APS SCIENCE 2020 Volume 2 • July 2021 ANL-21/06 Vol. 2 • Argonne National Laboratory

ANL-21/06 Vol.2
ISSN 1931-5007
July 2021

APS Science
2020 Volume 2

Research and engineering highlights from the Advanced Photon Source at Argonne National Laboratory

Includes APS research into the SARS-CoV-2 virus

Argonne
NATIONAL LABORATORY

ANL-21/06 Vol.2 • SSN 1931-5007 • July 2021

About Argonne National Laboratory
Argonne is a U.S. Department of Energy laboratory managed by UChicago Argonne, LLC under contract DE-AC02-06CH11357. The Laboratory's main facility is outside Chicago, at 9700 South Cass Avenue, Lemont, Illinois 60439. For information about Argonne and its pioneering science and technology programs, see www.anl.gov.

DOCUMENT AVAILABILITY
Online Access: U.S. Department of Energy (DOE) reports produced after 1991 and a growing number of pre-1991 documents are available free at OSTI.GOV (http://www.osti.gov/), a service of the US Dept. of Energy's Office of Scientific and Technical Information.

Reports not in digital format may be purchased by the public from the National Technical Information Service (NTIS):U.S. Department of Commerce National Technical Information Service
5301 Shawnee Rd
Alexandria, VA 22312
www.ntis.gov
Phone: (800) 553-NTIS (6847) or (703) 605-6000
Fax: (703) 605-6900
Email: orders@ntis.gov

Reports not in digital format are available to DOE and DOE contractors from the Office of Scientific and Technical Information (OSTI):
U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
www.osti.gov
Phone: (865) 576-8401
Fax: (865) 576-5728
Email: reports@osti.gov

Disclaimer
This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor UChicago Argonne, LLC, nor any of their employees or officers, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of document authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, Argonne National Laboratory, or UChicago Argonne, LLC.

ANL-21/06 Vol.2
ISSN 1931-5007
July 2021

APS Science 2020 Volume 2

Research and engineering highlights from the Advanced Photon Source at Argonne National Laboratory

Argonne is a U.S. Department of Energy (DOE) laboratory managed by UChicago Argonne, LLC.
The Advanced Photon Source is a DOE Office of Science user facility
operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Follow us: @advancedphoton Like us: Advanced Photon Source flickr: www.flickr.com/photos/97432701@N03/

Table of Contents

Access to Beam Time at the Advanced Photon Source

Five types of beam-time proposals are available at the APS: general user, partner or project user, collaborative access team (CAT) member, CAT staff, and APS staff. All beam time at the APS must be requested each cycle through the web-based Beam Time Request System. Each beam-time request (BTR) must be associated with one of the proposals mentioned above.

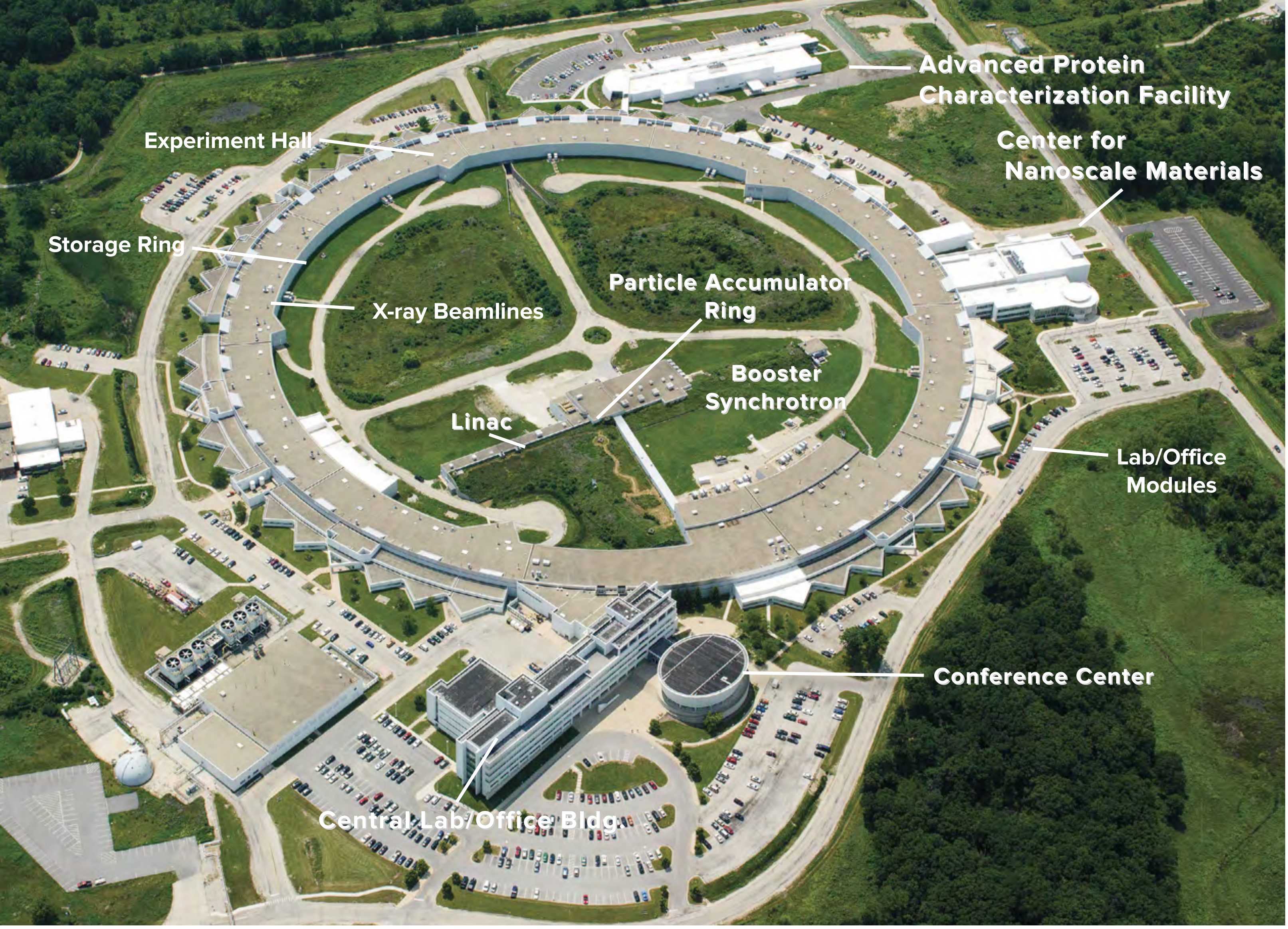
GENERAL-USER PROPOSALS AND BTRS Proposals are peer reviewed and scored by a General User Proposal Review Panel, and time is allocated on the basis of scores and feasibility. A new BTR must be submitted each cycle; each cycle, allocation is competitive. Proposals expire in two years or when the number of shifts recommended in the peer review has been utilized, whichever comes first.

PARTNER- OR PROJECT-USER PROPOSALS AND BTRS Proposals are peer reviewed by a General User Proposal Review Panel and reviewed further by a subcommittee of the APS Scientific Advisory Committee and by APS senior management. Although a new BTR must be submitted each cycle, a specific amount of beam time is guaranteed for up to three years.

CAT-MEMBER PROPOSALS from CAT members are typically much shorter and are reviewed by processes developed by individual CATs. Allocation/scheduling is determined by each CAT's management.

CAT AND APS STAFF-MEMBER PROPOSALS AND BTRS These proposals are also very short and are reviewed through processes developed by either the CAT or the APS. Each CAT/beamline determines how beam time is allocated/scheduled. Collaborative access team and/or APS staff may submit general-user proposals, in which case the rules for general-user proposals and BTRs are followed.

In addition to the above, the APS has developed an industrial measurement access mode (MAM) program to provide a way for industrial users to gain rapid access for one-time measurements to investigate specific problems. A MAM proposal expires after one visit. The APS User Information page (www.aps.anl.gov/Users-Information) provides access to comprehensive information for prospective and current APS users.



The Advanced Photon Source Facility at Argonne National Laboratory

The U.S. Department of Energy's Advanced Photn Source (APS) is one of the world's most productive x-ray light source facilities. Each year, the APS provides high-brightness x-ray beams to a diverse community of more than 5,000 researchers in materials science, chemistry, condensed matter physics, the life and environmental sciences, and applied research. Researchers using the APS produce over 2,000 publications each year detailing impactful discoveries, and solve more vital biological protein structures than users of any other x-ray light source research facility. APS x-rays are ideally suited for explorations of materials and biological structures; elemental distribution; chemical, magnetic, electronic states; and a wide range of technologically important engineering systems from batteries to fuel injector sprays, all of which are the foundations of our nation's economic, technological, and physical well-being.

The APS occupies an 80-acre site on the Argonne campus, about 25 miles from downtown Chicago, Illinois. It shares a site with the Center for Nanoscale Materials and the Advanced Protein Characterization Facility.

For directions to Argonne, see https://www.anl.gov/visiting-argonne.

CONTACT US

For more information about the APS send an email to apsinfo@aps.anl.gov or write to APS Info, Bldg. 401, Rm. A4113, Argonne National Laboratory, 9700 S. Cass Ave., Lemont, IL 60439.

To order additional copies of this, or previous, issues of *APS Science* send email to apsinfo@aps.anl.gov.

To download PDF versions of *APS Science* back issues go to
www.aps.anl.gov/Science/APS-Science

Visit the APS on the Web at
www.aps.anl.gov

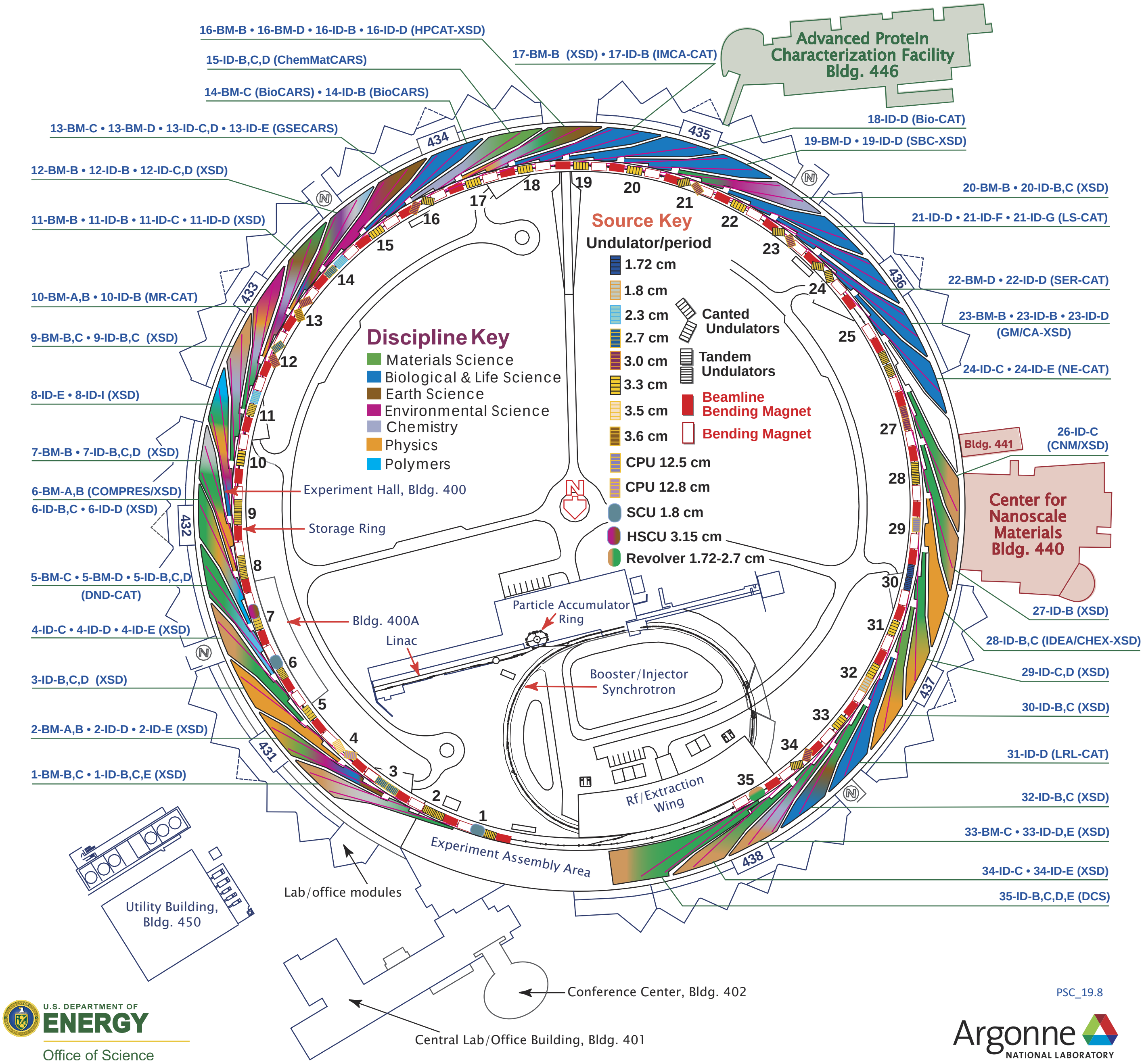
ARGONNE NATIONAL LABORATORY 400-AREA FACILITIES

ADVANCED PHOTON SOURCE

(**Beamlines**, **Disciplines**, and **Source Configuration**)

ADVANCED PROTEIN CHARACTERIZATION FACILITY

CENTER FOR NANOSCALE MATERIALS



U.S. DEPARTMENT OF ENERGY

Office of Science

Argonne NATIONAL LABORATORY

APS sectors: At the APS, a “sector” comprises the radiation sources (one bending magnet and nominally one insertion device, although the number of insertion devices in the straight sections of the storage ring can vary) and the beamlines, enclosures, and instrumentation that are associated with a particular storage ring sector. The APS has 35 sectors dedicated to user science and experimental apparatus. X-ray Science Division (XSD) sectors comprise those beamlines operated by the APS. Collaborative access team (CAT) sectors comprise beamlines operated by independent groups made up of scientists from universities, industry, and/or research laboratories both federal and private.

APS Beamlines

Key: Beamline designation • Sector operator • Disciplines • Techniques • Radiation source energy • User access mode(s) • General-user status

1-BM-B,C • **X-ray Science Division (XSD)** • Materials science, physics • Optics testing, detector testing, topography, white Laue single-crystal diffraction • 6-30 keV, 50-120 keV • On-site • Accepting general users

1-ID-B,C,E • XSD • Materials science, physics, chemistry, life science • High-energy x-ray diffraction, tomography, small-angle x-ray scattering, fluorescence spectroscopy, pair distribution function, phase contrast imaging • 41-136 keV, 45-116 keV • On-site • Accepting general users

2-BM-A,B • XSD • Physics, life sciences, geoscience, materials science • Tomography, phase contrast imaging • 10-170 keV, 11-35 keV • On-site • Accepting general users

2-ID-D • XSD • Life sciences, materials science, environmental science • Microfluorescence, micro x-ray absorption fine structure, nanoimaging, ptychography • 5-30 keV • On-site, remote, mail-in, beamline staff • Accepting general users

2-ID-E • XSD • Life sciences, environmental science, materials science • Microfluorescence, tomography • 5-20 keV • On-site, remote, mail-in, beamline staff • Accepting general users

3-ID-B,C,D • XSD • Physics, geoscience, life sciences, chemistry, materials science • Nuclear resonant scattering, high-pressure diamond anvil cell • 7-27 keV, 14.41-14.42 keV • On-site • Accepting general users

4-ID-C • XSD • Physics, materials science • Magnetic circular dichroism, x-ray magnetic linear dichroism, x-ray photoemission spectroscopy • 400-2800 eV • Remote • Accepting general users

4-ID-D • XSD • Physics, materials science • Anomalous and resonant scattering, magnetic x-ray scattering, magnetic circular dichroism, high-pressure diamond anvil cell • 2.7-40 keV • Remote • Accepting general users

4-ID-E • XSD • Materials science, physics • Synchrotron x-ray scanning tunneling microscopy (SX-STM), magnetic circular dichroism, x-ray photoemission spectroscopy • 400-1900 eV • On-site • Accepting general users

5-BM-C • **DuPont-Northwestern-Dow Collaborative Access Team (DND-CAT)** • Materials science, polymer science • Powder diffraction, tomography, wide-angle x-ray scattering • 10-42 keV • On-site, mail-in • Accepting general users

5-BM-D • DND-CAT • Materials science, polymer science, chemistry, environmental science • X-ray absorption fine structure, high-energy x-ray diffraction, general diffraction • 4.5-25 keV, 4.5-80 keV • On-site, mail-in • Accepting general users

5-ID-B,C,D • DND-CAT • Materials science, polymer science, chemistry, life science • Powder diffraction, x-ray standing waves, x-ray optics development/techniques, small-angle x-ray scattering, surface diffraction, x-ray reflectivity, wide-angle x-ray scattering • 6-17.5 keV • On-site, mail-in • Accepting general users

6-BM-A,B • **COMPRES/XSD** • Materials science, geoscience • Energy dispersive x-ray diffraction, high-pressure multi-anvil press, radiography, tomography • 20-200 keV • On-site • Accepting general users

6-ID-B,C • XSD • Physics, materials science • Magnetic x-ray scattering, anomalous and resonant scattering, general diffraction, grazing incidence diffraction • 4-38 keV • Remote • Accepting general users

6-ID-D • XSD • Physics, materials science • High-energy x-ray diffraction, powder diffraction, pair distribution function • 50-100 keV, 70-130 keV • Remote • Accepting general users

7-BM-B • XSD • Physics • Radiography, tomography, microfluorescence • 5-150 keV, 6-15 keV, 15-60 keV • On-site • Accepting general users

7-ID-B,C,D • XSD • Materials science, atomic physics, chemistry • Time-resolved x-ray scattering, time-resolved x-ray absorption fine structure, phase contrast imaging • 6-18 keV, 12-26 keV • On-site, remote • Accepting general users

8-ID-E • XSD • Materials science, polymer science, physics • Grazing incidence small-angle scattering, x-ray photon correlation spectroscopy • 7.35-7.35 keV, 10.9-10.9 keV • On-site, remote • Accepting general users

8-ID-I • XSD • Polymer science, materials science, physics • X-ray photon correlation spectroscopy, small-angle x-ray scattering • 7.35-7.35 keV, 10.9-10.9 keV • On-site, remote • Accepting general users

9-BM-B,C • XSD • Materials science, chemistry, environmental science • X-ray absorption fine structure, x-ray absorption near-edge structure • 2.1-22.5 keV • On-site, remote, mail-in • Accepting general users

9-ID-B,C • XSD • Chemistry, materials science, life sciences • Nano-imaging, microfluorescence, ultra-small-angle x-ray scattering, tomography, ptychography, x-ray absorption near-edge structure • 4.5-30 keV • On-site • Accepting general users

10-BM-A,B • **Materials Research (MR)-CAT** • Materials science, chemistry, environmental science, physics • X-ray absorption fine structure, time-resolved x-ray absorption fine structure, microfluorescence • 4-32 keV • On-site, remote, mail-in, observer, beamline staff • Accepting general users

