Neutron Day
Overview and Updates

Richard M. Ibberson

Oak Ridge, Tennessee

26th April, 2018

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

OAK RIDGE National Laboratory

Neutron Day Seminar Series: Instrumentation and Technique Development

Time	Event	Leader(s)
9:30–10:00 a.m.	Overview of Neutron Day and Updates	Richard Ibberson
10:00–10:30 a.m.	HFIR Cold Guide Hall Optimization and Beryllium Change	Georg Ehlers
10:30–10:45 a.m.	BREAK	
10:45–11:30 a.m.	Implementing the ORNL 3-Source Strategy	Ken Herwig
11:30–11:45 a.m.	Town Hall Q&A	
11:45 a.m.–12:15 p.m.	Grab lunch and head to breakout sessions	
12:15–1:15 p.m.	***Working Lunch*—BREAKOUT SESSIONS #1**	
Ground Floor (by spiral staircase)	• Polarization	Lee Robertson
Rm C250	• High Pressure Technique Development	Bianca Haberl
Rm C156	• Recommendations from recent instrument suite reviews	Dean Myles
Rm C152	• Engaging in instrument development process	Ken Herwig
1:15–1:30 p.m.	BREAK	
1:30–2:30 p.m.	**BREAKOUT SESSIONS #2**	
Ground Floor (by spiral staircase)	• Polarization	Lee Robertson
Rm C250	• High Pressure Technique Development	Bianca Haberl
Rm C152	• Recommendations from recent instrument suite reviews	Dean Myles
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2:30–2:45 p.m.	BREAK	
2:45–3:15 p.m.	Breakout Summaries (5-minute wrap-up per facilitator)	Breakout Facilitators
3:15–3:30 p.m.	Poster Summaries	GO! Students
3:30–5:00 p.m.	Poster Reception	GO! Students
5:00 p.m.	Adjourn	

GO! Students – Poster Session

Emily Armbruster

- Large Scale Structures, Neutron Scattering Division
- Capturing Hyper-Rotated Solution Structure of the *E. coli* Ribosome

Steven Dajnowicz

- Diffraction, Neutron Scattering Division
- Using Neutron Scattering, Diffraction, and Computational Methods to Identify the Molecular Determinants that Govern Pyridoxal 5'-Phosphate-Dependent Catalysis

Qing Huang

- Spectroscopy, Neutron Scattering Division
- Neutron Scattering Studies of Spin-1/2 Quantum Antiferromagnets with Strong Quantum Spin Fluctuations

GO! Students – Poster Session (cont'd)

Shiyun Jin

- Diffraction, Neutron Scattering Division
- Incommensurately Modulated Structures of Intermediate Plagioclase

Alessandro Mazza

- Large Scale Structures, Neutron Scattering Division
- Investigation of Ions and Induced Magnetism in Epitaxial Multi-layer Graphene

Gabriela Schroder

- Diffraction, Neutron Scattering Division
- Investigating enzyme catalytic mechanisms with neutrons: Tautomerization by the mammalian cytokine MIF

GO! Students – Poster Session (cont'd)

James Torres

- Detector Development, Neutron Technologies Division
- Structure and Dynamics of Interfacial Water near CuO Nanostructures. A neutron scattering study

Xin Wen

- Large Scale Structures, Neutron Scattering Division
- High Resolution Validation of Next Generation Turbulent Flow Models Using Neutron Beams, Laser Fluorescence and Liquid Helium

Jiayong Zhang

- Spectroscopy, Neutron Scattering Division
- Phonon Analysis using Real-Space Multigrid Method combined with VISION

Acknowledgements

Session leaders and facilitators

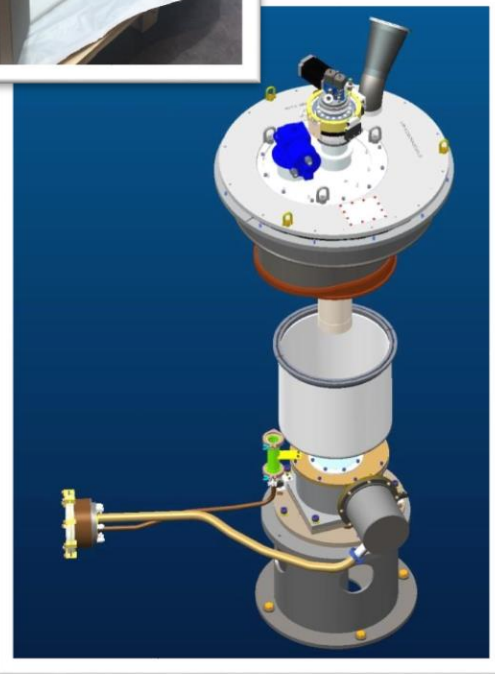
Neutron Day Committee:

- Matthias Frontzek
- Bianca Haberl
- Suzanne Parete-Koon
- Toni Sawyer
- Crystal Schrof
- Travis Williams
- Marie Yao

Instrument Improvement Projects add capabilities to the General User Program

- All 18 SNAP detector modules have received upgraded optics packages improving signal-to-noise by x3.5
- The new CNCS radial collimator supports larger sample environment equipment including the 8-T SNS magnet (and the future 14T magnet)
- Upgrade to the mechanics of the Liquids Reflectometer provide more robust, reliable system with the flexibility to explore new modes of operation
- Modifications to the EQ-SANS sample area enables a wide range of sample environment equipment
- 12 detectors have been relocated to the mid-plane on the newly installed West-side detector stands of POWGEN, completing mid-plane coverage
- Installation of the CORELLI vacuum isolation thimble allows more rapid sample and sample environment changes
- WAND^2 has received a new multi-wire, 2D pixelated detector with x4 vertical acceptance

