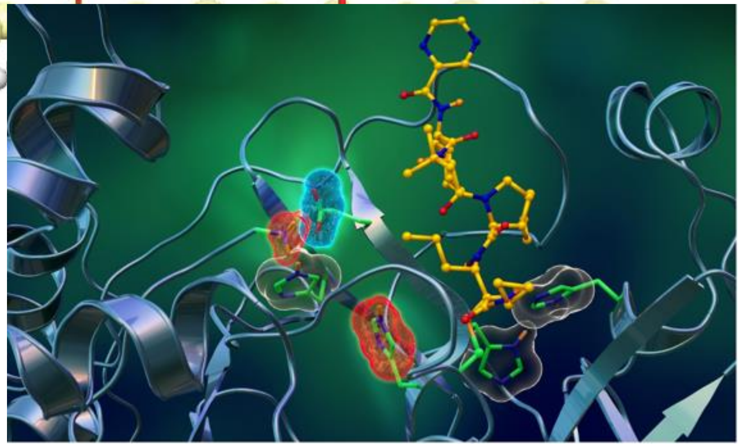












BACKUP

POWDER DIFFRACTION GROUP: Our Story…

- The current Powder Diffraction Group was formed after ORNL Reimagining, bringing together the previous Powder Team with group Computational CIS and Group Leader
- The powder diffraction group delivers a large percentage of publications and unique users for the SNS and HFIR

(**24%** of total SNS[27%] and HFIR[18%] instrument publications)

- The group delivers mail-in programs on NOMAD and POWGEN
- WAND^2 is part of the US-Japan Collaboration for Neutron Scattering