10-ID-B • MR-CAT • Materials science, environmental science, chemistry, physics • X-ray absorption fine structure, time-resolved x-ray absorption fine structure, microfluorescence, x-ray photoemission spectroscopy, x-ray emission spectroscopy • 4.8-32 keV, 15-65 keV • On-site, remote, mail-in, observer, beamline staff • Accepting general users

11-BM-B • XSD • Chemistry, materials science, physics • Powder diffraction • 15-33 keV • On-site, remote, mail-in • Accepting general users

11-ID-B • XSD • Chemistry, environmental science, materials science • Pair distribution function, high-energy x-ray diffraction • 58.66 keV, 86.7 keV • On-site, remote, mail-in • Accepting general users

11-ID-C • XSD • Materials science, chemistry, physics • High-energy x-ray diffraction, diffuse x-ray scattering, pair distribution function • 105.7 keV • On-site, remote • Accepting general users

11-ID-D • XSD • Chemistry, environmental science, materials science • Time-resolved x-ray absorption fine structure, time-resolved x-ray scattering • 6-25 keV • On-site, remote • Accepting general users

12-BM-B • XSD • Materials science, polymer science, chemistry, physics, environmental science • X-ray absorption fine structure, small-angle x-ray scattering, wide-angle x-ray scattering • 4.5-30 keV, 10-40 keV • On-site, remote, mail-in • Accepting general users

12-ID-B • XSD • Chemistry, materials science, life sciences, polymer science, physics • Small-angle x-ray scattering, grazing incidence small-angle scattering, wide-angle x-ray scattering, grazing incidence diffraction • 7.9-14 keV • On-site, remote • Accepting general users

12-ID-C,D • XSD • Chemistry, physics, materials science • Small-angle x-ray scattering, grazing incidence small-angle scattering, wide-angle x-ray scattering, surface diffraction • 4.5-40 keV • On-site • Accepting general users

13-BM-C • **GeoSoilEnviro Center for Advanced Radiation Sources (GSECARS)** • Geoscience, environmental science • Surface diffraction, high-pressure diamond anvil cell, single-crystal diffraction • 15-15 keV, 28.6-28.6 keV • On-site • Accepting general users

13-BM-D • GSECARS • Geoscience, environmental science • Tomography, high-pressure diamond anvil cell, high-pressure multi-anvil press • 4.5-100 keV • On-site • Accepting general users

13-ID-C,D • GSECARS • Geoscience, environmental science • Surface diffraction, microdiffraction, x-ray standing waves, x-ray absorption fine structure, resonant inelastic x-ray scattering, x-ray emission spectroscopy, high-pressure diamond anvil cell, high-pressure multi-anvil press • 4.9-45 keV, 10-75 keV • On-site • Accepting general users

13-ID-E • GSECARS • Geoscience, environmental science • Microfluorescence, micro x-ray absorption fine structure, microdiffraction, fluorescence spectroscopy • 2.4-28 keV, 5.4-28 keV • On-site • Accepting general users

14-BM-C • **BioCARS** • Life sciences • Macromolecular crystallography, fiber diffraction, biohazards at the BSL2/3 level • 8-14.9 keV • On-site, remote, beamline staff • Accepting general users

14-ID-B • BioCARS • Life sciences • Time-resolved crystallography, time-resolved x-ray scattering, Laue crystallography, wide-angle x-ray scattering, biohazards at the BSL2/3 level, macromolecular crystallography, serial crystallography • 7-19 keV • On site, remote, beamline staff • Accepting general users

15-ID-B,C,D • **ChemMatCARS** • Materials science, chemistry • Resonant diffraction (DAFS) – single-crystal, high-pressure diamond anvil cell – single crystal, photo-crystallography, single-crystal diffraction, liquid interface scattering, liquid interface spectroscopy, anomalous small-angle scattering • 5.5-32 keV, 10-70 keV • On-site, remote, mail-in • Accepting general users

16-BM-B • **High Pressure (HP)CAT-XSD** • Materials science, geoscience, chemistry, physics • White Laue single-crystal diffraction, energy dispersive x-ray diffraction, phase contrast imaging, radiography, pair distribution function • 10-120 keV • Remote • Accepting general users

16-BM-D • HPCAT-XSD • Materials science, geoscience, chemistry, physics • Powder angular dispersive x-ray diffraction, single-crystal diffraction, x-ray absorption near-edge structure, x-ray absorption fine structure, tomography • 6-45 keV • Remote • Accepting general users

16-ID-B • HPCAT-XSD • Materials science, geoscience, chemistry, physics • Microdiffraction, single-crystal diffraction • 18-50 keV • Remote • Accepting general users

16-ID-D • HPCAT-XSD • Materials science, geoscience, chemistry, physics • Nuclear resonant scattering, inelastic x-ray scattering (1-eV resolution), x-ray emission spectroscopy • 5-37 keV, 14.41-14.42 keV • Remote • Accepting general users

17-BM-B • XSD • Chemistry, materials science • Powder diffraction, pair distribution function • 27-51 keV • On-site, remote, mail-in • Accepting general users

17-ID-B • **Industrial Macromolecular Crystallography Association (IMCA)-CAT** • Life sciences • Macromolecular crystallography, multi-wavelength anomalous dispersion, microbeam, single-wavelength anomalous dispersion, large unit cell crystallography • Subatomic (<0.85 Å) resolution • 6-20 keV • On-site, remote, mail-in • Accepting general users

18-ID-D • **Biophysics (Bio)-CAT** • Life sciences • Fiber diffraction, micro-diffraction, small-angle x-ray scattering, time-resolved x-ray scattering • 3.5-35 keV • On-site, remote, mail-in • Accepting general users

19-BM-D • **Structural Biology Center (SBC)-XSD** • Life sciences • Multi-wavelength anomalous dispersion, macromolecular crystallography, single-wavelength anomalous dispersion • 6-18.5 keV • Remote, on-site, mail-in • Accepting general users

19-ID-D • SBC-XSD • Life sciences • Macromolecular crystallography, multi-wavelength anomalous dispersion, subatomic (<0.85 Å) resolution, large unit cell crystallography, single-wavelength anomalous dispersion, serial crystallography • 6-19 keV • On-site, remote, mail-in • Accepting general users

20-BM-B • XSD • Materials science, environmental science, chemistry • X-ray absorption fine structure, microfluorescence • 2.7-32 keV, 2.7-35 keV • On-site, remote, mail-in • Accepting general users

20-ID-B,C • XSD • Materials science, environmental science, chemistry • X-ray absorption fine structure, x-ray Raman scattering, micro x-ray absorption fine structure, microfluorescence, x-ray emission spectroscopy • 4.3-27 keV, 7-52 keV • On-site, remote, mail-in • Accepting general users

21-ID-D • **Life Sciences (LS)-CAT** • Life sciences • Macromolecular crystallography • 6.5-20 keV • On-site, remote, mail-in • Accepting general users

21-ID-F • LS-CAT • Life sciences • Macromolecular crystallography • 12.7 keV • Remote, on-site, mail-in • Accepting general users

21-ID-G • LS-CAT • Life sciences • Macromolecular crystallography • 12.7 keV • On-site, remote, mail-in • Accepting general users

22-BM-D • **Southeast Regional (SER)-CAT** • Life sciences • Macromolecular crystallography, single-wavelength anomalous dispersion, multi-wavelength anomalous dispersion • 8-16 keV • On-site, remote • Accepting general users

22-ID-D • SER-CAT • Life sciences • Macromolecular crystallography, multi-wavelength anomalous dispersion, single-wavelength anomalous dispersion, microbeam • 6-16 keV • On-site, remote • Accepting general users

23-ID-B • **National Institute of General Medical Sciences and National Cancer Institute (GM/CA)-XSD** • Life sciences • Macromolecular crystallography, microbeam, large unit cell crystallography, subatomic (<0.85 Å) resolution, multi-wavelength anomalous dispersion, single-wavelength anomalous dispersion • 3.5-20 keV • On-site, remote • Accepting general users

23-ID-D • GM/CA-XSD • Life sciences • Macromolecular crystallography, microbeam, large unit cell crystallography, subatomic (<0.85 Å) resolution, multi-wavelength anomalous dispersion, single-wavelength anomalous dispersion, serial crystallography • 11-13.5 keV • On-site, remote • Accepting general users

24-ID-C • **Northeastern (NE)-CAT** • Life sciences • Macromolecular crystallography, microdiffraction, single-wavelength anomalous dispersion, single-crystal diffraction, microbeam, multi-wavelength anomalous dispersion, subatomic (<0.85 Å) resolution • 6.5-20 keV • On-site, remote • Accepting general users

24-ID-E • NE-CAT • Life sciences • Macromolecular crystallography, microbeam, microdiffraction, single-wavelength anomalous dispersion, single-crystal diffraction • 12.68 keV • On-site, remote • Accepting general users

26-ID-C • **Center for Nanoscale Materials (CNM)/XSD** • Physics, materials science • Nanodiffraction, nano-imaging, coherent x-ray scattering • 7-12 keV • On-site, remote, mail-in, observer, beamline staff • Accepting general users

27-ID-B • XSD • Physics, materials science, chemistry • Resonant inelastic x-ray scattering • 5-14 keV • On-site • Accepting general users

29-ID-C,D • XSD • Physics, materials science • Resonant soft x-ray scattering, angle-resolved photoemission spectroscopy • 250-2200 eV, 2200-3000 eV • Remote, mail-in • Accepting general users

30-ID-B,C • XSD • Physics, materials science, geoscience, life sciences • Inelastic x-ray scattering (1-meV resolution), nuclear resonant scattering • 23.7-23.9 keV • On-site • Accepting general users

31-ID-D • **Lily Research Laboratories (LRL)-CAT** • Life sciences • Macromolecular crystallography, single-wavelength anomalous dispersion • 5-22 keV • Mail-in • Accepting general users

32-ID-B,C • XSD • Materials science, life sciences, geoscience • Phase contrast imaging, radiography, transmission x-ray microscopy, tomography • 7-40 keV • On-site • Accepting general users

33-BM-C • XSD • Materials science, physics, chemistry • Diffuse x-ray scattering, general diffraction, powder diffraction, x-ray reflectivity, grazing incidence diffraction, anomalous and resonant scattering • 5-35 keV • On-site • Accepting general users

33-ID-D,E • XSD • Materials science, physics, chemistry, environmental science • Anomalous and resonant scattering, diffuse x-ray scattering, general diffraction, surface diffraction, surface diffraction (UHV), x-ray reflectivity • 5-30 keV • On-site • Accepting general users

34-ID-C • XSD • Materials science, physics • Coherent x-ray scattering • 5-15 keV • On-site, remote • Accepting general users

34-ID-E • XSD • Materials science, physics, environmental science, geoscience • Microdiffraction, Laue crystallography, microbeam, microfluorescence • 7-30 keV • On-site • Accepting general users

35-ID-B,C,D,E • **Dynamic Compression Sector (DCS)** • Physics, materials science, geoscience • Time-resolved x-ray scattering, phase contrast imaging, radiography • 7-35 keV, 7-100 keV, 24-24 keV • On-site, remote • Accepting general users

Farewell & Welcome

Stephen Streiffer

July 2021

What to give the person who thinks they have everything?

Make them the director of the Advanced Photon Source, and then they really will have everything.

This is my last “Welcome” column in these APS highlights books. As you may or may not know, I’ve accepted the position of Argonne Deputy Laboratory Director for Science & Technology. To say I leave with mixed emotions is the quintessential understatement.

While the prospect of new challenges is exciting to be sure, it has been a highpoint in my life and an honor to serve as the fifth APS director; one does not leave a position like this without careful consideration.

There are many remarkable things about this job, but truly, the most remarkable are (in no set order) the people and the dazzling science this facility enables.

Our staff, our users, our sponsors, our Argonne colleagues, the students and public servants who cross one’s path; the APS seems to be a magnet that draws to it the best people who bring curiosity and fierce intellect and a desire to reach into the unknown and bring out new knowledge.

And the science! This is the twenty-first issue in this series of highlights books (https://www.aps.anl.gov/Science/APS-Science). These and the science highlights on our website (https://www.aps.anl.gov/APS-Science-Highlight/All) taken together number in the hundreds, and yet, they do not even begin to account for all the knowledge that has flowed from the APS.

At time I’m writing this, we are in the final laps of a lengthy and exacting search for the sixth APS director.I want to thank all of the candidates for their interest, their time, and their ideas about the future of the APS and x-ray science. I also want to thank Kathy Harkay of the Accelerator Systems Division, Jim Bluemond of Argonne Human Resources, and the rest of the selection committee for steering the selection process to its outstanding conclusion.

The next director is coming into this job at the best possible time: on the eve of an excitingly reimagined and upgraded APS that will join the elite ranks of the world’s next-generation light sources. The APS Upgrade Project will provide our outstanding user community with the tools they deserve. As they have for the past 25 years, they will use the new APS to continually enrich every aspect of our lives and support our national health and well-being.

I know you all will give the new director your full, unflagging support, just like you did for me.

And I will be cheering you on!

All my best,
Stephen Streiffer
Argonne Deputy Laboratory Director for Science & Technology and
Interim Associate Laboratory Director for
Photon Sciences.

APS Upgrade Update

Bob Hettel

August 2021

As one would expect, a project like upgrading the APS is a massive endeavor. It requires years of planning and design work before anything can be built, and review after review by the DOE to make sure we are on track and have properly estimated our schedule and budget. This is all important and necessary work on the path toward a fully realized project–but the effort is worth it, given the up to 500-fold increase in performance the APS Upgrade Project (APS-U) will deliver upon completion.

The construction phase of the APS-U officially began in 2019. In the past two years, incredible progress toward the realization of the APS-U has been achieved, despite the uncertainties the COVID pandemic has introduced. The project will replace the 25-year-old APS storage ring with a state-of-the-art multi-bend achromat lattice, with many more bending magnets and magnet-focusing cells. Also included in the project are nine “feature beamlines” that will exploit the very high brightness and transverse coherence of the x-ray produced in the new ring, two of which will be housed in a new Long Beamline Building (LBB); many new permanent magnet and superconducting insertion devices; and enhancements to multiple other existing x-ray beamlines.

If there is a theme that describes our plan, it is this: full speed ahead.

Our current schedule has the APS suspending operations in April of 2023 for one year as we replace the current storage ring. We will see increasing on-site activity between now and then as industrial deliveries increase and on-site acceptance tests, and sub-assembly efforts ramping up.

Here are just some of the achievements at the time of writing, August 2021:

- We have received more than 1000 storage ring magnets, out of the 1321 total needed for the upgrade project multi-bend achromat magnet lattice. The magnets (dipoles, quadrupoles, and sextupoles) are all being carefully measured upon arrival to certify their acceptance for installation.
- More than 1500 storage ring magnet power supplies have been received and accepted.
- With the arrival of the initial support structures, each weighing 20 tons, first practice assemblies of storage ring magnet modules have been completed and lessons fed back into the process such that future assemblies can be done efficiently and successfully.
- We installed three shielded enclosures at beamline 28-ID and are installing five shielded enclosures at beamline 25-ID.
- We installed beam position monitors at Sector 25 after receiving them from our colleagues at Brookhaven National Laboratory.
- In one of the more outwardly visible signs of progress, construction of the LBB is well along, with all foundation and ironwork complete.
- A major decision modifying the injection scheme from a vertical design to a horizontal design was made, lowering the risk to the project while maintaining performance.

Other designs of the accelerator and beamlines are very close to completion, and the final design of the new beamline instruments progressed with help from our partner laboratories.

Once completed, the APS will be a global leader among the fourth-generation storage-ring x-ray light sources, delivering not only world-class, intensely bright hard x-rays but tightly focused ones as well.

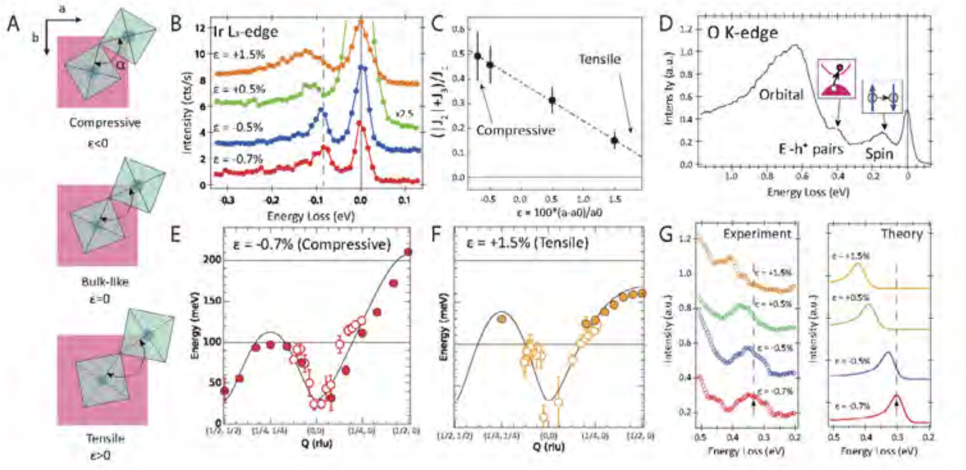
The upgraded APS will allow our users to conduct small-beam scattering and spectroscopy, coherent scattering and imaging, and x-ray photon correlation spectroscopy at resolutions unattainable by today’s x-ray light sources. It will allow researchers to see things at scale they’ve never seen before. This extreme level of detail will enable new discoveries in biofuels, energy storage, medicine, and other fields, and help us understand everything from the structure of the Earth to the makeup of the human brain.

When it is completed, it will be thanks to the dedicated people who worked and are working tirelessly to bring this project to fruition. With all of us working together, the APS-U will be a brilliant jewel in the crown of the DOE science mission.

Robert Hettel
Project Director, APS Upgrade Project

Engineering Materials and Applications

Exploring New Ways to Fine Tune Strontium-Iridium-Oxide Thin Films for Spintronics



Spintronics is the rapidly approaching future of electronics, expanding the capabilities of all our devices by exploiting not only the electron's charge but its subatomic spin. But a more exotic technology calls for more exotic materials, particularly those that can be precisely tailored for specific properties. Especially promising in this regard is the class of antiferromagnetic perovskite oxides, hosting many handy characteristics including superconductivity, magnetoresistance, and Mott insulator-type behaviors. In such a framework, the presence of high spin-orbit coupling allows additional leverage to control the magnetic structure through lattice deformations. A team of experimenters from a diverse international group of institutions used the APS and two other x-ray light sources to explore the intricately entangled spin and orbital degrees of freedom and the lattice structure of strontium-iridium-oxide (Sr_2IrO_4) by inducing epitaxial strain on thin films to create lattice distortions. Their work, published in the *Proceedings of the National Academy of Sciences of the United States of America*, provides an unprecedented level of understanding of the electron-lattice interactions in this important thin-film material and points to possibilities for customizing its properties for new applications. — Mark Wolverton

Read the entire *APS Science* article here.