CNCS collimator



CORELLI VIT

WAND^2 Detector

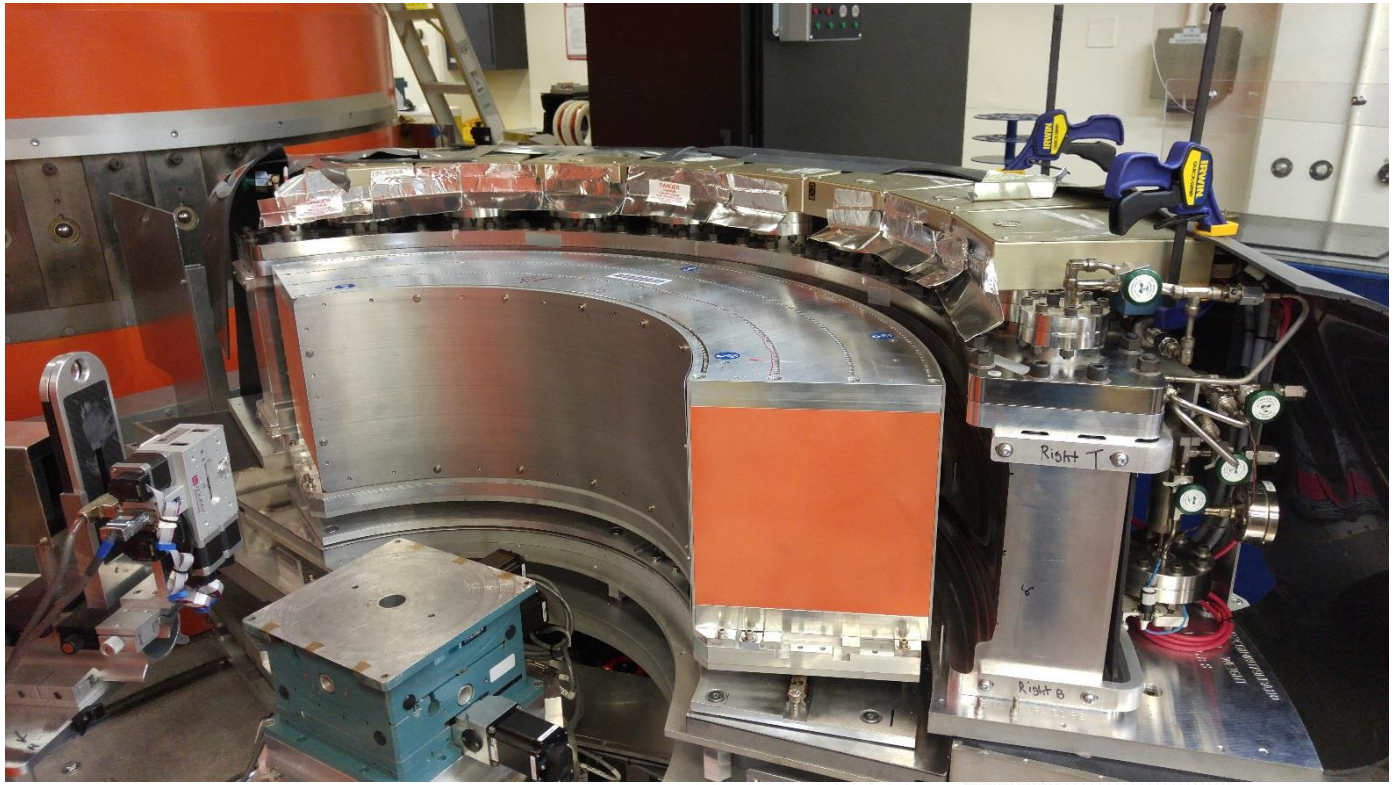
WAND² on HB-2C ready for general user program

Completion of $4 M 2-year project

Kudos to:
Mathias Frontzek, Katie Andrews,
Mike Harrington, Miljko Bobrek,
Rob Knudson, Marie Xingxing Yao,
Klemen Vodopivec, Matthew Pearson,
Mariano Ruiz-Rodriguez, Ross Whitfield,
Amy Black Jones, Van Graves, Kevin Berry,
Eric Griffis,…(and others..)

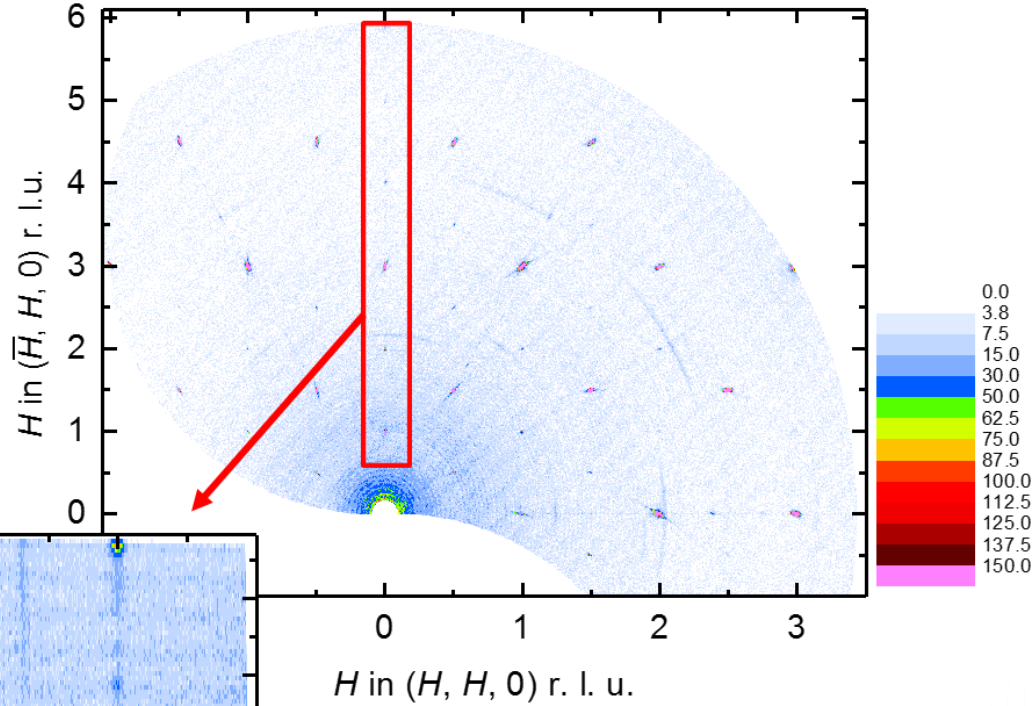
HFIR Craft - deserve big praise!