See: Eugenio Paris[1*], Yi Tseng[1], Ekaterina M. Pärschke[2, 3], Wenliang Zhang[1], Mary H. Upton[4], Anna Efimenko[5], Katharina Rolfs[1, 6], Daniel E. McNally[1], Laura Maurel[1, 7], Muntaser Naamneh[1], Marco Caputo[1], Vladimir N. Strocov[1], Zhiming Wang[8], Diego Casa[4], Christof W. Schneider[1], Ekaterina Pomjakushina[1], Krzysztof Wohlfeld[9], Milan Radovic[1], and Thorsten Schmitt[1**], "Strain engineering of the charge and spin-orbital interactions in Sr_2IrO_4," Proc. Natl. Acad. Sci. U.S.A. **117**(40), 24764 (October 6, 2020).
DOI: 10.1073/pnas.2012043117

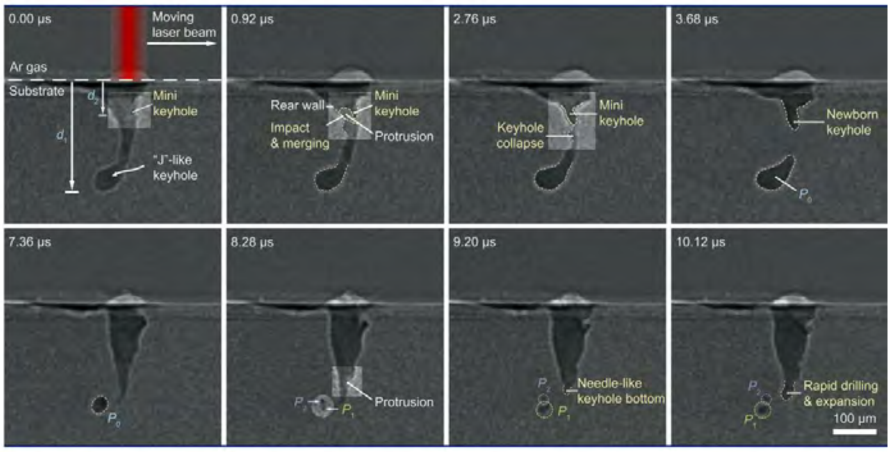
Author affiliations: [1]Paul Scherrer Institut, [2]University of Alabama at Birmingham, [3]Institute of Science and Technology Austria, [4]Argonne National Laboratory, [5]European Synchrotron Radiation Facility, [6]Physikalisch-Technische Bundesanstalt Berlin, [7]ETH Zurich, [8]Chinese Academy of Sciences, [9]Institute of Theoretical Physics

Correspondence: * eugenio.paris@psi.ch, ** thorsten.schmitt@psi.ch

The work at PSI is supported by the Swiss National Science Foundation (SNSF) through Project 200021_178867, the NCCR (National Centre of Competence in Research) MARVEL (Materials' Revolution: Computational Design and Discovery of Novel Materials) and the Sinergia network Mott Physics Beyond the Heisenberg Model (MPBH) (SNSF Research Grants CRSII2_160765/1 and CRSII2_141962). K. W. acknowledges support by the Narodowe Centrum Nauki Projects 2016/22/E/ST3/00560 and 2016/23/B/ST3/00839. E. M. P. and M. N. acknowledge funding from the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie Grant Agreements 754411 and 701647, respectively. M. R. was supported by the Swiss National Science Foundation under Project 200021–182695. This research used resources of the APS, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357.

XSD Inelastic X-ray & Nuclear Resonant Scattering Group 27-ID-B station

Defining the Laser Speed Limit for 3-D Printing with Metal



Metal objects manufactured by 3-D printing often contain tiny holes which can weaken the final product, making it more prone to corrosion or breaking under stress. Researchers using the APS detailed how such pores are created and defined the best combination of laser energy and scanning speed to avoid causing the defects. Their results were published in the journal *Science*. Laser bed powder fusion is the most commonly used additive manufacturing process for metal parts. A laser, guided by a computer, scans over a bed of metal powder, melting it and fusing it to the already hardened layer below. The laser beam creates a keyhole, a deep, roughly cylindrical gap that extends through the powder and into the metal. Laser reflections within the keyhole actually increase energy absorption and increase the efficiency of the process, but sometimes the keyhole can become unstable and break apart, leaving behind voids that get trapped in the finished product. To understand the dynamics of this process, the researchers performed high-speed x-ray imaging experiments. to image the fusion process as the laser moved across a powdered titanium alloy, Ti-6Al-4V, which also contained small amounts of vanadium and aluminum. The high-brightness x-rays from the APS gave them access to a temporal resolution below 1 nanosecond, spatial resolution in micrometers, and imaging at megahertz frame rates, allowing them to watch the formation of keyholes and pores. – Neil Savage

Read the entire *APS Science* highlight here.

See: Cang Zhao[1,2*], Niranjan D. Parab[3‡], Xuxiao Li[4], Kamel Fezzaa[3], Wenda Tan[4], Anthony D. Rollett[5**], and Tao Sun[6***], "Critical instability at moving keyhole tip generates porosity in laser melting," Science **370(**6520), 1080 (27 November 2020). DOI: 10.1126/science.abd1587 Figure Copyright © 2020, American Association for the Advancement of Science

Author affiliations: [1]Tsinghua University, [2]Key Laboratory for Advanced Materials Processing Technology, [3]Argonne National Laboratory, [4]University of Utah, [5]Carnegie Mellon University, [6]University of Virginia

Correspondence: * cangzhao@tsinghua.edu.cn, ** rollett@andrew.cmu.edu, *** ts7qw@virginia.edu ‡Present address: Intel Corporation

The authors acknowledge A. Deriy and F. De Carlo at the APS, and Z. Guo and W. Chen at Purdue University for their technical support of the beamline experiments. The work was supported by the start-up fund from the Department of Mechanical Engineering at Tsinghua University, the start-up fund from the University of Virginia, the Department of Defense Office of Economic Adjustment under award ST1605-17-02, the National Aeronautics and Space Administration (NASA) University Leadership Initiative program under grant 80NSSC19M0123, and the National Science Foundation under grant 1752218. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

XSD Imaging Group station 32-ID-B,C

(Solar) Power to the Perovskites

Solar power generates a growing slice of the world's electricity, and industry is always on the hunt for better solar technology. Lead iodide perovskites are promising candidates that match the efficiency of current technologies and cost less, but most of them are less stable than the industry standard. Recently, materials scientists have found that two-dimensional (2-D) lead iodide perovskites are more stable than three dimensional (3-D) ones, and that mixing 2-D and 3-D versions created solar cells that combined the stability of the 2-D phase with the efficiency of the 3-D version. Now, a group of researchers has used the APS to examine how 2-D lead iodide perovskites form in real time. They found a method to enhance the quality of the 2-D cells, and now have a basis for rationally designing manufacturing techniques for high-quality commercial lead iodide perovskite solar cells. This work was published in the journal *Advanced Materials*. – Kim Krieger

Read the entire *APS Science* article here.

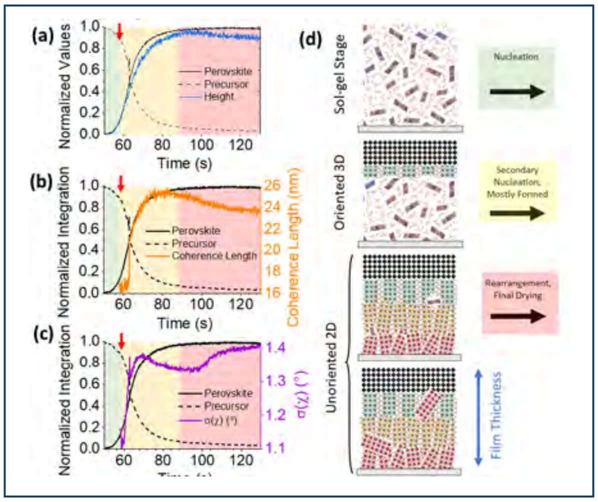
See: Justin M. Hoffman[1], Joseph Strzalka[2], Nathan C. Flanders[1], Ido Hadar[1], Shelby A. Cuthriell[1], Qingteng Zhang[2], Richard D. Schaller[1,2], William R. Dichtel[1], Lin X. Chen[1,2]*, and Mercouri G. Kanatzidis[1]**, "In Situ Grazing-Incidence Wide-Angle Scattering Reveals Mechanisms for Phase Distribution and Disorientation in 2D Halide Perovskite Films," Adv. Mater. **32,** 2002812 (2020). DOI: 10.1002/adma.202002812 Figure © 2020 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim

Author affiliations: [1]Northwestern University, [2]Argonne National Laboratory

Correspondence: * l-chen@northwestern.edu, ** m-kanatzidis@northwestern.edu

This work was supported by the Office of Naval Research (ONR) under grant N00014-20-1-2725. This project was supported in part by a fellowship award through the National Defense Science and Engineering Graduate (NDSEG) Fellowship Program, sponsored by the Air Force Research Laboratory (AFRL), the Office of Naval Research, and the Army Research Office (ARO). Part of this work was done through Dr. Hsinhan Tsai's user proposal (GUP-61829) at the Advanced Photon Source. N.C.F is partially supported by the Center for Light Energy Activated Redox Processes (LEAP), an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences under Award # DE-SC0001059. L.X.C. is partially support by the Solar Energy Photochemistry program of the U. S. DOE Office of Science-Basic Energy Sciences, through Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Dynamics & Structure Group 8-ID-E station



Testing the Mettle of Lithium Metal Batteries

Lithium-based batteries need improvement. Lithium-ion batteries are lightweight with high energy density, and therefore commonly used in phones, laptops, and electric vehicles. However, they have limited charge capacity, which is inherent to their structure and which restricts the range of electric cars and shortens how long we can talk on our phones before recharging. A newer type of battery, made of lithium metal instead of lithium ions, could hold much more charge. But first we need to solve key material challenges associated with these batteries. In particular, lithium metal batteries are prone to shorting and material damage when the lithium metal meets the ceramic parts of the battery. This can sharply limit the battery's useful life. A group of researchers used the APS to image the lithium-ceramic interface and explain why the damage occurs. Their research, which could lead to a new generation of much better batteries made of lithium metal, was published in *Applied Energy Materials*. – Kim Krieger

Read the entire *APS Science* article here.

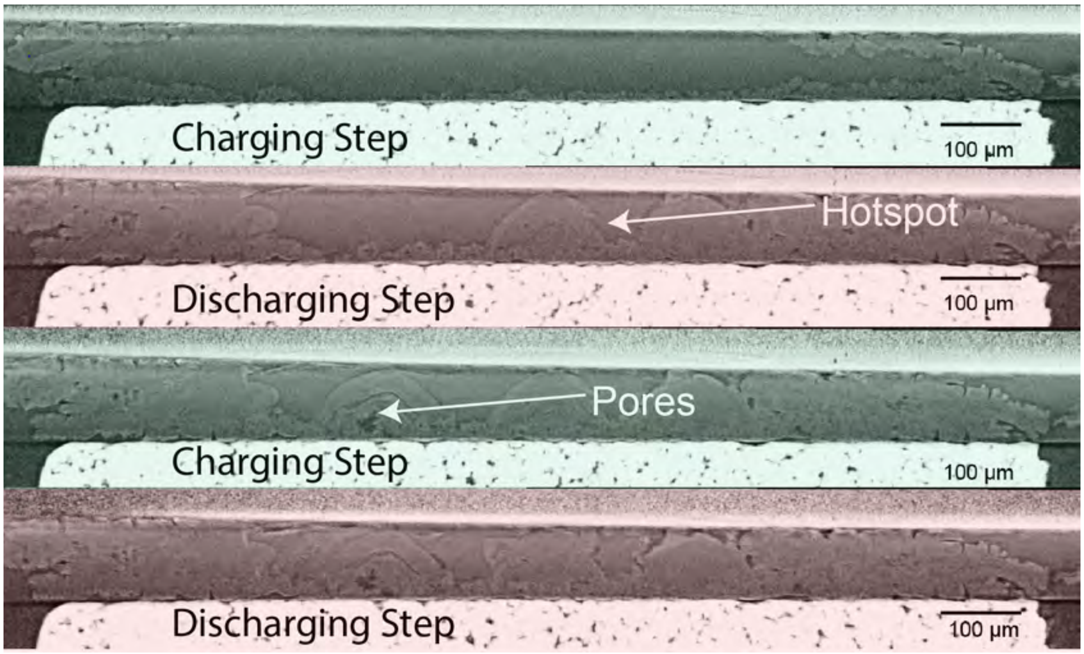
See: Marm B. Dixit[1], Ankit Verma[1], Wahid Zaman[1], Xinlin Zhong[1], Peter Kenesei[2], Jun Sang Park[2], Jonathan Almer[2], Partha P. Mukherjee[3], and Kelsey B. Hatzell[1]*, "Synchrotron Imaging of Pore Formation in Li Metal Solid-State Batteries Aided by Machine Learning," ACS Appl. Energy Mater. **3**, 9534 (2020). DOI: 10.1021/acsaem.0c02053

Author affiliations: [1]Vanderbilt University, [2]Argonne National Laboratory, [3]Purdue University

Correspondence: * kelsey.b.hatzell@vanderbilt.edu

K.B.H. and M.B.D. acknowledge support from National Science Foundation (NSF) Grant 1847029. K.B.H. and W.Z. acknowledge support from NSF Grant 1821573. P.P.M. and A.V. acknowledge financial support in part from a Scialog program sponsored jointly by Research Corporation for Science Advancement and the Alfred P. Sloan Foundation, which includes a grant to Purdue University by the Alfred P. Sloan Foundation. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Materials Physics & Engineering Group 1-ID-B,C,E station



Using Strain to Control an Iron-Based, High-Temperature Superconductor

The onset of superconductivity in nearly all high-temperature superconductors is a complex phenomenon that is linked to the appearance of certain electronic and magnetic orderings. More specifically, as the temperature of these materials is lowered, their electrons arrange into a nematic ordering reminiscent of that found in liquid crystal displays. Similarly, an antiferromagnetic ordering also typically arises at low temperatures. It appears that superconductivity in these compounds can be suppressed or enhanced by the strength of their nematic electron ordering and magnetism. In this study researchers set out to vary the nematic electron ordering in an iron-based superconductor by squeezing and stretching it, during experiments performed at low temperatures. The induced stresses caused distortions in the material's crystalline lattice that were precisely measured by x-ray diffraction experiments performed at the APS and published in *Nature Physics*. The experiments demonstrated the capability to dramatically promote or suppress superconductivity by applying small amounts of strain. The ability to vary a material's superconductivity using purely mechanical means is an important advance in the effort to harness superconductivity for use in a wide variety of applications. – Philip Koth

Read the entire *APS Science* article here.

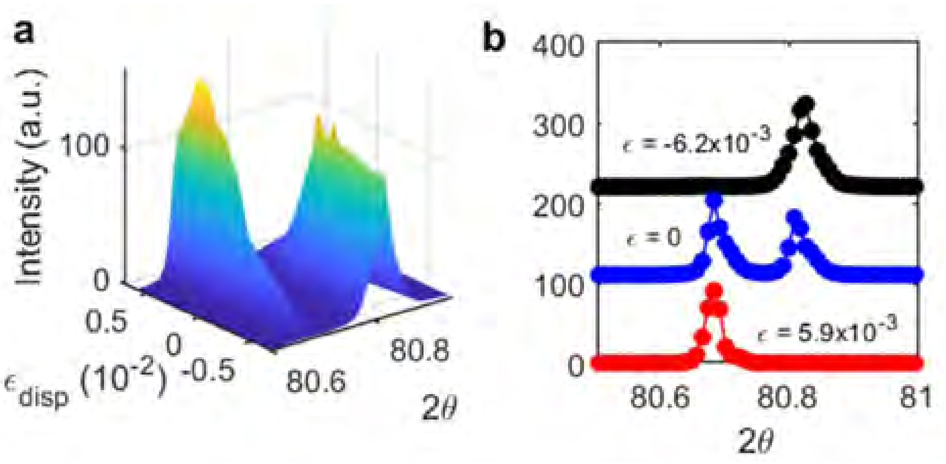
See: Paul Malinowski[1], Qianni Jiang[1], Joshua J. Sanchez[1], Joshua Mutch[1], Zhaoyu Liu[1], Preston Went[1], Jian Liu[2], Philip J. Ryan[3] Jong-Woo Kim[3], and Jiun-Haw Chu[1]*, "Suppression of superconductivity by anisotropic strain near a nematic quantum critical point," Nat. Phys. **16,** 1189 (December 2020). DOI: 10.1038/s41567-020-0983-9

Author affiliations: [1]University of Washington, [2]University of Tennessee, [3]Argonne National Laboratory

Correspondence: * jhchu@uw.edu

This work was mainly supported by National Science Foundation (NSF) MRSEC at UW (DMR-1719797) and the Gordon and Betty Moore Foundation's EPiQS Initiative, grant GBMF6759 to J.-H.C. The development of strain instrumentation is supported as part of Programmable Quantum Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences under award DE-SC0019443. The integration of x-ray diffraction with *in situ* strain is supported by the Air Force Office of Scientific Research Young Investigator Program under grant FA9550-17-1-0217 and the Defense University Research Instrumentation Program Award FA9550-19-1-0180. J.L. acknowledges support from the NSF under grant no. DMR- 1848269. J.-H.C. acknowledges the support of the David and Lucile Packard Foundation and the State of Washington-funded Clean Energy Institute. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Magnetic Materials Group 6-ID-B,C station



Some New and Unexpected Wrinkles in a Spin-Triplet Superconductor Under Pressure

A practical quantum computer is the next major goal for computer science, offering processing speeds impossible for classical systems through the use of "qubits" instead of conventional bits. Many different technological pathways toward this goal are being pursued, some of them involving the phenomenon of superconductivity. Harnessing such an unconventional property of matter requires unconventional materials, however, so the quest for novel superconducting materials is vital, and sometimes leads to unexpected places, such as the compound uranium ditelluride (UTe_2). Although known for decades, UTe_2 was only recently found to harbor an unusual flavor of superconductivity called "spin-triplet" topological superconductivity that might facilitate quantum computers. Researchers using x-ray beams from the APS found that UTe_2 reveals some further intriguing characteristics when subjected to applied pressures. A greater understanding of its unusual qualities will clearly be needed before it can be determined whether it's a viable candidate for quantum computing technology, but further detailed studies no doubt promise more surprising discoveries and yet-unknown potential. The work appeared in *Science Advances*. — Mark Wolverton

Read the entire *APS Science* article here.