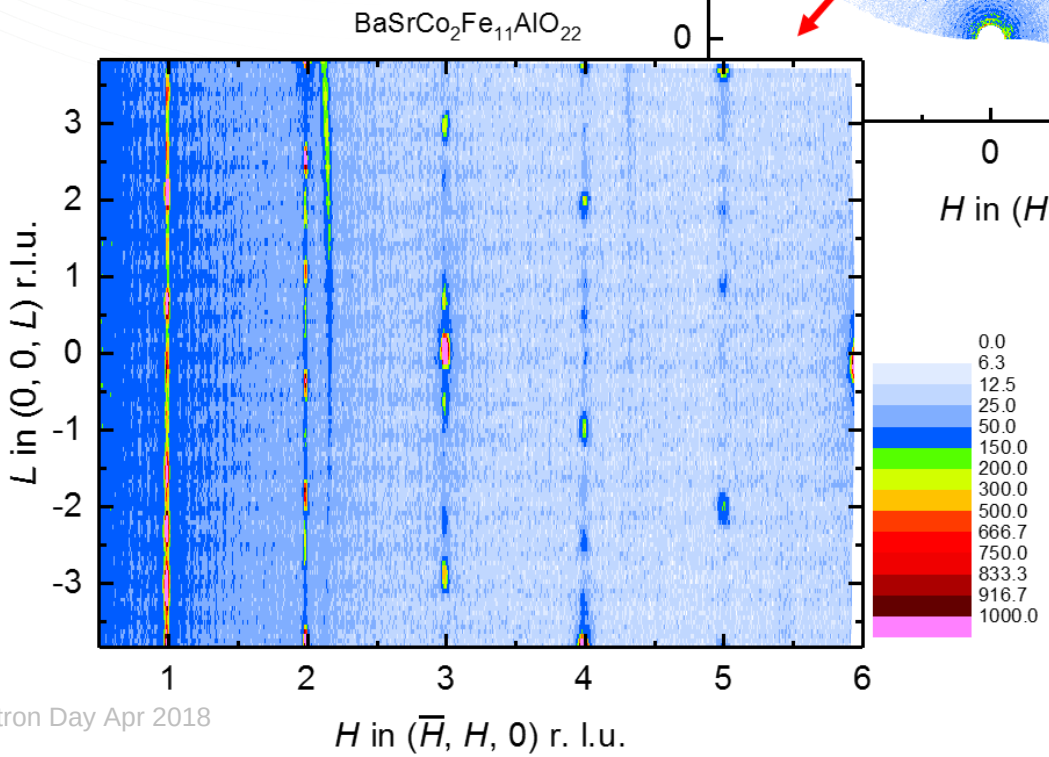
Help from Brookhaven National Laboratory:
Neil Schaknowski, Joe Mead, John Kuczewski



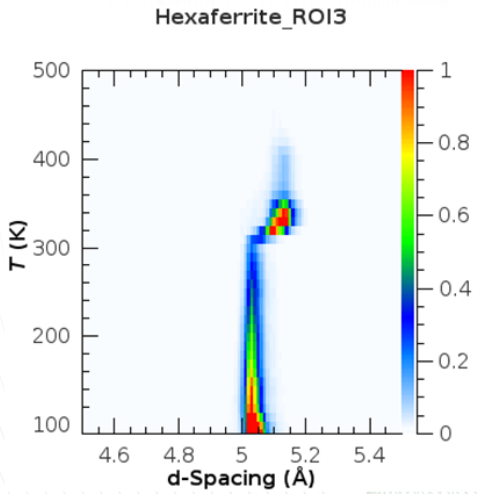
WAND²: $BaSrCo_2Fe_{11}AlO_{22}$ Y-type hexaferrite

- Out of plane coverage will help solving complex crystallographic and magnetic structures





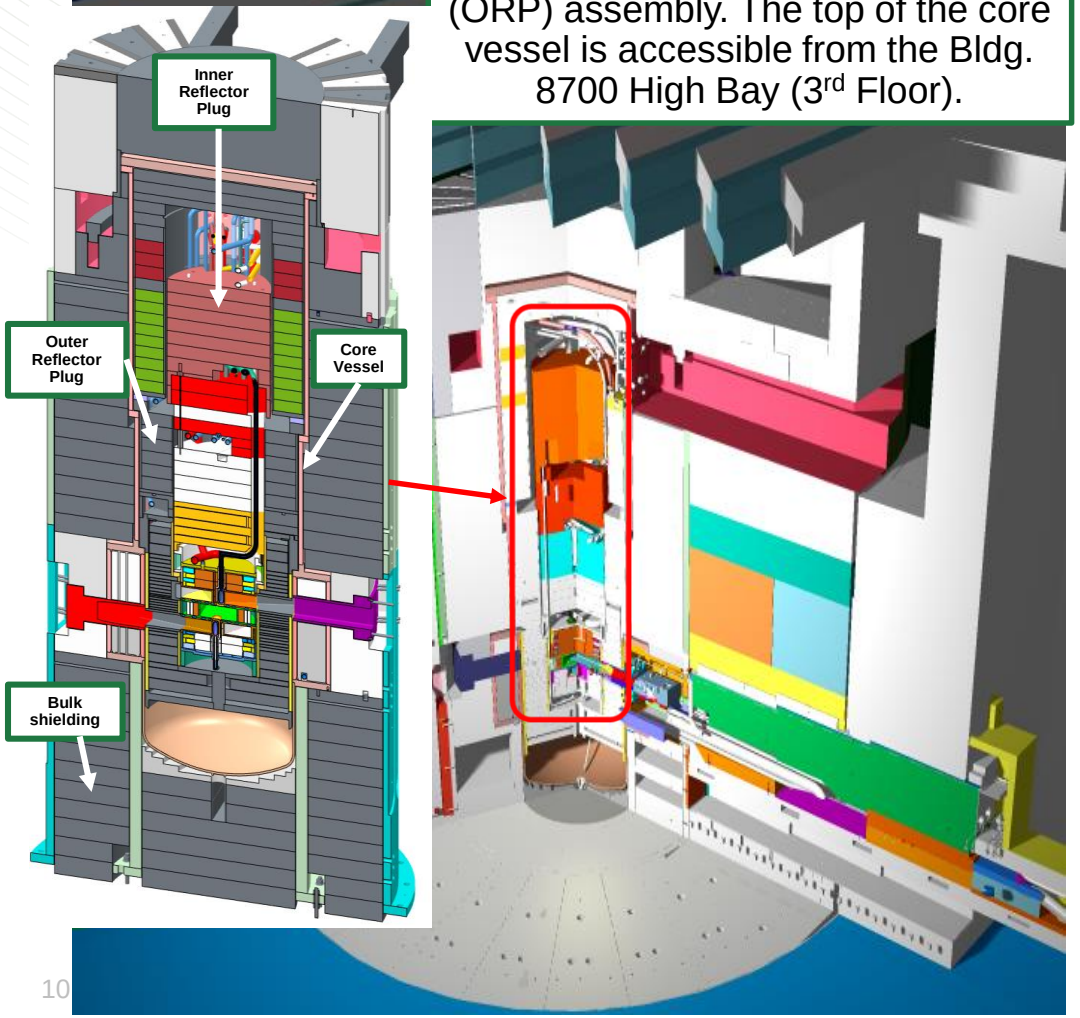
- Event mode allows filtering after the experiment