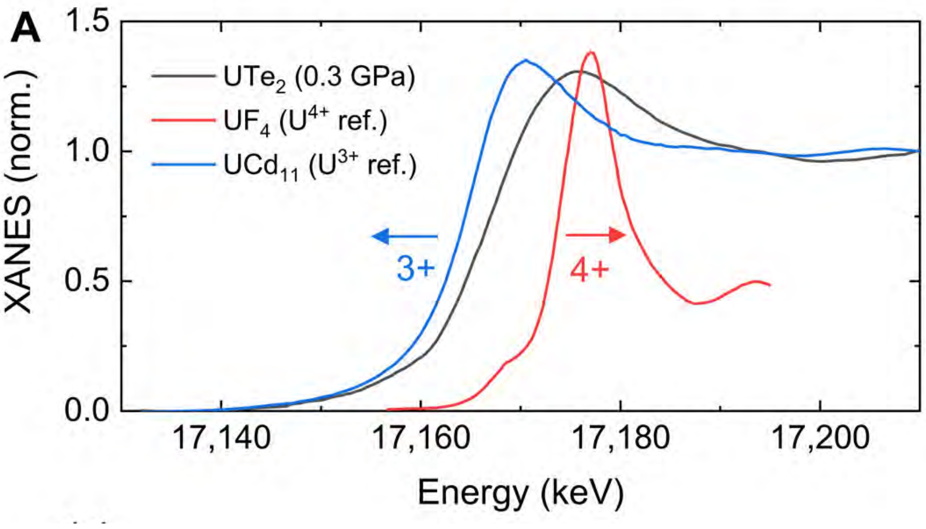
See: S. M. Thomas[1*], F. B. Santos[1,2], M. H. Christensen[3], T. Asaba[1], F. Ronning[1], J. D. Thompson[1], E. D. Bauer[1], R. M. Fernandes[3], G. Fabbris[4], and P. F. S. Rosa[1], "Evidence for a pressure-induced antiferromagnetic quantum critical point in intermediate-valence UTe_2," Sci. Adv. **6,** eabc8709 (14 October 2020). DOI: 10.1126/sciadv.abc8709 Figure © 2020 American Association for the Advancement of

Author affiliations: [1]Los Alamos National Laboratory, [2]Universidade de Sao Paulo (EEL-USP), [3]University of Minnesota, [4]Argonne National Laboratory

Correspondence * smthomas@lanl.gov

The experimental work at Los Alamos was performed under the auspices of the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences, Division of Materials Science and Engineering, under project "Quantum Fluctuations in Narrow-Band Systems." F. B. S. was supported by FAPESP under grant nos. 2016/11565-7 and 2018/20546-1. Theory work (M.H.C. and R.M.F.) was supported by the U.S. DOE Office of Science-Basic Energy Sciences, Materials Science and Engineering Division, under award no. DE-SC0020045. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Magnetic Materials Group 4-ID-D station



Unraveling the Secrets of Twisted Crystals

An ideal crystal, by definition, is made up of a series of identical repeating units forming a lattice in all directions. But at least 25% of molecular crystals that grow from the melt are twisted, screwing themselves into unusual shapes, and breaking that symmetry. One international group of scientists used the APS to help uncover the mechanism that causes a particular crystal to twist. The scientists performed high-resolution synchrotron powder x-ray diffraction at the APS, which allowed the team to identify structural disorder at the scale of 10s of nanometers. The team used the data they got from the diffraction study along with other data obtained through cryo-transmission electron microscopy. Combining the two allowed them to identify the crystallographic orientation of the lamellae. Their results were published in the journal *Angewandte Chemie International Edition*.— Neil Savage

Read the entire *APS Science* article here.

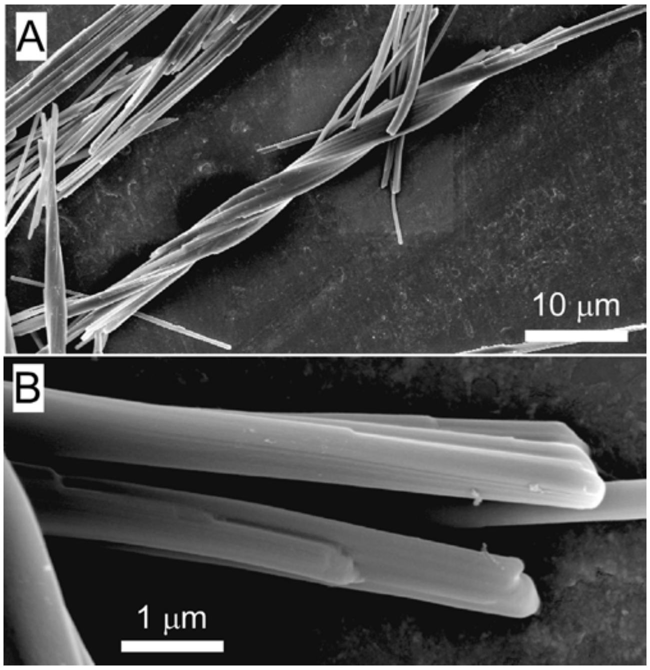
See: Alexander G. Shtukenberg[1*], Ran Drori[2***], Elena V. Sturm[3], Netta Vidavsky[4], Asaf Haddad[5], Jason Zheng[1], Lara A. Estroff[6], Haim Weissman[5], Sharon G. Wolf[5], Eyal Shimoni[5], Chao Li[1], Noalle Fellah[1], Efi Efrati[5****], and Bart Kahr[1**], "Crystals of Benzamide, the First Polymorphous Molecular Compound, Are Helicoidal," Angew. Chem. Int. Ed. **59**, 14593 (2020). DOI: 10.1002/anie.202005738

Author affiliations: [1]New York University, [2]Yeshiva University, [3]University of Konstanz, [4]Ben-Gurion University of the Negev, [5]Weizmann Institute of Science, [6]Cornell University

Correspondence: * shtukenberg@mail.ru, ** bart.kahr@nyu.edu, *** rdrori@yu.edu, **** efi.efrati@weizmann.ac.il

This work was primarily supported by the New York University Materials Research Science and Engineering Center (MRSEC) program of the National Science Foundation (NSF) under award number DMR-1420073. Funding support was also provided by the NSF (DMR-1608374, with a supplement through the United States–Israel Binational Science Foundation, DMR-BSF 2015670). This work made use of the Cornell Center for Materials Research Shared Facilities which are supported through the NSF MRSEC program (grant DMR-1719875). We are grateful to Lynn W. Ribaud and Saul D. Lapidus for providing assistance in collecting synchrotron powder diffraction data at the APS. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Structural Science Group 11-BM-B station



Revealing the Source of Unusually High Strength in Sintered Aluminum

A team of researchers set out to determine the factors behind the unusually high strength of certain sintered metals. Sintering (making a powdered material coalesce into a solid or porous mass by heating it—and usually also compressing it—without liquefaction) can produce intricate forms with unusual properties. Generally speaking, the strength of a sintered object increases as its grain size decreases. However, the strengths of some very fine-grained sintered materials are much higher than theory predicts. To understand the source of this unexpected strength, the researchers used a technique called differential aperture x-ray microscopy (DAXM) to probe sintered aluminum samples possessing grain sizes of either 5 μm)or 1 μm. The DAXM experiments, carried out at the APS, revealed the dislocation densities within the grains. Dislocations are crystalline defects that contribute to the strength of sintered materials. The researchers found that the dislocation density for the sample featuring 5-μm-size grains could theoretically explain its exceptional strength. In contrast, dislocation densities in the 1-μm grain sample were much too small to account for its strength, implying that another factor must be responsible. These insights, published in the journal *Materials Letters*, improve the overall understanding of fine grain-sized metals and should ultimately enable improved control of their properties. — Philip Koth

Read the entire *APS Science* article here.

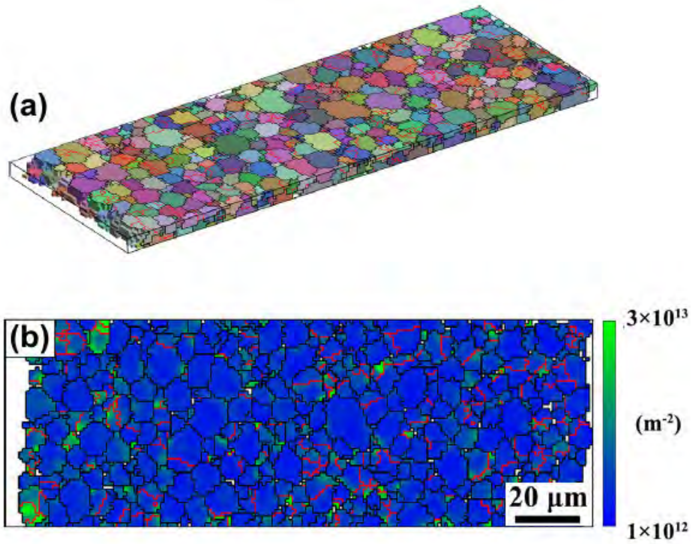
See: C.L. Zhang[1], A. Godfrey[1*], Y. Zhang[2], G.L. Wu[3], R. Xu4, W. Liu[4], and D. Juul Jensen[2], "Dislocation density in fine grain-size spark-plasma sintered aluminum measured using high brightness synchrotron radiation," Mat. Lett. **269**, 127653 (2020). DOI: 10.1016/j.matlet.2020.127653 Figure © 2020 Elsevier B.V. All rights reserved.

Author affiliations: [1]Tsinghua University, [2]Technical University of Denmark, [3]Chongqing University, [4]Argonne National Laboratory

Correspondence: * awgodfrey@mail.tsinghua.edu.cn

Financial support from the National Natural Science Foundation of China (project numbers 51471095 and 51671113) is gratefully acknowledged. Y.Z. and D.J.J. acknowledge support from the European Research Council (ERC grant agreement No.788567) for part of the work. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357.

XSD Surface Scattering & Diffraction Group 34-ID-E station



A Cold-Spray Solution for AM Metal Fatigue

Additive manufacturing (AM) techniques of various forms are becoming ever more prominent and important in many industries, thanks to their efficiency, versatility, and economy compared to traditional fabrication methods. Before AM can fully complement or even supplant more established manufacturing techniques, however, some persistent problems need to be addressed, such as the increased fragility and reduced structural integrity of some AM-fabricated products. One possible answer is the combination of metal AM technologies with cold spraying (CS), in which a supersonic jet of fine powder is used to coat an object to repair or protect it. Already a popular technique in conventional manufacturing, CS also promises to enhance the durability of AM-produced metal parts, especially those with complex geometries subject to repeated stresses and loading. To investigate the possibilities, experimenters examined the behavior of CS-coated, AM-fabricated stainless steel under cyclical loading using the APS. The work, published in the journal *Additive Manufacturing*, shows that the integration of additive manufacturing with the cold spray coating process can offer an intriguing way to overcome such limitations and further increase the versatility of additive manufacturing techniques. – Mark Wolverton

Read the entire *APS Science* article here.

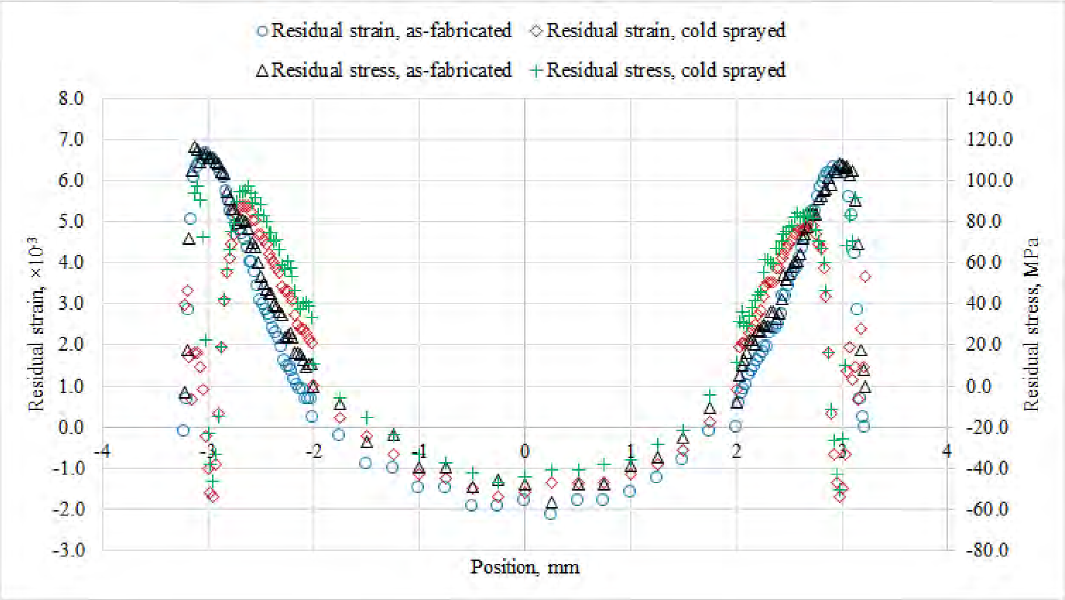
See: Davoud M. Jafarlou[1], Gehn Ferguson[2], Kyle L. Tsaknopoulos[3], Andrew Chihpin Chuang[4], Aaron Nardi[2], Danielle Cote[3], Victor Champagne[2], and Ian R. Grosse[1]*, “Structural integrity of additively manufactured stainless steel with cold sprayed barrier coating under combined cyclic loading,” Additive Manu. 35, 101338 (2020).
DOI: 10.1016/j.addma.2020.101338

Author affiliations: [1]University of Massachusetts, [2]CCDC Army Research Laboratory, [3]Worcester Polytechnic Institute, [4]Argonne National Laboratory

Correspondence: * grosse@ecs.umass.edu

This research was accomplished through a cooperative research agreement with the U.S. Army Research Laboratory, Contract: W911NF-15-2-0024, “Intelligent Processing of Materials by Design.” This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

XSD Materials Physics & Engineering 6-BM-A,B station



Electronic and Magnetic Materials

A Strain-Induced Charge Carrier-Type Crossover in a Complex Oxide

Epitaxial thin films of lanthanum cobaltite ($LaCoO_{3-\delta}$) under tensile strain—the elongation of a material via application of a tensile force—are ferromagnetic, whereas the bulk material is not. No clear understanding of this surprising phenomenon has yet emerged. Also, while the magnetism of this material has been heavily studied, relatively little attention has been paid to electronic transport, due to the insulating nature of the strain-stabilized ferromagnetic state. Here, researchers grew epitaxial $LaCoO_{3-\delta}$ films on a variety of substrates that induced lattice mismatches ranging from 1.4% of compression to 2.5% of tensile strain. They then studied the structure, magnetism, and electronic transport of the films using synchrotron x-ray diffraction at the APS as well as an array of other techniques; the results were published in *Physical Review Materials*. Ferromagnetism was observed under tension, polarized neutron reflectometry indicating a relatively uniform magnetization depth profile. Electrically, the films were found to have similar semiconducting properties to bulk $LaCoO_{3-\delta}$. Hall effect measurements, however, revealed a striking and unanticipated inversion of the majority carrier type, from p-type under compression to n-type under tension. This can be understood based on strain-induced orbital population changes, exposing a previously undetected link between magnetism and electronic transport in thin films of this material. — Chris Palmer

Read the entire *APS Science* article here.

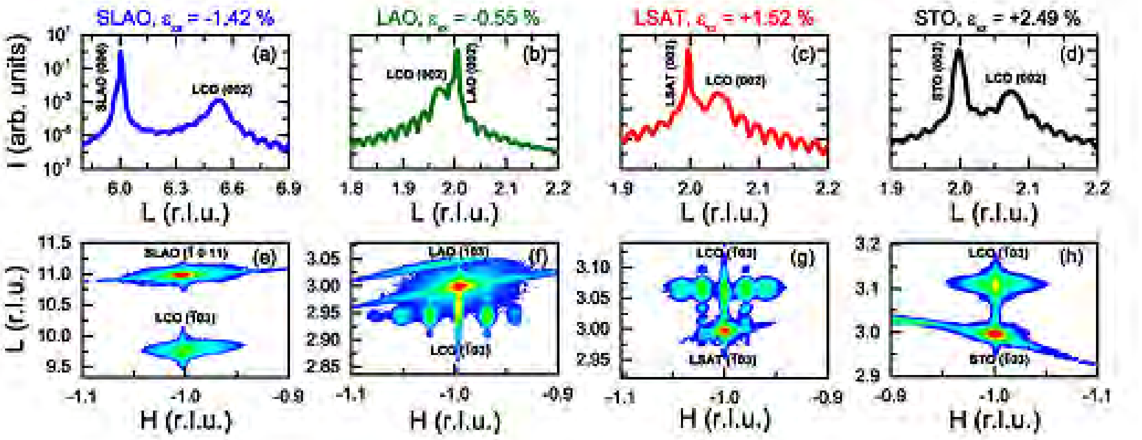
See: Vipul Chaturvedi[1], Jeff Walter[1, 2], Arpita Paul[1], Alexander Grutter[3], Brian Kirby[3], Jong Seok Jeong[1], Hua Zhou[4], Zhan Zhang[4], Biqiong Yu[1], Martin Greven[1], K. Andre Mkhoyan[1], Turan Birol[1], and Chris Leighton[1]*, "Strain-induced majority carrier inversion in ferromagnetic epitaxial $LaCoO_{3-\delta}$ thin films," Phys. Rev. Mater. **4**, 034403 (2020). DOI:10.1103/PhysRevMaterials.4.034403 Figure ©2020 American Physical Society

Author affiliations: [1]University of Minnesota, [2]Augsburg University, [3]NIST, [4]Argonne National Laboratory

Correspondence: * leighton@umn.edu

This work was supported primarily by the U.S. Department of Energy (DOE) through the University of Minnesota (UMN) Center for Quantum Materials under Grant No. DESC- 0016371. Computational work by A.P. was supported by the National Science Foundation (NSF) through the UMN MRSEC under Award No. DMR-1420013. Parts of this work were performed in the Characterization Facility, UMN, which receives partial support from the NSF through the MSREC. This research used resources of the APS, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357.

XSD Surface Scattering & Microdiffraction Group 33-ID-D,E station



Revealing the Mechanism of an Otherworldly Metal-Insulator Transition

Hexagonal iron monosulfide (h-FeS), also known as troilite (Fig.1), isn't exactly a material one encounters every day. Mostly it's found in meteorites originating from the Moon or Mars, and it has also been identified on those worlds *in situ* by astronauts and space probes, although it was first discovered in the Earth's crust. But aside from its exotic origins, it features an intriguing crystal structure with multiferroic properties that make it a leading candidate for new technologies such as spintronics. Researchers used the APS to investigate that potential by using high-brightness x-rays to study the tightly-coupled interplay of the lattice, magnetic, and electronic degrees of freedom in h-FeS, which can provide insight into the possible design and tailoring of multiferroic and spintronic materials. The work was published in *Nature Physics*. — Mark Wolverton

Read the entire *APS Science* article here.