Kakurai, Nakajima, Frontzek, et al.

The ~32-ton Inner Reflector Plug (IRP) moderates the neutrons created in the mercury target and reflects them to the beam lines. IRP-01 was operated beyond end-of-life (40 GW-hrs) which resulted in water leaks and degraded neutronic performance. Lethally radioactive, it was remotely replaced in February, 2018.

The IRP is installed in the Core Vessel and Outer Reflector Plug (ORP) assembly. The top of the core vessel is accessible from the Bldg. 8700 High Bay (3rd Floor).



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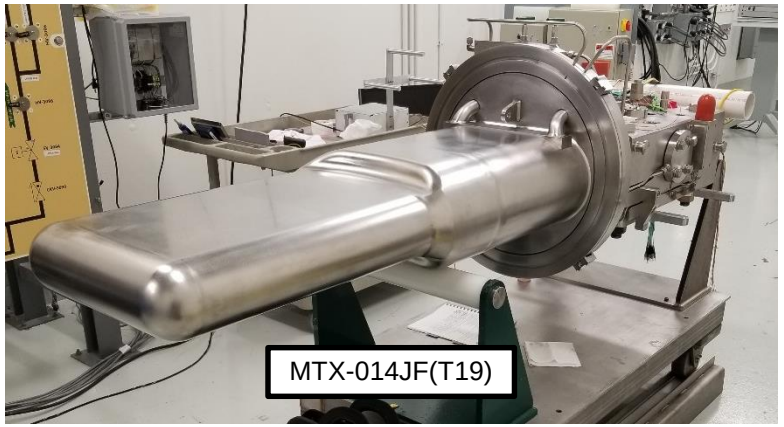
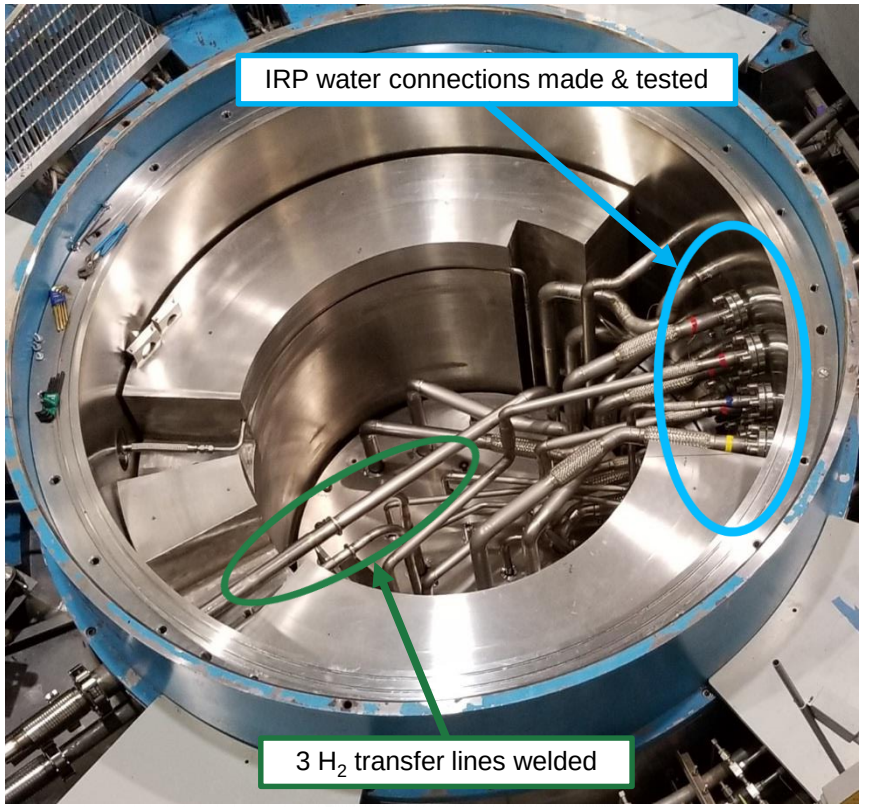
Beam-on-target is likely May 12th – 16th, Cryogenic Moderator System (CMS) progress dependent. The success-oriented plan is:





Pressurize H_2 side with helium; evacuate surrounding insulating vacuum jackets and confirm no helium leaks