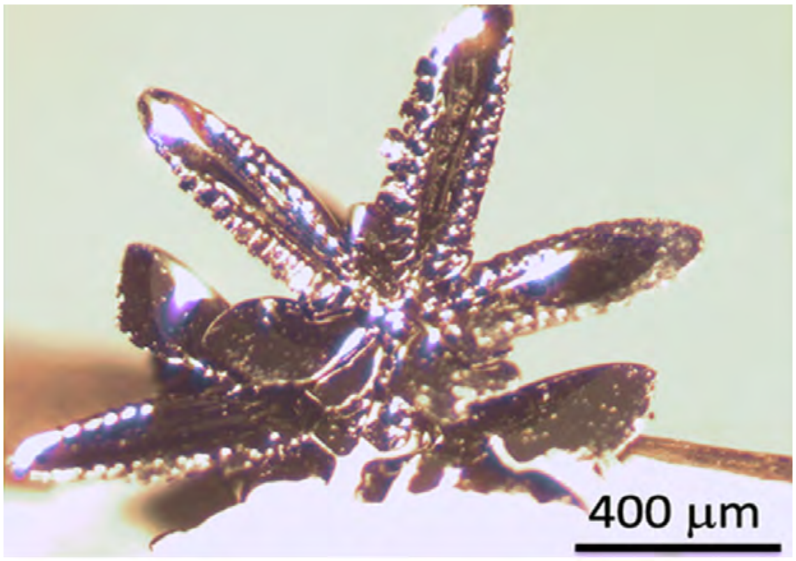
See: Dipanshu Bansal[1*], Jennifer L. Niedziela[2], Stuart Calder[2], Tyson Lanigan-Atkins[1], Ryan Rawl[3], Ayman H. Said[4], Douglas L. Abernathy[2], Alexander I. Kolesnikov[2], Haidong Zhou[3], and Olivier Delaire[1**], "Magnetically driven phonon instability enables the metal–insulator transition in h-FeS," Nat. Phys. **16**, 669 (June 2020).
DOI: 10.1038/s41567-020-0857-1

Author affiliations: [1]Duke University, [2]Oak Ridge National Laboratory, [3]University of Tennessee, [4]Argonne National Laboratory

Correspondence: * dipanshu.bansal@duke.edu, ** olivier.delaire@duke.edu

Neutron and x-ray scattering measurements were supported by the US Department of Energy (DOE) Office of Science-Basic Energy Sciences, Materials Sciences and Engineering Division, under the Early Career award no. DE-SC0016166. Analysis of results and writing of the manuscript was supported by the U.S. DOE Office of Science-Basic Energy Sciences, Materials Sciences and Engineering Division, under award no. DE-SC0019978. H.Z. (sample synthesis) thanks the support from the National Science Foundation NSF-DMR-1350002. The use of Oak Ridge National Laboratory's Spallation Neutron Source and High Flux Isotope Reactor was sponsored by the Scientific User Facilities Division, Basic Energy Sciences, U.S. DOE. Theoretical calculations were performed using resources of the National Energy Research Scientific Computing Center, a U.S. DOE Office of Science User Facility supported by the Office of Science of the U.S. DOE under contract no. DE-AC02-05CH11231. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Inelastic X-ray & Nuclear Resonant Scattering Group 30-ID-B,C station



Probing Thin-Film Superconductivity at the Picoscale

For nearly a decade, scientists have investigated the high-temperature superconductivity of an iron-based thin film consisting of a single layer of iron selenide (FeSe) on a substrate of strontium titanate ($SrTiO_3$). This FeSe/$SrTiO_3$ material becomes superconducting at the highest temperature of any thin film. Past research indicated that the interface between the FeSe monolayer and its substrate plays a crucial role in the material's remarkable superconducting properties. In spite of the importance of this interface, there has been uncertainty about many of its fundamental features, such as the distance between the FeSe monolayer and the substrate. To determine this and other key features, researchers in this study from Yale University with their colleagues employed high-brightness x-rays at the APS to help resolve the interfacial structure of FeSe/$SrTiO_3$ samples at the picoscale, equivalent to one-thousandth of a nanometer. It is anticipated that the new data about the interfacial landscape, published in the journal *Science Advances*, will guide development of refined theoretical models, not only of superconductivity in the FeSe/$SrTiO_3$ system but of thin-film superconductivity in general. Understanding the exact mechanisms responsible for thin-film superconductivity is essential for applying these materials to practical high-temperature superconducting devices. – Philip Koth

Read the entire *APS Science* article here.

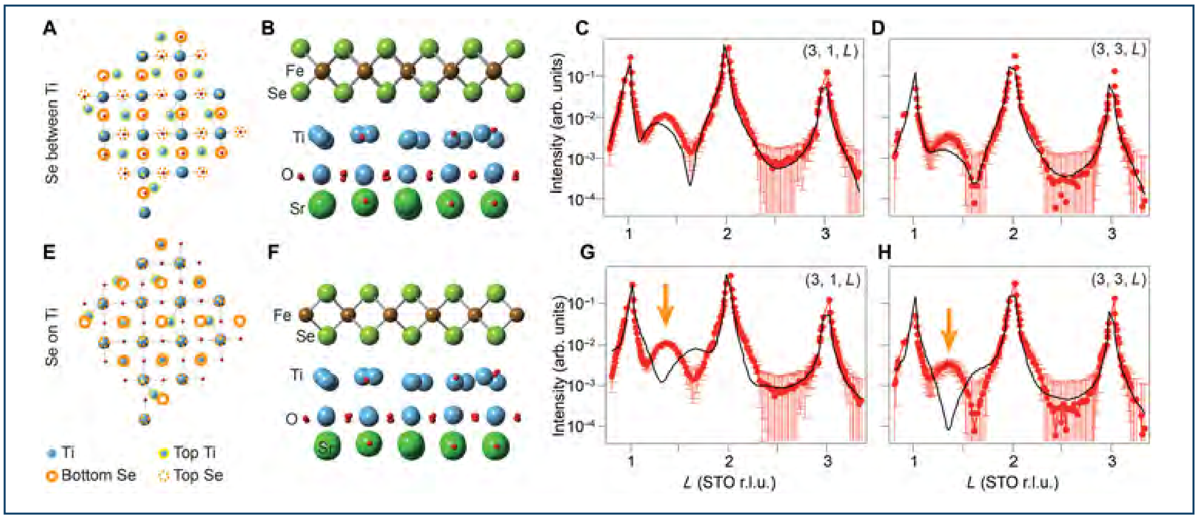
See: Rui Peng[1,2*], Ke Zou[1‡], M. G. Han[4], Stephen D. Albright[1], Hawoong Hong[4], Claudia Lau[1], H. C. Xu[1,2], Yimei Zhu[3], F. J. Walker[1**], and C. H. Ahn[1***], "Picoscale structural insight into superconductivity of monolayer FeSe/$SrTiO_3$," Sci. Adv. **6**, eaay4517 (8 April 2020). DOI: 10.1126/sciadv.aay4517

Author affiliations: [1]Yale University, [2]Fudan University, [3]Brookhaven National Laboratory, [4]Argonne National Laboratory ‡Present address: University of British Columbia

Correspondence: * pengrui@fudan.edu.cn, ** fred.walker@yale.edu,*** charles.ahn@yale.edu

This work was supported by AFOSR grant FA9550-15-1-0472. The work at Brookhaven National Laboratory was supported by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences, under contract no.DESC0012704. TEM sample preparation using FIB was performed at the Center for Functional Nanomaterials, Brookhaven National Laboratory. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Surface Scattering & Microdiffraction Group 33-ID-D,E station



Ultrafast X-rays Track Charge Flows in a Promising Photovoltaic Material

A class of materials known as lead halide perovskites (LHPs) show remarkable potential for use in optoelectronic applications. Given the urgency to derive more of our energy renewably, LHPs hold out great promise as materials for thin-film solar cells that are both highly efficient and inexpensive to produce. Although LHPs have been extensively studied, the exact process of how an incident photon is converted into an electrical charge and then migrates within the material has remained open to debate. To resolve this mystery, researchers performed x-ray transient absorption (XTA) on two different types of thin-film LHPs. In experiments carried out at the APS, a team of researchers from two DOE national laboratories used XTA to detect the creation and movement of electrical carriers within the thin films. The experiments revealed exactly how the crystalline structure of thin-film LHP is excited by incident photons, as well as how the resulting charged regions behave within the material. The experiments also showed that the photo-generated charges behaved differently in the two LHPs. These direct observations of photo-induced charges and their movement within thin-film LHPs should improve the theoretical framework used to describe these materials, thereby hastening their practical use for solar power and other applications. The results were published in *The Journal of Physical Chemistry Letters*. — Philip Koth

Read the entire *APS Science* article here.

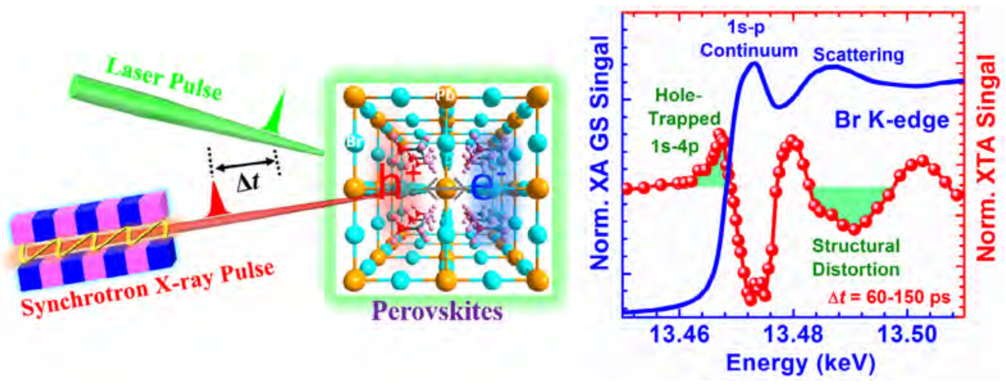
See: Cunming Liu[1]*, Hsinhan Tsai[2], Wanyi Nie[2], David Gosztola[1], and Xiaoyi Zhang[1]**, “Direct Spectroscopic Observation of the Hole Polaron in Lead Halide Perovskites,” J. Phys. Chem. Lett. **11**, 6256 (2020).
DOI: 10.1021/acs.jpclett.0c01708 Figure © 2020 American Chemical Society

Author affiliations: [1]Argonne National Laboratory, [2]Los Alamos National Laboratory

Correspondence: * lcmingsc@gmail.com, ** xyzhang@anl.gov

This work was supported by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences, under Contract DE-AC02-06CH11357. The laser system at 11-ID-D of the APS was funded through New Facility and Mid-scale Instrumentation grants to the Chemical Sciences and Engineering Division of Argonne National Laboratory (ANL) (PI, Lin X. Chen). W.N. acknowledges the Director’s quantum initiative funding from Laboratory Directed Research Directions (LDRD) program at Los Alamos National Laboratory (LANL). H.T. acknowledges the financial support from a Robert Oppenheimer (JRO) Distinguished Postdoc Fellowship at LANL. This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the DOE Office of Science by LANL (Contract 89233218CNA000001). Use of the Center for Nanoscale Materials, an Office of Science user facility, was supported by the U.S. DOE Office of Science-Basic Energy Sciences, under Contract No. DE-AC02-06CH11357. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357.

XSD Time Resolved Research Group 11-ID-D station



Frustrated Antiferromagnet Jarosite Collapses under Pressure

The antiferromagnetic mineral jarosite, $KFe_{3(}OH)_6(SO4)_2$, has been intensely studied for several decades, in part because its high-spin Fe^{3+} ions are arrayed on a corner-sharing triangular (kagomé) lattice, which ensures magnetic frustration. In fact, jarosite has one of the most highly frustrated two-dimensional lattices known to exist. Frustrated magnets are materials whose localized magnetic moments, or spins, interact through competing interactions that cannot be simultaneously satisfied, creating the possibility that lattice manipulation can produce exotic magnetic phases of commercial value. Extensive theoretical work has hinted at a rich phase diagram for frustrated kagomé antiferromagnets like jarosite, but experimental evidence remained lacking until very recently. Since applied high pressure shortens interatomic distances, the technique offers a route to accessing magnetic variants of frustrated parent lattices that may be difficult to access synthetically at ambient conditions. For this reason, researchers working at the APS and the National Synchrotron Light Source II investigated the pressure-temperature phase diagram of jarosite at pressures up to 121 GPa. Upon finding that jarosite's antiferromagnetic magnetic order unexpectedly disappeared at ~45 GPa, they went on to probe for an explanation of this surprising behavior by characterizing the structural, electronic, and magnetic changes in jarosite through the phase transition using a suite of in situ diamond anvil cell techniques. Their results were published in *Physical Review Letters*.

– Vic Comello

Read the entire *APS Science* article here.

See: Ryan A. Klein[1], James P. S. Walsh[1], Samantha M. Clarke[2], Zhenxian Liu[3], E. Ercan Alp[4], Wenli Bi[5], Yue Meng[4], Alison B. Altman[1], Paul Chow[4], Yuming Xiao[4], M. R. Norman[4**], James M. Rondinelli[1***], Steven D. Jacobsen[1****], Danilo Puggioni[1*****], and Danna E. Freedman[1*], "Pressure-Induced Collapse of Magnetic Order in Jarosite," Phys. Rev. Lett **125**, 077202 (2020). DOI: 10.1103/PhysRevLett.125.077202

Author affiliations: [1]Northwestern University, [2]Lawrence Livermore National Laboratory, [3]University of Illinois at Chicago, [4]Argonne National Laboratory, [5]University of Alabama at Birmingham

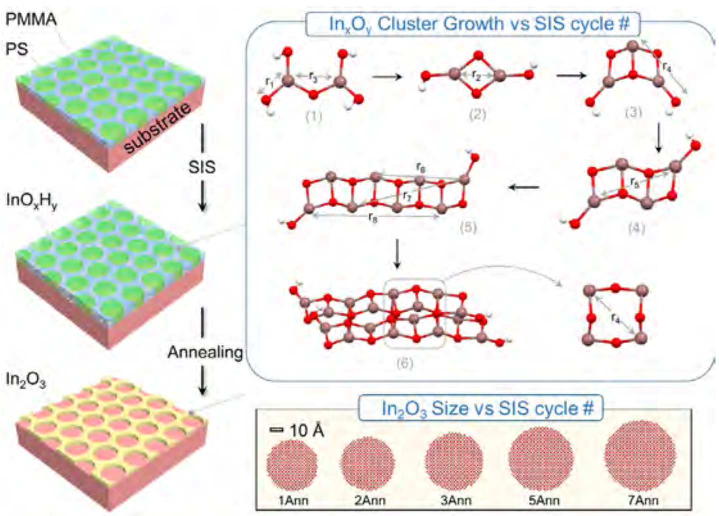
Correspondence: * danna.freedman@northwestern.edu, ** norman@anl.gov, *** jrondinelli@northwestern.edu, **** s-jacobsen@northwestern.edu, ***** Danilo Puggioni*****

Creating and understanding magnetic frustration in synthetically derived materials was supported by the Army Research Office (W911NF1810006). Initial work to develop high-pressure methodologies was supported by the Air Force Office of Scientific Research (FA9550-17-1-0247). S. D. J. acknowledges support from the Capital/U.S. Department of Energy (DOE) Alliance Center (CDAC) for beamtime at HPCAT-XSD, the National Science Foundation (NSF) (EAR-1452344), and the David and Lucile Packard Foundation. D. P. and J. M. R. acknowledge the Army Research Office under Grant No. W911NF-15-1-0017 for financial support and the Department of Defense High Performance Computing Modernization Program (DOD-HPCMP) for computational resources. W. B. was partially supported by the Consortium for Materials Properties Research in Earth Sciences (COMPRES). M. R. N. is supported by the Materials Sciences and Engineering Division, Basic Energy Sciences, Office of Science, U.S. DOE. Part of this work was performed under the auspices of the DOE by Lawrence Livermore National Security, LLC, under Contract No. DE-AC52-07NA27344. The gas loading was also partially supported by COMPRES under the NSF Cooperative Agreement EAR-1634415. HPCAT-XSD operations are supported by the DOE-National Nuclear Security Administration's Office of Experimental Sciences. The National Science Foundation—Earth Sciences (EAR-1634415) and Department of Energy—Geosciences (DE-FG02-94ER14466) support GeoSoilEnviroCARS. Experiments at GeoSoilEnviroCARS station 13-BM-C were conducted under the Partnership for Extreme Crystallography (PX^2), which is also supported by COMPRES. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

HPCAT-XSD 16-ID-B, 16-ID-D, and 16-BM-D stations; GSECARS 13-BM-C station; XSD Inelastic X-ray & Nuclear Resonant Scattering Group 3-ID-B,C,D station

Soft Materials and Liquids

Tracking the Early Stages of Sequential Infiltration Synthesis



Sequential infiltration synthesis (SIS) is a rapid and efficient method for forming inorganic solids within polymers via alternating exposure to vapor-phase chemical precursors. The resulting hybrid of organic/inorganic materials can then be annealed or etched to remove the organic matrix and yield wholly inorganic materials with exquisite nanoscale morphological complexity inherited from the initial organic polymer template. Potential applications extend to virtually all technologies in which periodic nanomaterial structures are desirable, including optoelectronics, sensors, membranes, photonic crystals, dielectric materials, and electronics. However, the earliest stages of SIS growth remain a mystery, including the atomic structure of nuclei and the evolution of local coordination environments, before and after polymer template removal. Researchers used synchrotron x-ray analysis at the APS to reveal the structural evolution of inorganic cluster growth and crystallization resulting from SIS in polymeric templates. They found that early SIS cycles resulted in I_nO_xHy cluster growth with high aspect ratios (i.e., a length many times that of their width). Additional SIS cycles resulted in the formation of a three-dimensional network. Annealing the mixed inorganic/polymer films in air removed the PMMA template and consolidated the as-grown clusters into cubic $_In_{2O}3$ (indium oxide) nanocrystals. Additional structural details depended on SIS cycle number. These results, published in the journal *ACS Nano*, suggest I_nO_xHy clusters can be modeled as multinuclear clusters with bonding patterns related to those in $_In_2O3$. In(O$_H$)3 (indium hydroxide) crystal structures, meanwhile, suggested that SIS may be an efficient route to producing 3D arrays of discrete-atom-number clusters. In addition, this new approach to characterizing structural growth within the polymer provides fundamental insights into the electrical conductivity of nanoscale electrodes. The APS Upgrade Project, when completed, will enable the study of amorphous and nanocrystalline thin films during formation with unprecedented combination of spatial and structural resolution at 11-ID-D. — Chris Palmer

Read the entire *APS Science* article here.

See: Xiang He[1], Ruben Z. Waldman[2], David J. Mandia[1], Nari Jeon[1], Nestor J. Zaluzec[1], Olaf J. Borkiewicz[1], Uta Ruett[1], Seth B. Darling[1, 2], Alex B. F. Martinson[1]* and David M. Tiede[1]**, "Resolving the Atomic Structure of Sequential Infiltration Synthesis Derived Inorganic Clusters," ACS Nano **14**, 14846 (2020). DOI: 10.1021/acsnano.0c03848 Figure © 2020 American Chemical Society

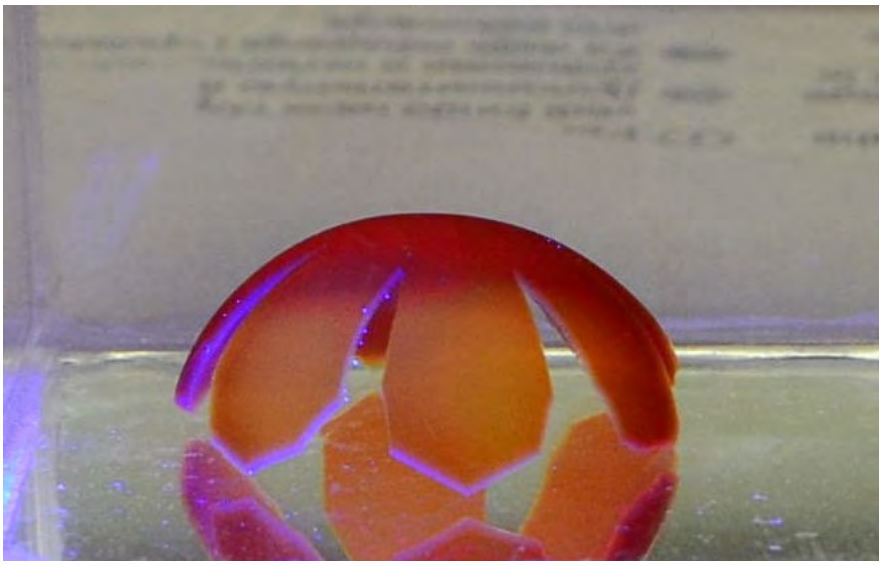
Author affiliations: [1]Argonne National Laboratory, [2]The University of Chicago

Correspondence: * martinson@anl.gov, ** tiede@anl.gov

This work was funded by the Advanced Materials for Energy-Water Systems (AMEWS) Center, an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences. This research used resources of the Advanced Photon Source and the Center for Nanoscale Materials, both U.S. DOE Office of Science User Facilities operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

XSD Structural Science Group 11-ID-B station & XSD Spectroscopy Group 20-BM-B station

Bringing to Light the Polymers that Mimic Biomolecular Machines



A growing amount of research has been geared toward creating synthetic soft matter that produces mechanical work through motion in response to external stimuli. Materials like these are inspired by biological tissues and could eventually be used as artificial muscles in many applications, such as manufacturing and chemical production, or even drug delivery. Researchers have explored several different forms of external stimuli for these applications, such as heat, pH (the relative amount of free hydrogen and hydroxyl ions), and redox reactions, but light is particularly attractive because of its non-invasive nature and the possibility of localizing the stimulus. An important gap in this field could be filled by the use of supramolecular polymers that can spontaneously reconfigure by forming noncovalent bonds, similar to natural materials such as cytoskeletal filaments. Hybrid systems in which monomers of these supramolecular polymers are chemically bonded to stimuli-responsive covalent polymer networks could have advantages such as strengthening and providing structure for the covalent polymers. Users of the APS from Northwestern University have accomplished this goal, reporting in *Nature Materials* the synthesis of a supramolecular-covalent hybrid polymer that contracts when exposed to visible light. Consequently, films and objects made of this material move when illuminated, exhibiting actions such as bending, crawling, or rotating.

— Christen Brownlee

Read the entire *APS Science* article here.

See: Chuang Li, Aysenur Iscen, Hiroaki Sai, Kohei Sato, Nicholas A. Sather, Stacey M. Chin, Zaida Álvarez, Liam C. Palmer, George C. Schatz*, and Samuel I. Stupp**, “Supramolecular–covalent hybrid polymers for light-activated mechanical actuation,” Nat. Mater. **19**, 900 (August 2020). DOI: /10.1038/s41563-020-0707-7

Author affiliation: Northwestern University

Correspondence: * g-schatz@northwestern.edu, ** s-stupp@northwestern.edu

This work was supported by the Center for Bio-Inspired Energy Science (CBES), an Energy Frontiers Research Center (EFRC) funded by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences under award number DE-SC0000989. Z. A. received postdoctoral support from the Beatriu de Pinós Fellowship 2014 BP A 00007 (Agència de Gestió d’Ajust Universitaris i de Recerca, AGAUR) and the Paralyzed Veterans of America (PVA) (grant no. PVA17_RF_0008). DND-CAT is supported by Northwestern University, The Dow Chemical Company, and DuPont de Nemours, Inc. X-ray scattering data was collected using an instrument funded by the National Science Foundation under Award Number 0960140. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

DND-CAT 5-ID-B,C,D station

A Simple Switch in Lanthanide Separations

Rare earths are a set of 17 elements, 15 lanthanides plus yttrium and scandium, which have an outsized importance in several industrial sectors, notably as catalysts in the refining of crude oil into gasoline products. These metals have also been widely used as alloys to impart strength and hardness to other metals. More recently, the demand for lanthanide elements has been rising due to their use in other industrial applications, such as permanent magnets used in electric vehicles and wind turbines. All these applications have driven research into the efficient separation of lanthanides from their mixtures. The main technological barrier in obtaining lanthanides is chemically separating individual rare-earth elements from each other. Solvent extraction has been the preeminent industrial process for the separation of lanthanides, but its mechanisms are not clearly understood. In this study, published in the journal *Nanoscale*, researchers used small angle x-ray scattering at the APS to investigate the correlation between extraction performance and the structure of the complex fluids and interfaces involved in extraction. Their results can be used to more efficiently extract the desired lanthanides. – Chris Palmer

Read the entire *APS Science* article here.

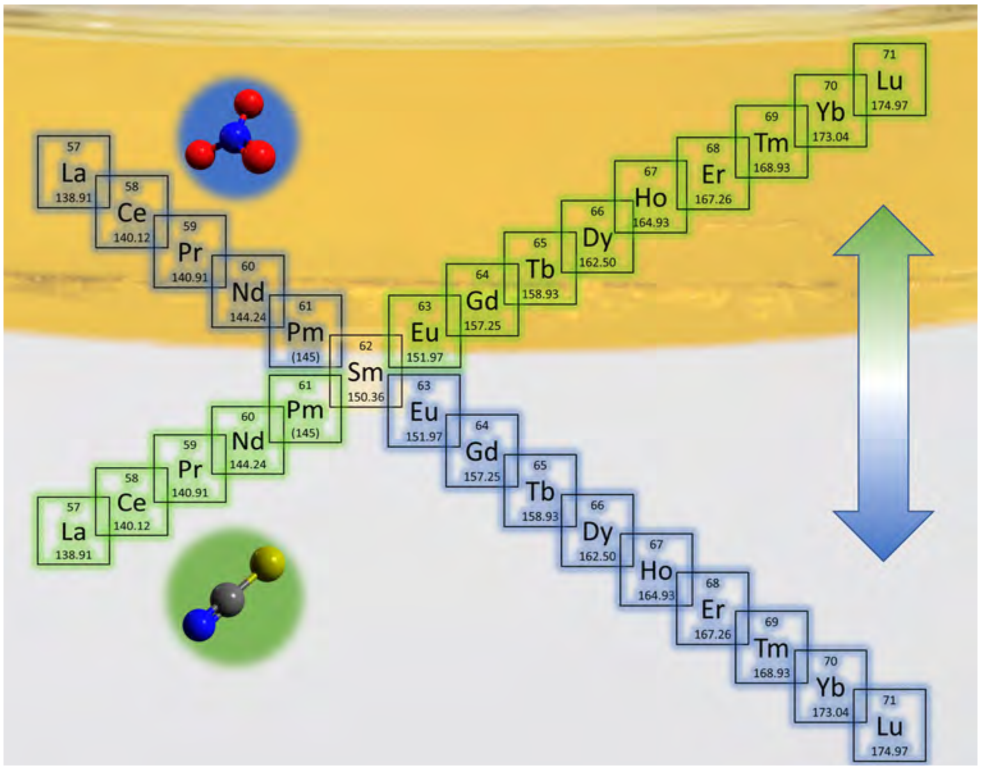
See: Srikanth Nayak, Kaitlin Lovering, and Ahmet Uysal *, “Ion-specific clustering of metal–amphiphile complexes in rare earth separations,” Nanoscale **12**, 20202 (2020). DOI: 10.1039/d0nr04231e

Author affiliation: Argonne National Laboratory

Correspondence: * ahmet@anl.gov

The authors thank Soenke Seifert (XSD) for his help in conducting SAXS experiments, and Byeongdu Lee (XSD) for his suggestions in analyzing the SAXS data. This work was supported by the U.S. DOE Office of Science-Basic Energy Sciences, Division of Chemical Sciences, Geosciences, and Biosciences, under contract DE-AC02-06CH11357. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. DOE Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract No. DE-AC02-06CH11357.

XSD Chemical & Materials Science Group 12-ID-C,D station



Chemical Science

Boosting the Performance of a Lower-Cost Fuel Cell Catalyst

Fuel cells hold tremendous appeal in the energy sector, especially for transportation applications, as they offer the possibility of providing pollution-free power. However, achieving efficient cost-effective fuel cells, especially for the automotive industry, remains a challenge, with one key obstacle being the costly platinum-containing catalysts. Lower-cost platinum-group, metal-free catalysts, such as those based on cobalt (Co), are under investigation, but have exhibited lower activity and durability than those based on platinum. To improve performance, researchers studied the atomic structure of a Co-based catalyst using the APS. These studies were also correlated with results from scanning transmission electron microscopy coupled with electron energy loss characterization performed at the DOE's Oak Ridge National Laboratory. Together the findings from these studies published in *Nature Cataslysis*, along with fuel cell performance and durability data, supports Co-based catalysts as potential game-changers in the race to establish fuel cells as a sustainable energy solution. – Erika Gebel Berg

Read the entire *APS Science* article here.

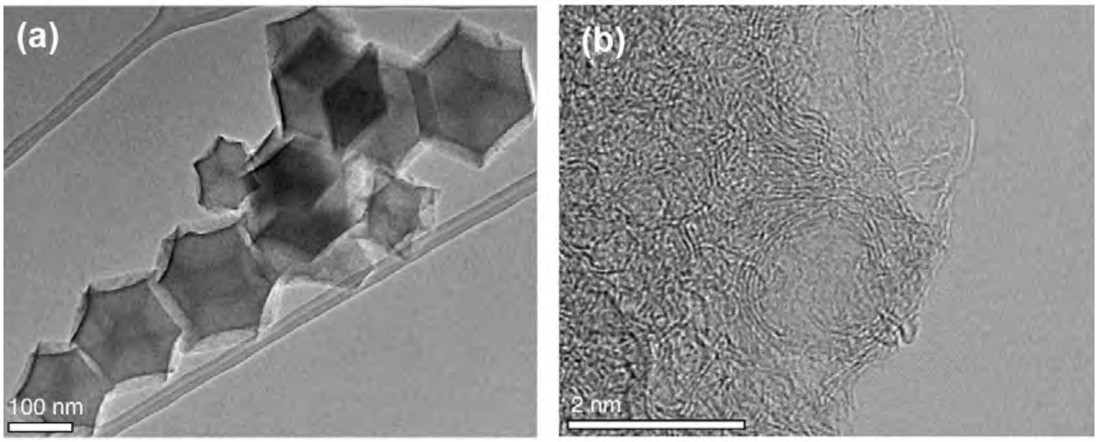
See: Xiaohong Xie[1], Cheng He[2], Boyang Li[3], Yanghua He[4], David A. Cullen[5], Evan C. Wegener[6], A. Jeremy Kropf[6], Ulises Martinez[7], Yingwen Cheng[8], Mark H. Engelhard[1], Mark E. Bowden[1], Miao Song[1], Teresa Lemmon[1], Xiaohong S. Li[1], Zimin Nie[1], Jian Liu[1], Deborah J. Myers[6], Piotr Zelenay[7], Guofeng Wang[3], Gang Wu[4]*, Vijay Ramani[2]**, and Yuyan Shao[1]***, "Performance enhancement and degradation mechanism identification of a single-atom Co–N–C catalyst for proton exchange membrane fuel cells," Nat. Catal. **3**, 1044 (December 2020). DOI: /10.1038/s41929-020-00546-1

Author affiliations: [1]Pacific Northwest National Laboratory, [2]Washington University in St Louis, [3]University of Pittsburgh, [4]The State University of New York (University at Buffalo), [5]Oak Ridge National Laboratory, [6]Argonne National Laboratory, [7]Los Alamos National Laboratory, [8]Northern Illinois University

Correspondence: * gangwu@buffalo.edu, ** ramani@wustl.edu, *** yuyan.shao@pnnl.gov

The authors acknowledge support from the U.S. Department of Energy (DOE) Energy Efficiency and Renewable Energy, Hydrogen and Fuel Cell Technologies Office (DOE-EERE-HFTO) through the Electrocatalysis consortium (ElectroCat) and the DOE program managers, D. Papageorgopoulos, S. Thompson, D. Peterson and G. Kleen. The EMSL(grid.436923.9) is a U.S. DOE Office of Science user facility sponsored by the Biological and Environmental Research program. Pacific Northwest National Laboratory is operated by Battelle for the U.S. DOE under contract DE-AC05- 76RLO1830. MRCAT at the Advanced Photon Source (APS), a DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02- 06CH11357. The Materials Research Collaborative Access Team is supported both by the DOE and the MR-CAT member institutions. Use of the Center for Nanoscale Materials and Advanced Photon Source, both Office of Science user facilities, was supported by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences, under Contract No. DE-AC02-06CH11357.

MR-CAT 10-ID-B station



Sniffing Out a Better Covalent Organic Framework

Covalent organic frameworks (COFs) have great potential as materials for batteries, sensors, and “smart” membranes that selectively admit or reject other molecules. But current manufacturing methods find COFs awkward to work with. Now, a team of researchers has developed a method of preparing COFs as inks that can be sprayed onto many different surfaces. They proved the concept by building an acoustic sensor to detect meat spoilage. They used the APS to characterize the device and show its nanoscale structure was indeed what they had hoped. Their work, published in the journal *Advanced Materials*, will open the way to effective manufacturing techniques to make COFs commercially viable materials.able energy solution. – Kim Krieger

Read the entire *APS Science* article here.

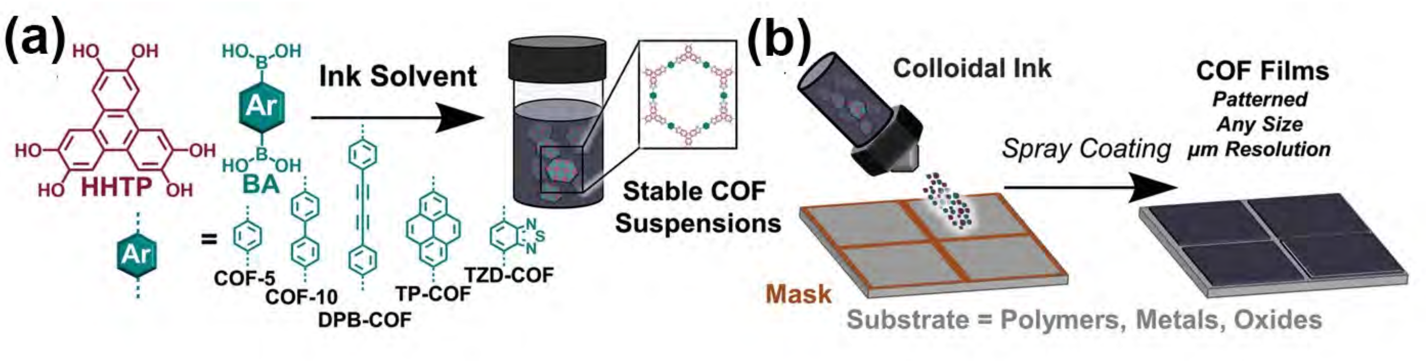
See: Austin M. Evans[1], Nathan P. Bradshaw[1], Brian Litchfield[2], Michael J. Strauss[1], Bethany Seckman[2], Matthew R. Ryder[3], Ioannina Castano[1], Christopher Gilmore[2], Nathan C. Gianneschi[1], Catherine R. Mulzer[2***], Mark C. Hersam[1*], and William R. Dichtel[1**], “High-Sensitivity Acoustic Molecular Sensors Based on Large-Area, Spray-Coated 2D Covalent Organic Frameworks,” Adv. Mater. **32**, 2004205 (2020). DOI: 10.1002/adma.202004205 Figure © 2020 Wiley-VCH GmbH

Author affiliations: [1]Northwestern University, [2]DuPont Electronics and Imaging, [3]Oak Ridge National Laboratory

Correspondence: * m-hersam@northwestern.edu, ** wdichtel@northwestern.edu, *** catherine.mulzer@dupont.com

The authors acknowledge the Army Research Office for a Multidisciplinary University Research Initiatives (MURI) award under grant number W911NF-15- 1-0447. N.P.B. and A.M.E. also acknowledge the Department of Energy (DOE) (Grant DE-SC0019356) for support of the 2D COF spray coating work. A.M.E. (DGE-1324585), M.J.S. (DGE-1842165), I.C. (DGE-1842165), and N.P.B. were supported by National Science Foundation (NSF) Graduate Research Fellowships. A.M.E., M.J.S., and I.C were supported by Ryan Fellowships provided by the International Institute of Nanotechnology. N.P.B. and M.C.H. acknowledge the DOE (Grant DE-SC0019356) and the NSF (Grant DMR-1720139) for support of the 2D COF spray coating work. M.R.R. acknowledges the U.S. DOE Office of Science-Basic Energy Sciences for research funding and the National Energy Research Scientific Computing Center (NERSC), a U.S. DOE Office of Science User Facility, operated under Contract No. DE-AC02-05CH11231, for access to supercomputing resources. DND-CAT is supported by Northwestern University, E.I. DuPont de Nemours & Co., and the Dow Chemical Company. This work has also made use of the IMSERC, EPIC, Keck II, and NUANCE facilities at Northwestern University, which have received support from the Soft and Hybrid Nanotechnology Experimental (SHyNE) Resource (NSF ECCS-1542205), the MRSEC program (NSF DMR-1720139) at the Materials Research Center, the Keck Foundation, the State of Illinois, and International Institute for Nanotechnology (IIN). This research used resources of the Advanced Photon Source and Center for Nanoscale Materials, both U.S. DOE Office of Science User Facilities operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE- AC0206CH11357.

XSD CMS Group 12-ID-C,D station, DND-CAT 5-ID-B,C,D station, XSD DYS Group 8-ID-E station



Two from APS Collect Best Paper Award at SC20

An innovative collaboration between computer and computational scientists from the Argonne Data Science and Learning Division, the Electrical and Computer Engineering Department at the University of Illinois at Urbana-Champaign, and Vincent De Andrade (formerly with the XSD Imaging Group) and Doga Gursoy (XSD Computational X-ray Science Group) garnered the Best Paper Award at the SC20 virtual conference for "Petascale XCT: 3D Image Reconstruction with Hierarchical Communications on Multi-GPU Nodes."

Wojcik of XSD Earns 2020 R&D 100 Award

Michael J. Wojcik (XSD Optics Group) was a co-winner of a 2020 R&D 100 Award for the x-ray polarizing beam splitter, the first-ever instrument to combine an x-ray polarizer and an x-ray beam splitter using a single cubic crystal to separate an incoming x-ray beam into two polarized beams, enabling the measurement of both components simultaneously.

Shu of XSD Named an Argonne Distinguished Fellow

Deming Shu (XSD) was named an Argonne Distinguished Fellow upon unanimous recommendation by the Argonne Laboratory Director's Oversight Council for Hiring and Promotions. Distinguished Fellow is the highest scientific/engineering rank at Argonne, held by only a small fraction (approximately 3%) of the research staff.

Chen of ChemMatCARS Wins DECTRIS Award 2020 for Work on *In Situ* Structural Analysis of Metal-Organic Frameworks

Yu-Sheng Chen, research professor at the University of Chicago and Operations Manager for the ChemMatCARS Sector 15 x-ray beamllnes at the APS received the 2020 DECTRIS Award sponsored by the DECTRIS detector manufacturer for studies of metal-organic frameworks carried out at ChemMatCARS. The awarded work was published in the journal *Nature Chemistry* and highlighted on the APS web site.

APS User Dichtel Receives Prestigious Blavatnik National Award in Chemistry

Northwestern University organic chemist and APS user William Dichtel was named the National Laureate in Chemistry by the 2020 Blavatnik National Awards for Young Scientists. The Blavatnik Family Foundation and the New York Academy of Sciences honored the three National Laureates for their work in the awards' disciplines of life sciences, physical sciences and engineering, and chemistry. Dichtel is the first Laureate ever selected from Northwestern.