Complete clean-up of the H_2 side of CMS

Cooldown helium refrigerator and H_2 transfer lines (with helium) and confirm no helium leaks

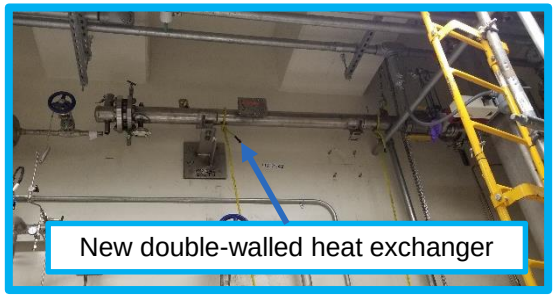
Install target T19

Warm up CMS

Install H_2 transfer line covers and core vessel shielding

Cool down CMS with H_2

April 26 27 28 29 30 May 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16



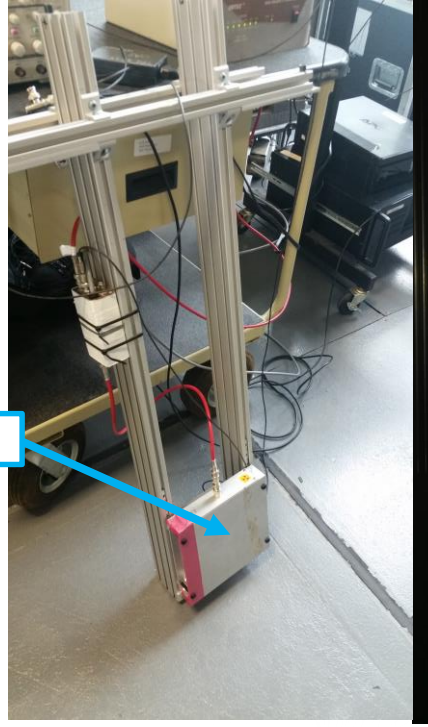
Complete Reflector Water System (HWS #4) D_2O modifications

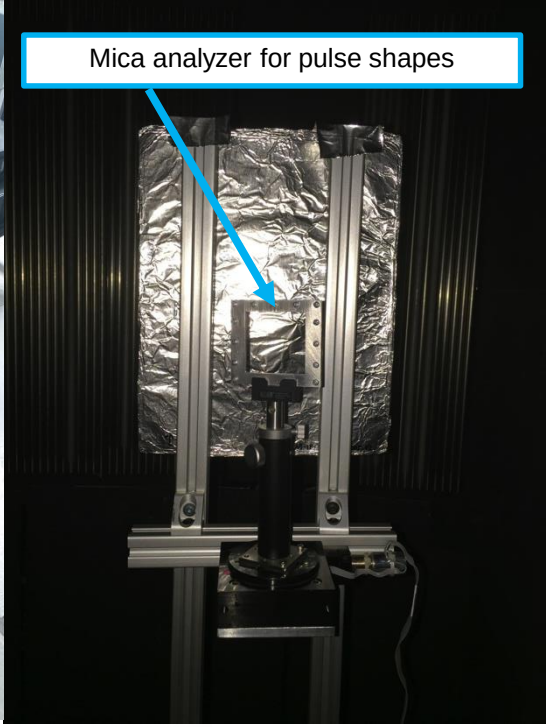
Fill HWS #4 drain tank with D_2O

Complete HWS #4 functional tests

Neutronics characterization measurements to confirm performance consistent with expectations; comparable spectra and pulse shapes, similar power dependence

Point of contact: Erik Iverson (NTD)





Pre-beam estimate of delayed neutron component

Spectrum and Pulse Shapes for Decoupled H_2 (1-3)

Spectrum and Pulse Shapes for Decoupled H_2O (7-9)

Spectrum for Decoupled H_2 (10-12)

Spectrum and Pulse Shapes for Decoupled H_2O (7-9)

May 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 1 2

Set up on SNAP

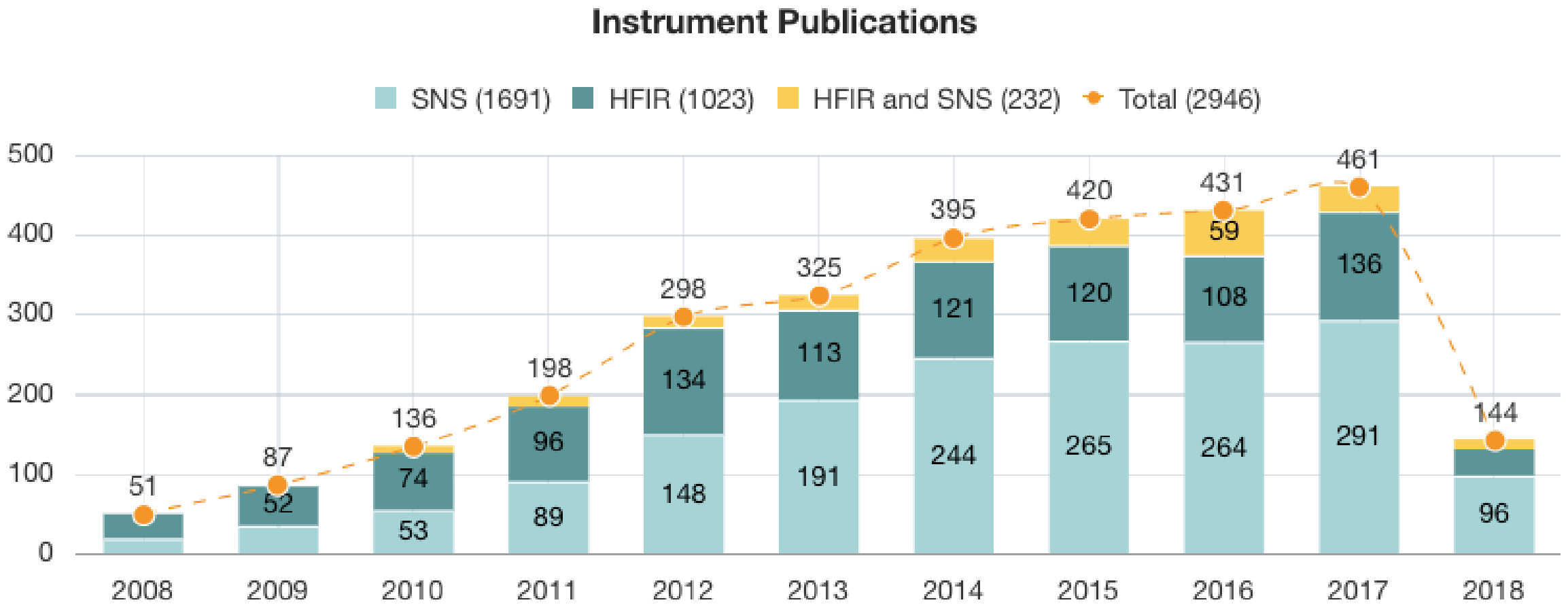
Set up on VULCAN

Set up on POWGEN

Backup for SNAP

Set up on CORELLI

Instrument publications through April 11, 2018



Each publication is counted once as related to only SNS instrument(s), only HFIR instrument(s), or to both SNS and HFIR instruments.

DOE high-impact publications (Jan-Apr 2018)

D. Bansal, J. Niedziela, R. Sinclair, V. O. Garlea, D. L. Abernathy, S. X. Chi, Y. Ren, H. D. Zhou, O. Delaire, "Momentum-resolved observations of the phonon instability driving geometric improper ferroelectricity in yttrium manganite." Nature Communications 9(1), 15 (January 2018). BL-14B (HYSPEC), BL-18 (ARCS), HB-3 (TAX)

S. Bordacs, D. G. Farkas, J. S. White, R. Cubitt, L. M. Debeer-Schmitt, T. U. Ito, I. Kezsmarki, "Magnetic Field Control of Cycloidal Domains and Electric Polarization in Multiferroic BiFeO3." Physical Review Letters 120(14), 147203 (April 2018). CG-2 (GP-SANS)

D. Fobes, S. Zhang, S. Z. Lin, P. Das, N. J. Ghimire, E. D. Bauer, J. D. Thompson, L. W. Harriger, G. Ehlers, A. A. Podlesnyak, R. I. Bewley, A. P. Sazonov, V. Hutanu, F. Ronning, C. D. Batista, M. Janoschek, "Tunable emergent heterostructures in a prototypical correlated metal." Nature Physics, (March 2018). BL-5 (CNCS)

E. A. Goremychkin, H. Park, R. Osborn, S. Rosenkranz, J. P. Castellan, V. R. Fanelli, A. D. Christianson, M. B. Stone, E. D. Bauer, K. J. McClellan, D. D. Byler, J. M. Lawrence, "Coherent band excitations in CePd3: A comparison of neutron scattering and ab initio theory." Science 359(6372), 186-191 (January 2018). BL-18 (ARCS)

B. Li, H. Wang, Y. Kawakita, Q. Zhang, M. Feygenson, H. L. Yu, D. Wu, K. Ohara, T. Kikuchi, K. Shibata, T. Yamada, X. K. Ning, Y. Chen, J. Q. He, D. Vaknin, R. Q. Wu, K. Nakajima, M. G. Kanatzidis, "Liquid-like thermal conduction in intercalated layered crystalline solids." Nature Materials 17, 226–230 (January 2018). BL-1B (NOMAD)

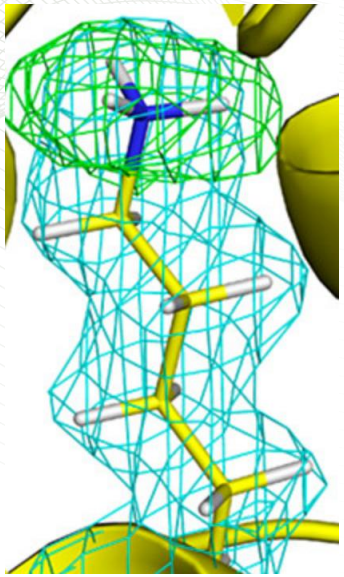
Z. Y. Li, Y. Cho, X. Li, X. Y. Li, A. Aimi, Y. Inaguma, J. A. Alonso, M. T. Fernandez-Diaz, J. Q. Yan, M. C. Downer, G. Henkelman, J. B. Goodenough, J. S. Zhou, "New mechanism for ferroelectricity in the perovskite Ca2-xMnxTi2O6 synthesized by spark plasma sintering." Journal of the American Chemical Society 146(6), 2214–2220 (February 2018). BL-11A (POWGEN)

G. L. Sternhagen, S. Gupta, Y. Zhang, V. T. John, G. J. Schneider, D. H. Zhang, "Solution Self-Assemblies of Sequence-Defined Ionic Peptoid Block Copolymers." Journal of the American Chemical Society, (2018). BL-6 (EQ-SANS), CG-3 (Bio-SANS)

T. A. Strobel, A. J. Ramirez-Cuesta, L. L. Daemen, V. S. Bhadram, T. Jenkins, C. Brown, Y. Q. Cheng, "Quantum Dynamics of H2 Trapped within Organic Clathrate Cages." Physical Review Letters 120(12), 120402 (March 2018). BL-16B (VISION)

B. Yang, W. Ming, M. Du, J. K. Keum, A. Puretzky, C. M. Rouleau, J. Huang, D. B. Geohegan, X. P. Wang, K. Xiao, "Real-Time Observation of Order-Disorder Transformation of Organic Cations Induced Phase Transition and Anomalous Photoluminescence in Hybrid Perovskites." Advanced Materials, 1705801 (April 2018). BL-12 (TOPAZ)

Substrate Binding Induces Conformational Changes in a Class A β-lactamase that Prime it for Catalysis



(Left) Neutron data from MaNDi enables the protonation states of key residues to be determined such as Lys 73 which is fully protonated $–ND_3^+$ in the absence of the substrate. (Right) Image of the front cover of ACS Catalysis which shows a cartoon representation of the Toho-1 β-lactamase structure with beta sheets (blue), helices (gold), and surface rendering (white).