Ren of XSD is the 2020 Gopal K. Shenoy Award for Excellence in Beamline Science Recipient

Yang Ren (XSD Structural Science Group) was named the recipient of the 2020 Gopal K. Shenoy Award for Excellence in Beamline Science at the APS. He was acknowledged for creating a world-leading high-energy x-ray diffraction beamline and user program for comprehensive atomic structure studies of condensed matter. Ren was cited for his work on high-energy x-ray diffraction, evolving it from a "niche"' technique to a mainstream capability enabling leading-edge research on atomic structures and generating major impact in many areas of condensed matter physics and material science, including battery materials, catalysts, ferroelectrics and multiferroics, ceramics, metals and alloys, and materials science under extreme conditions.

Tsai Earns 2020 APSUO Rosalind Franklin Young Investigator Award

Hsinhan (Dave) Tsai of Los Alamos National Laboratory was the recipient of the 2020 APS Users Organization Rosalind Franklin Young Investigator Award for his prolific record of high-impact achievements, driving innovations in instrumental capabilities, fostering new collaborations, and continuing research into opto-electronic applications of perovskites, pushing the boundaries of grazing-incidence wide-angle x-ray scattering (GIWAXS) with simultaneous auxiliary probes and GIWAXS coupled with characterization at other beamlines.

APS User Chen Receives Award in Experimental Physical Chemistry

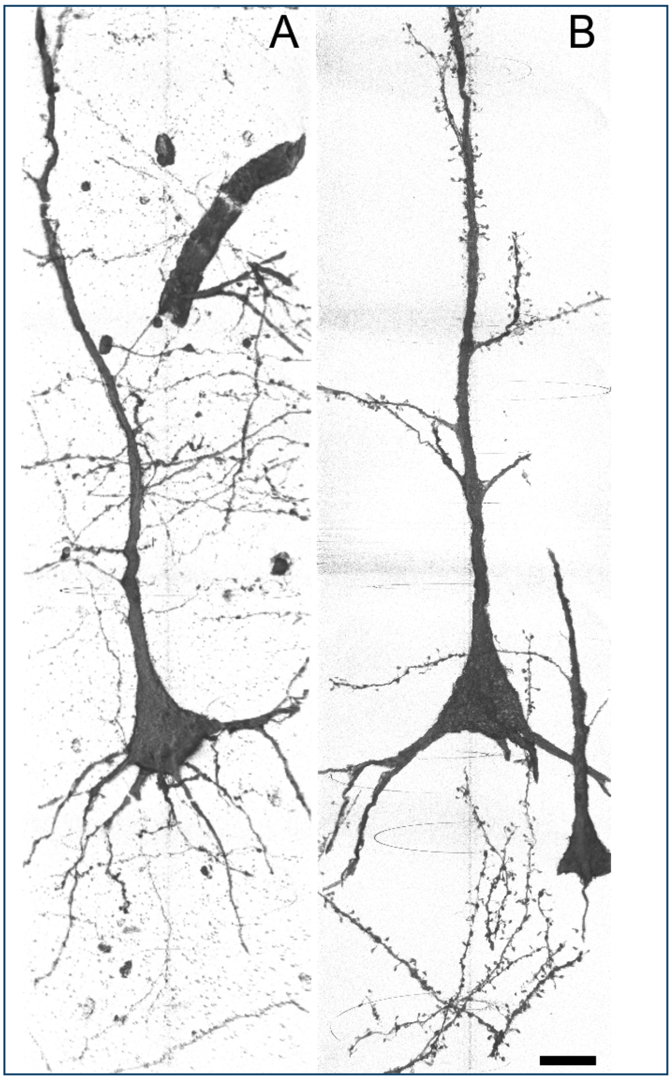
The Physical Chemistry Division of the American Chemical Society awarded Lin X. Chen (Argonne and Northwestern University) the 2020 Award in Experimental Physical Chemistry for her fundamental contributions to the elucidation of excited state structures, dynamics, and energetics of light harvesting systems through state-of-the art experimental techniques.

Life Science

Uncovering New Insights about the Brains of Individuals with Schizophrenia

Compared to the general population, patients with severe mental disorders—such as schizophrenia and bipolar disorder—often die 10-20 years earlier than those without a mental illness. There is no cure for these severe mental disorders, and patients must rely on expensive medication therapies and counseling sessions to manage their conditions. Despite the need for better ways to manage and treat severe mental disorders, there is still little known about the causes of these diseases and how these diseases progress. A team of scientists are attempting to use new techniques to better understand how diseases like schizophrenia develop over time. In a recent study published in the journal *Translational Psychiatry*, this international, multi-institution research team utilized synchrotron radiation nanotomography to analyze the structures of brain tissues from individuals with and without schizophrenia. They discovered that neuronal structures that allow neurons to communicate with each other are different in individuals with schizophrenia and that the structural dissimilarity observed varied from patient to patient. Essential to this work was the hard x-ray nanotomography performed at the APS and at the SPring-8 x-ray light source (Japan).

– Stephen Taylor



Read the entire *APS Science* article here.

See: Ryuta Mizutani[1]*, Rino Saiga[1], Yoshiro Yamamoto[1], Masayuki Uesugi[2], Akihisa Takeuchi[2], Kentaro Uesugi[2], Yasuko Terada[2], Yoshio Suzuki[3], Vincent De Andrade[4], Francesco De Carlo[4] Susumu Takekoshi[5], Chie Inomoto[5], Naoya Nakamura[5], Youta Torii[6], Itaru Kushima[6, 7], Shuji Iritani[6,8], Norio Ozaki[6], Kenichi Oshima[8, 9], Masanari Itokawa[8, 9], and Makoto Arai[9], "Structural diverseness of neurons between brain areas and between cases," Transl. Psychiatr. **11**, 49 (2021). DOI: 10.1038/s41398-020-01173-x

Author affiliations: [1]Tokai University, [2]Japan Synchrotron Radiation Research Institute, [3]High Energy Accelerator Research Organization KEK, [4]Argonne National Laboratory, [5]Tokai University School of Medicine, [6]Nagoya University Graduate School of Medicine, [7]Nagoya University Hospital, [8]Tokyo Metropolitan Matsuzawa Hospital, [9]Tokyo Metropolitan Institute of Medical Science

Correspondence: * mizutanilaboratory@gmail.com

This work was supported by Grants-in-Aid for Scientific Research from the Japan Society for the Promotion of Science (nos. 21611009, 25282250, and 25610126), and by the Japan Agency for Medical Research and Development under grant nos. JP18dm0107087, JP18dm0107088, JP18dm0107108, JP19dm0107087, JP19dm0107088h0004, and JP19dm0107108. The synchrotron radiation experiments at SPring-8 were performed with the approval of the Japan Synchrotron Radiation Research Institute (JASRI) (proposal nos. 2011A0034, 2015A1160, 2015B1101, 2016B1041, 2018A1164, 2018B1187, and 2019B1087). This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

XSD Imaging Group 32-ID-B,C station

A Framework for an Anti-Cancer Light Therapy

Where cancer is concerned, sometimes the treatment can be as bad as the disease, with invasive surgeries and aggressive chemotherapies taking a great toll on the health of patients. The search for effective noninvasive cancer treatments remains an active area of research. One promising strategy that is already in use as a cancer treatment is photodynamic therapy, which involves using light in combination with a photosensitizer to generate reactive oxygen species and kill cancer cells. The approach has been limited by current photosensitizers, which have a number of drawbacks. Researchers are developing novel photosensitizers, such as nanoscale metal-organic framework-stabilized bacteriochlorins, to overcome these limitations. In this study, researchers from The University of Chicago characterized these new photosensitizers using the APS. They also took it a step further, testing the treatment strategy in cancer cells and animal models. Their results, published in the *Journal of the American Chemical Society*, shine new light on PDT as an effective and safe treatment for cancer. — Erika Gebel Berg

Read the entire *APS Science* article here.

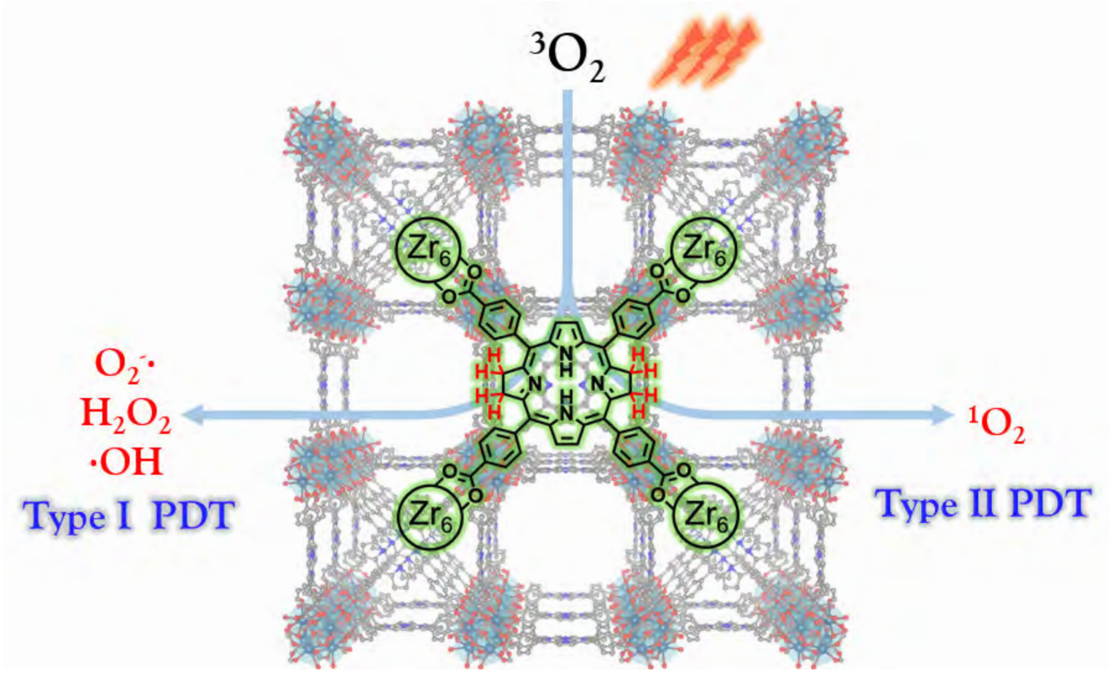
See: Taokun Luo, Kaiyuan Ni, August Culbert, Guangxu Lan, Zhe Li, Xiaomin Jiang, Michael Kaufmann, and Wenbin Lin*, “Nanoscale Metal–Organic Frameworks Stabilize Bacteriochlorins for Type I and Type II Photodynamic Therapy,” J. Am. Chem. Soc. **142**, 7334 (2020). DOI: 10.1021/jacs.0c02129 Figure © 2020 American Chemical Society

Author affiliation: The University of Chicago

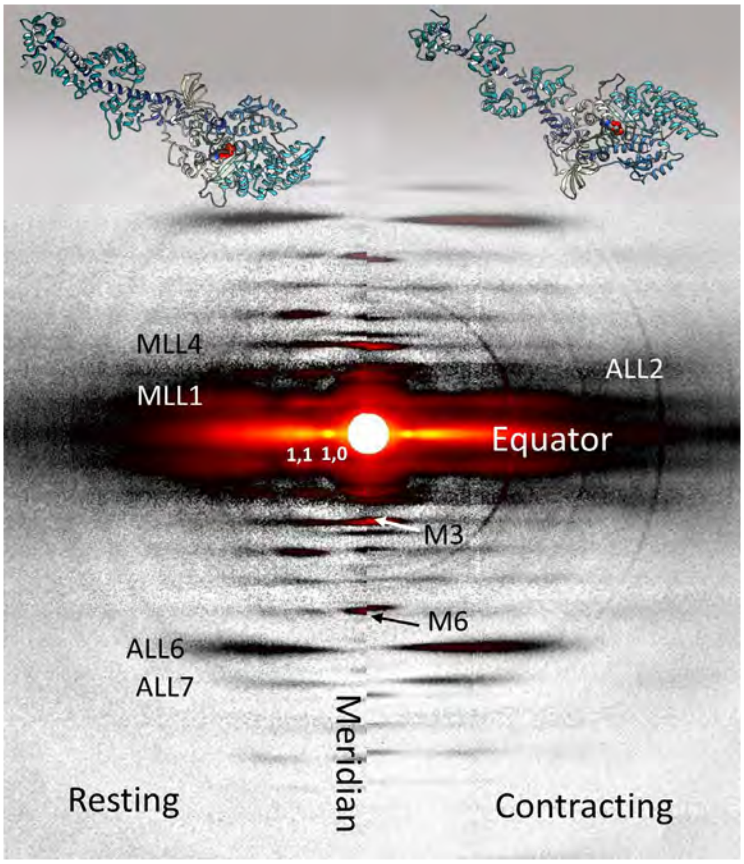
Correspondence: * wenbinlin@uchicago.edu

We thank Yang Song, Xuanyu Feng, Yunhong Pi, and Wenbo Han for experimental help. We acknowledge the National Cancer Institute (U01-CA198989) and The University of Chicago Medicine Comprehensive Cancer Center (NIH CCSG: P30 CA014599) for funding support. ChemMatCARS is principally supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under Grant NSF/ CHE-1834750. Use of the Advanced Photon Source, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the U.S. DOE under Contract DE-AC02-06CH11357.

ChemMatCARS 15-ID-B,C,D station



Relaxation at the Molecular Level



The molecular interactions between the proteins myosin and actin that generate force during muscle contraction are some of the most well-studied molecular interactions in biology. However, there are some congenital skeletal muscle disorders and types of heart failure where relaxation of the muscle, rather than the force generation part of the cycle, appears to be the problem, and there are currently no available treatments that affect relaxation specifically. A more detailed understanding of the dynamics of the relaxation process could help in the development of treatments that maintain or increase force generation while repairing defects in relaxation. Recent work conducted at the APS used a unique transgenic mouse model, time-resolved small-angle x-ray diffraction, and molecular dynamics simulations to discover more about how myosin and actin interact during skeletal muscle relaxation. This research, published in the *Journal of Physiology*, demonstrates that this type of small-angle x-ray analysis may be of great value for uncovering the information needed to identify new treatments for neuromuscular disorders associated with impaired muscle relaxation kinetics.bending, crawling, or rotating.

– Sandy Field

Read the entire *APS Science* article here.

See: Weikang Ma[1*], Matthew Childers[2], Jason Murray[2], Farid Moussavi-Harami[2], Henry Gong[1], Robert Weiss[3], Valerie Daggett[2], Thomas Irving[1], and Michael Regnier[2], "Myosin dynamics during relaxation in mouse soleus muscle and modulation by 2′-deoxy-ATP," J. Physiol. **598**(22), 5165 (2020). DOI: 10.1113/JP280402

Author affiliations: [1]Illinois Institute of Technology, [2]University of Washington, [3]Cornell University

Correspondence: * wma6@iit.edu

The research was supported by National Institutes of Health (NIH) R01 HL128368, NIH R56 AG055594, NIH RM1 GM131981, and NIH U01 HL122199 to M.R., and K08 HL128826 to F.M.H. Use of the BioCAT facility was supported by grant 9 P41 GM103622 from the National Institute of General Medical Sciences of the National Institutes of Health. Use of the Pilatus 3 1M detector was provided by grant 1S10OD018090-01 from NIGMS. Research was also supported by the National Energy Research Scientific Computing Center, supported by the U.S. Department of Energy (DOE) Office of Biological Research, which is supported by the U.S. DOE under contract no. DE-AC02-05CH11231. The research reported in this publication was also supported by the National Institute of Arthritis and Musculoskeletal and Skin Diseases of the National Institutes of Health under Award Number P30AR074990. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

Bio-CAT 18-ID-D station

Bromine is Not Useful as a Paleo-Diet Indicator

Human diets are determined by both environmental and social considerations. People eat what is available, what they are technologically able to obtain, and what their social group considers to be appropriate. One tool to identify the dietary choices of ancient people is the chemical composition of recovered human skeletal tissue. Researchers using high-brightness x-rays from the APS analyzed bromine in human bones and teeth excavated from Pre-Columbian archeological sites and found that bromine concentrations were close to the lower detection limit, suggesting that bromine is not a good indicator of paleo-human diet. These results were published inthe journal *Archaeometry*. — Dana Desonie

Read the entire *APS Science* article here.

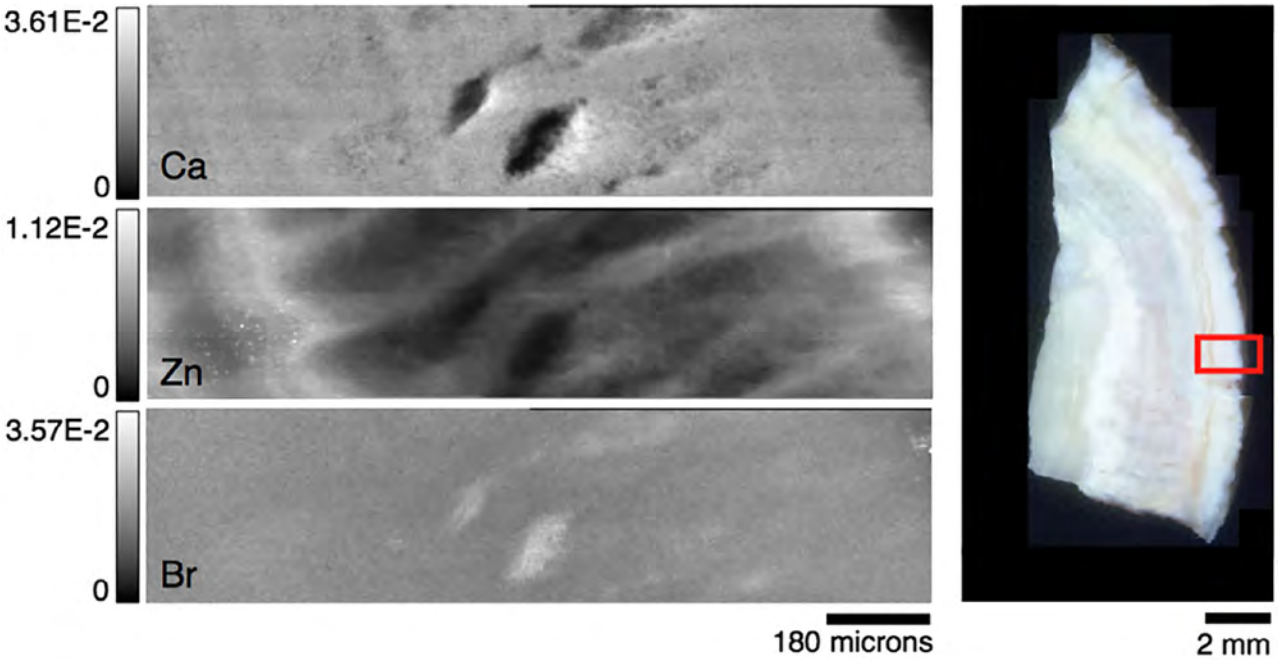
See: M. S. Kozachuk[1], T. K. Sham[2], R. R. Martin[2]*, and A. J. Nelson[2], “Bromine, a Possible Marine Diet Indicator? A Hypothesis Revisited,” Archaeometry **62**(6), 1267 (2020). DOI: 10.1111/arcm.12590 Figure © 2020 University of Oxford

Author affiliations: [1]Canadian Nuclear Laboratories, [2]The University of Western Ontario

Correspondence: * rrhm@uwo.ca

This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357, and the Canadian Light Source and its funding partners for the use of station 20-ID.