Work performed at ORNL SNS's BL-11B, Macromolecular Neutron Diffractometer (MaNDi), sponsored by DOE Office of Science, Scientific User Facilities Division. This work was supported by the Laboratory Directed Research and Development Program at Oak Ridge National Laboratory (ORNL) and by the National Science Foundation Graduate Research Fellowship under Grant No. 2017219379. Results shown in this report are derived from work performed at Argonne National Laboratory (ANL), Structural Biology Center at the Advanced Photon Source. ANL is operated by UChicago Argonne, LLC, for the U.S. DOE, Office of Biological and Environmental Research, under contract DE-AC02-06CH11357. This research used resources of the National Energy Research Scientific Computing Center, a DOE Office of Science User Facility supported by the Office of Science of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231.

Scientific Achievement

The study fills in considerable detail on the structure and energetics of the proton relay network in the active site of a class A β-lactamase in the pre-covalent complex.

Significance and Impact

Understanding the catalytic mechanism of β-lactamases is important for developing strategies to overcome multi drug resistant bacteria.

Research Details

- Neutron and X-ray crystallography was used to determine the structure and protonation states of the catalytic residues Lys73 and Glu166 in the enzymes active site with and without the clinical antibiotic cefotaxime
- Using these structures we performed QM/MM free energy simulations to model the initial proton transfer steps in the reaction to quantify the role of the substrate cefotaxime in facilitating the reaction. We found that proton transfer from Lys73 to Glu166 is more thermodynamically favorable when the substrate is bound.

Langan, Patricia; Vandavasi, Venu Gopal; Cooper, Sarah; Weiss, Kevin; Ginell, Stephan; Parks, Jerry; Coates, Leighton. "Substrate binding induces conformational changes in a Class A β-lactamase that primes it for catalysis" (ACS Catalysis). 2018, 8, pp 2428–2437


ACTION
THIS DAY
IRAN L. THOMAS
ACS Catalysis
ACS Publications
ACS Catalysis
ACS Publications

Shear thickening electrolyte built from sterically stabilized colloidal particles (in-situ rheology on USANS)

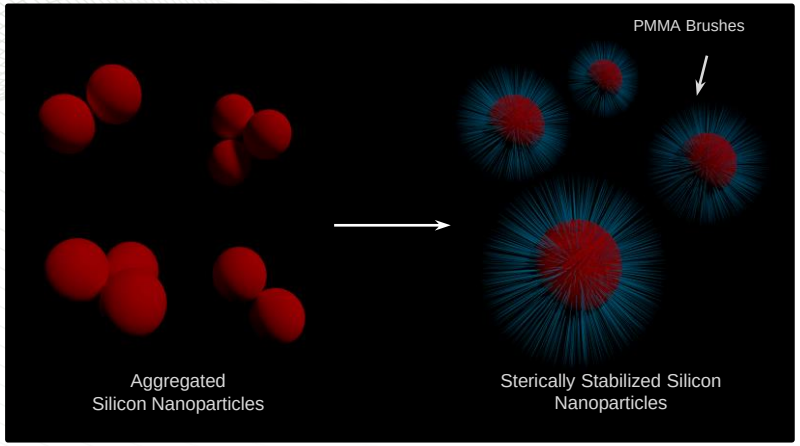
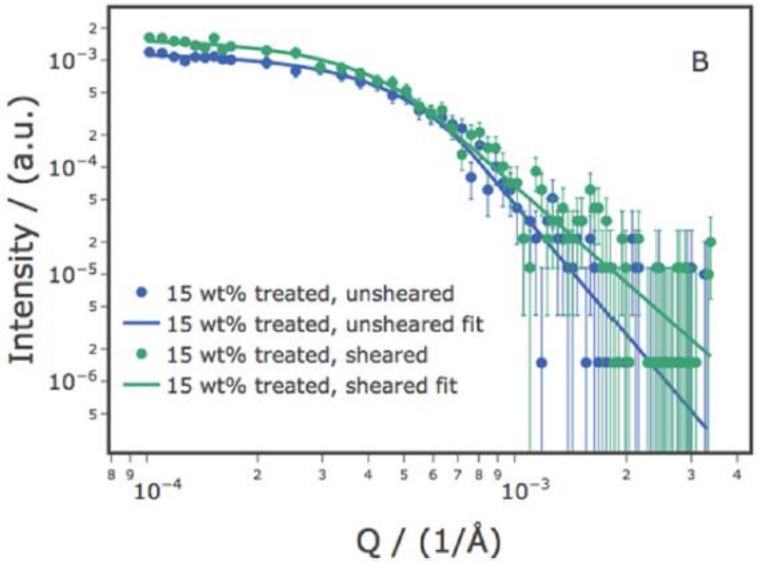


Image shows the depiction of the aggregation of bare silica particles in solution. Once coated with surface tethered PMMA brushes, the particles are sterically stabilized and the aggregation behaviour is diminished while keeping shear-thickening effects.



Scientific Achievement

Researchers demonstrated a method to prepare shear-thickening electrolytes consisting of silica nanoparticles in conventional liquid electrolytes.

Significance and Impact

These electrolytes rapidly and reversibly stiffen to solid-like behaviors in the presence of external shear or high impact, which is promising for improved lithium ion battery safety, especially in electric vehicles.

Research Details

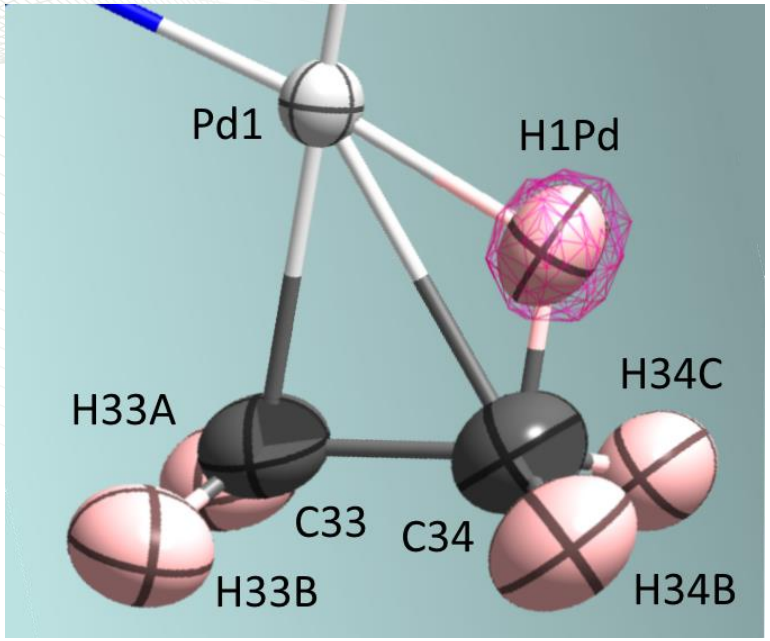
- USANS measurements were performed under shear to confirm stabilization.
- Conductivity tests were performed over 24-hour period to track stability.
- Coulombic efficiency was tracked using coin cells to confirm that Poly(methyl methacrylate) PMMA-coated silica colloid electrolytes are viable for lithium batteries.

B. Shen, et al., “Shear Thickening Electrolyte Built from Sterically Stabilized Colloidal Particles,” *ACS Appl. Mater. Interfaces (2018)* DOI:10.1021/acsami.7b19441

Work performed at ORNL SNS’s BL-1A, USANS, sponsored by DOE Office of Science, Scientific User Facilities Division.

OAK RIDGE National Laboratory

Neutrons reveal the long sought after β-Agostic Bonds



The negative nuclear scattering density obtained from single crystal neutron diffraction revealed the position of the agostic hydrogen atom (labeled H1Pd) in a β-agostic Pd polymerization intermediate.

Xu H., Hu C.T., Wang X.P., Diao T., Structural Characterization of β-Agostic Bonds in Pd-Catalyzed Polymerization *Organometallics*, **36**, *21*, 4099–4102 (2017). DOI: 10.1021/acs.organomet.7b00666

Scientific Achievement

We reported the first structural characterization of palladium agostic complexes, critical intermediates in catalytic reactions, such as olefin polymerization reactions that have eluded structural characterization and been long sought after by synthetic chemists.

Significance and Impact

Characterization of the agostic structure offers important insight into the fundamental understanding of agostic bonds and the mechanism of polymerization for polymers with increased strength and toughness.

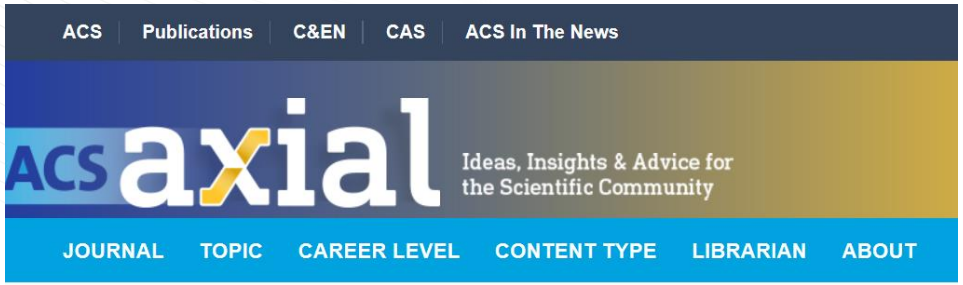
Research Details

- Crystallography, including X-ray and neutron diffraction, provides unambiguous proof of β-agostic bonds in cationic (α-diimine)Pd agostic complexes.
- Single crystal neutron diffraction was used to assign the H atom position of the β-agostic Pd polymerization intermediate.
- A crystal of 0.31 mm^3 in volume was used for data collection on the SNS TOPAZ instrument.

Work performed at the ORNL Spallation Neutron Source's TOPAZ beam line was supported by the Scientific User Facilities Division, Office of Basic Energy Sciences, US Department of Energy.

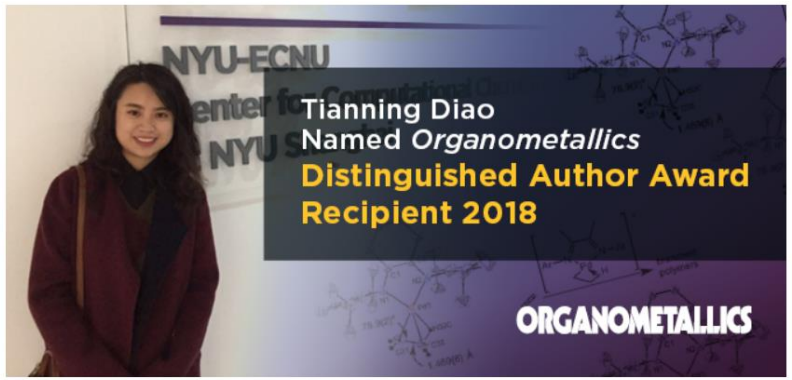
Distinguished publication award for TOPAZ user

The paper was published October 23, 2017 and received the 2018 Organometallics Distinguished Author Award on April 14, 2018 in recognition of work on the first structural characterization of palladium agostic complexes using single crystal X-ray and neutron diffraction.



Tianning Diao Named Organometallics Distinguished Author Award Recipient

By Mia Fields-Hall



Tianning Diao, Assistant Professor of Chemistry at New York University, is the 2018 recipient of the Organometallics Distinguished Author Award. Diao's group recently published the first structural characterization of palladium agostic complexes. These are intermediates in polymerization reactions that have eluded structural characterization and been long sought after by synthetic chemists. This finding offers important insight into chemical bonding.

http://axial.acs.org/2018/04/19/tianning-diao-organometallics/

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