XSD Spectroscopy Group 20-ID-B,C station



What Bacterial Pathogens Can Teach Us about Protein Folding

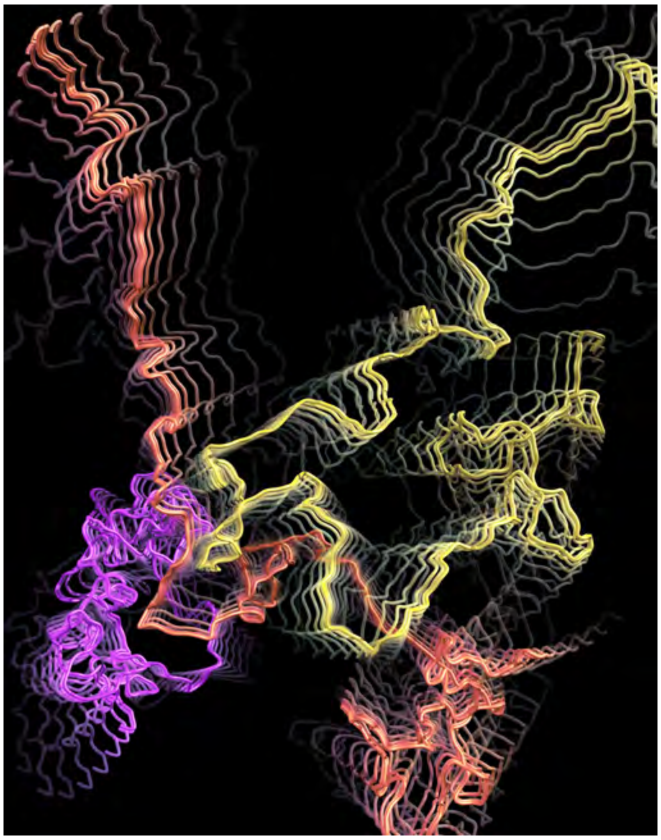


Image created by Kristina Davis, University of Notre Dame. (Image used with permission)

Protein folding is one of the fascinating unanswered questions in biology. How does an amino acid sequence that is unfolded when it leaves the ribosome manage to fold properly into a highly ordered, lightning-fast enzyme or sturdy structural protein? Why don't all the proteins in the cell instead just stick to each other, aggregating into a big mess? A unique model system in bacteria may hold some of the answers to these questions. The system involves the study of what are termed autotransporter proteins, which pathogenic bacteria secrete as virulence factors for infection. These proteins are synthesized in the bacterial cytoplasm and cross one membrane into the bacterial periplasm. Autotransporter proteins then remain in an unfolded state in the periplasm until they pass through the outer bacterial membrane, folding properly along the way. This highly specialized protein folding process has attracted the attention of a team of researchers who have used this bacterial system as a model to determine what allows these unique proteins to maintain their disordered state in the periplasm. The work includes studies carried out at the APS and was published in the journal *Proceedings of the National Academy of Sciences of the United States of America*. The authors believe their work will provide important information toward understanding basic questions of protein folding and tests long-held theories about how this remarkable biological process works. — Sandy Field

Read the entire *APS Science* article here.

See: Micayla A. Bowman[1], Joshua A. Riback[2], Anabel Rodriguez[1], Hongyu Guo[1], Jun Li[1], Tobin R. Sosnick[2]*, and Patricia L. Clark[1]**, "Properties of protein unfolded states suggest broad selection for expanded conformational ensembles," Proc. Natl. Acad. Sci. U.S.A. 117(38), 23356 (September **22**, 2020). DOI: 10.1073/pnas.2003773117

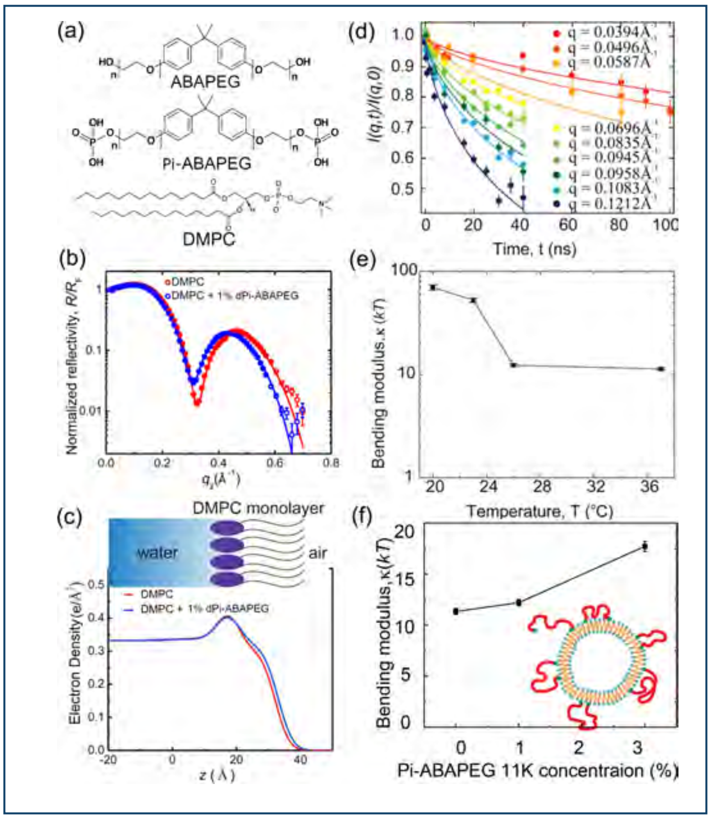
Author affiliations: [1]University of Notre Dame, [2]The University of Chicago

Correspondence: * trsosnic@uchicago.edu, ** pclark1@nd.edu

We thank Srinivas Chakravarthy (Bio-CAT) for assistance with the SAXS measurements and Gina Jozwiak for assistance with RNA quantification and protein purification. This work was supported by grants from the National Institutes of Health (GM130122 [T.R.S. and P.L.C.] and GM055694 [T.R.S.]), the W. M. Keck Foundation (P.L.C.), and the National Science Foundation (MCB 1516959 [C. R. Matthews]). Use of the Advanced Photon Source, an Office of Science User Facility, operated for the Department of Energy (DOE) Office of Science by Argonne National Laboratory, was supported by the DOE under Contract DEAC02-06CH11357.

Bio-CAT 18-ID-D station

Making Better Drugs by Controlling Membrane Mechanics



Cellular membranes are the body's wall of defense against nefarious invaders, with the tricky task of blocking the bad guys while letting beneficial molecules come and go. Scientists are beginning to learn membranes' secrets and are using this knowledge to develop pharmaceuticals that can help secure the perimeter. Recently, researchers developed a potential membrane-targeting treatment—called end-phosphorylated polyethylene glycol triblock copolymer (Pi-ABAPEG)—for infections caused by pathogens that attack the epithelium, a thin protective layer of cells that lines the outer surface of organs and blood vessels. To probe the mechanism behind Pi-ABAPEG's protective effect, the researchers studied interactions between the copolymer and a membrane model using a number of advanced instruments including the APS. Together, these measurements, published in the journal *Soft Matter*, painted a detailed picture of how Pi-ABAPEG protects cells from pathogens, providing insights that could bolster the next generation of pharmaceutical defenses. — Erika Gebel Berg

Read the entire *APS Science* article here.

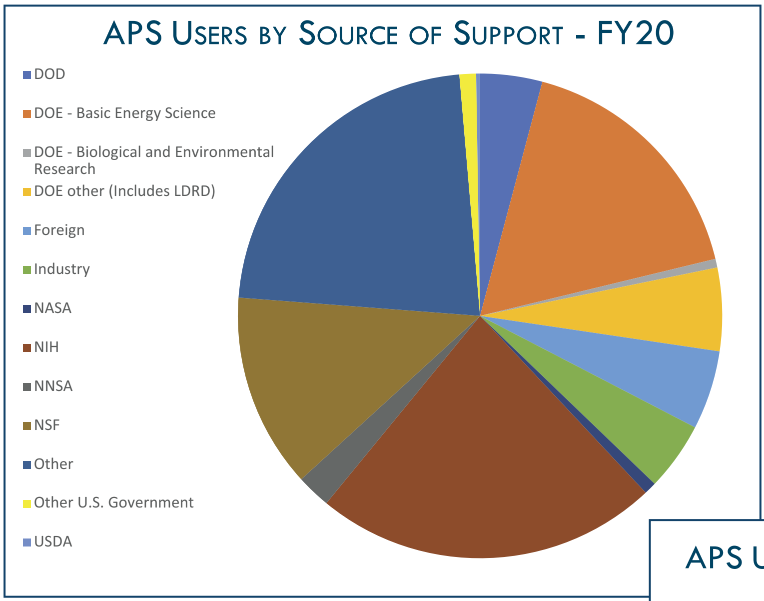
See: Jing Yu[1,2], Jun Mao[1,2], Michihiro Nagao[3,4], Wei Bu[2], Binhua Lin[2], Kunlun Hong[5], Zhang Jiang[1], Yun Liu[3,6], Shuo Qian[5], Matthew Tirrell[1,2]*, and Wei Chen[1,2]**, "Structure and dynamics of lipid membranes interacting with antivirulence end-phosphorylated polyethylene glycol block copolymers," Soft Matter, **16**, 983 (2020). DOI: 10.1039/c9sm01642b

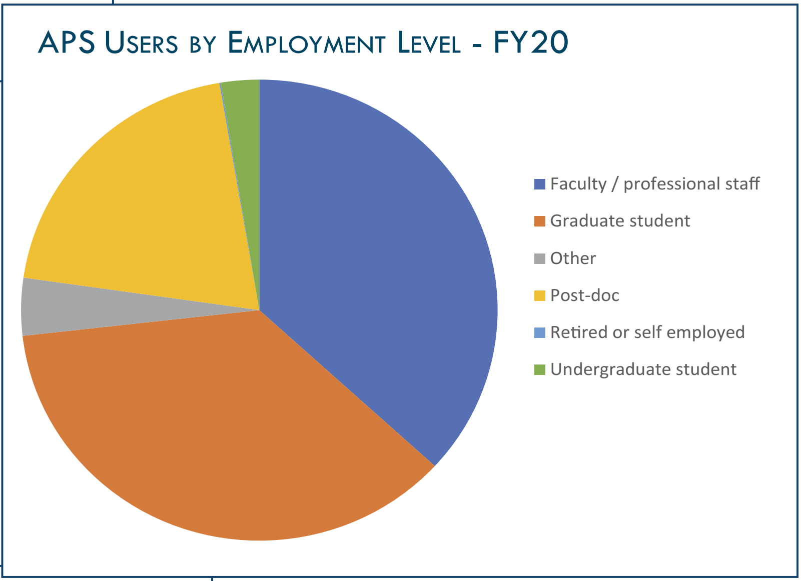
Author affiliations: [1]Argonne National Laboratory, [2]The University of Chicago, [3]National Institute of Standards and Technology, [4]Indiana University, [5]Oak Ridge National Laboratory, [6]University of Delaware

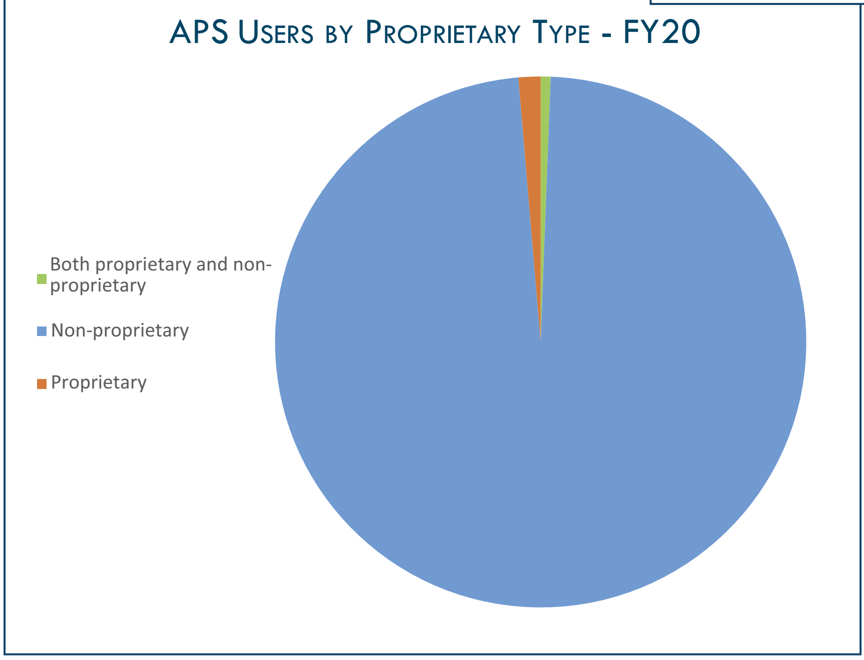
Correspondence: ** wchen@anl.gov, * mtirrell@uchicago.edu

Work in the Center for Molecular Engineering and the Materials Science Division of Argonne National Laboratory was supported by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences, Materials Science and Engineering Division. M. N. and Y. L. acknowledge funding support of cooperative agreement 70NANB15H259 and 70NANB15H260, respectively, from NIST, U.S. Department of Commerce. Access to the NG3-SANS instrument and NGA-NSE spectrometer was provided by the Center for High Resolution Neutron Scattering, a partnership between NIST and the National Science Foundation (NSF) under Agreement No. DMR-1508249. ChemMatCARS is supported by the Divisions of Chemistry (CHE) and Materials Research (DMR), National Science Foundation, under grant number NSF/CHE-1834750. A portion of the synthesis was conducted at the Center for Nanophase Materials Sciences at ORNL, which is a DOE Office of Science user facility. Part of the SANS was done on the CG-3 Bio-SANS instrument at the HFIR, which is sponsored by the Office of Biological & Environmental Research in the DOE's Office of Science. This research used resources of the Advanced Photon Source and the Center for Nanoscale Materials, U.S. DOE Office of Science user facilities operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

ChemMatCARS 15-ID-B,C,D station


APS Users by Source of Support - FY20
DOD
DOE - Basic Energy Science
DOE - Biological and Environmental Research
DOE other (Includes LDRD)
Foreign
Industry
NASA
NIH
NNSA
NSF
Other
Other U.S. Government
USDA


APS Users by Employment Level - FY20
Faculty / professional staff
Graduate student
Other
Post-doc
Retired or self employed
Undergraduate student


APS Users by Proprietary Type - FY20
Both proprietary and non-proprietary
Non-proprietary
Proprietary

Structural Biology

New, Potent Inhibitors of an Enzyme Essential for SARS-Cov-2 Viral Replication

At the root of the devastating COVID-19 pandemic is the SARS- CoV-2 virus. One of the enzymes essential for this virus to function is PLpro, which is a protease that cleaves large viral proteins into smaller proteins. The proteolytic activity of this enzyme ultimately enables viral spread. In a recent study by an international research team that carried out investigations at the APS, a chemical screen was done to identify irreversible inhibitors that are highly selective for PLpro. Using the APS high-brightness x-ray beams, the authors generated crystal structures of two particular potent inhibitors—VIR250 and VIR251—in complex with PLpro, allowing for a structural understanding of how these compounds mediate their inhibition. This work was published in the journal *Science Advances*. — Alicia Surrao

Read the entire *APS Science* article here.

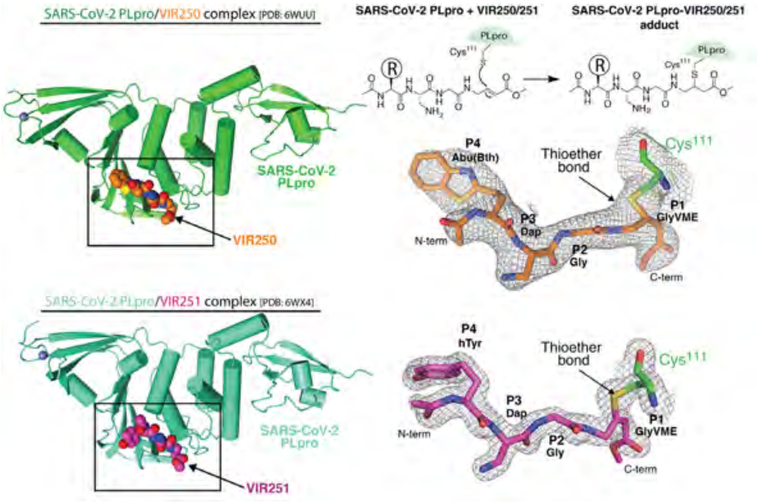
See: Wioletta Rut[1]*, Zongyang Lv[2, 3]*, Mikolaj Zmudzinski[1], Stephanie Patchett[4], Digant Nayak[2,3], Scott J. Snipas[5], Farid El Oualid[6], Tony T. Huang[4]**, Miklos Bekes[7]***‡, Marcin Drag[1,5]*****, Shaun K. Olsen[2, 3]****, "Activity profiling and crystal structures of inhibitor bound SARS-CoV-2 papain-like protease: A framework for anti–COVID-19 drug design," Sci. Adv. **6**: eabd4596 (16 October 2020). DOI: 10.1126/sciadv.abd4596

Author affiliations: [1]Wroclaw University of Science and Technology, [2]Medical University of South Carolina, [3]University of Texas Health Science Center at San Antonio, [4]New York University School of Medicine, [5]Sanford Burnham Prebys Medical Discovery Institute, [6]UbiQ Bio B.V., [7]Independent Consultant

Correspondence: * wioletta.rut@pwr.edu.pl, ** tony.huang@nyulangone.org, , *** miklosbekes@icloud.com, **** olsens@uthscsa.edu, ***** marcin.drag@pwr.edu.pl ‡Present address: Arvinas, Inc.

This project was supported by the National Science Center grant 2015/17/N/ST5/03072 (Preludium 9) in Poland (W.R.) and the "TEAM/2017-4/32" project, which is carried out within the TEAM program of the Foundation for Polish Science, co-financed by the European Union under the European Regional Development Fund (M.D.). W.R. is a beneficiary of a START scholarship from the Foundation for Polish Science. The Northeastern Collaborative Access Team beamlines are funded by the National Institute of General Medical Sciences from the National Institutes of Health (P30 GM124165). Research reported in this publication was supported by CPRIT RR200030 and NIH R01 GM115568 (S.K.O.), ES025166 (T.T.H.), and GM099040 (S.J.S.). Z.L. is a Hollings Cancer Center Postdoctoral Fellow, and S.P. is an American Cancer Society Postdoctoral Fellow (PF-18-235- 01-RMC). This research used resources of the APS, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357. Extraordinary facility operations were supported in part by the DOE Office of Science through the National Virtual Biotechnology Laboratory, a consortium of DOE national laboratories focused on the response to COVID-19, with funding provided by the Coronavirus CARES Act.

NE-CAT 24-ID-C station



A Template for Inhibiting SARS-CoV-2 Replication

When SARS-CoV-2, the virus responsible for the disease COVID-19, infects a person's cells, it provides the instructions to make the proteins responsible for viral replication and release. An essential step in this process is the cleaving of a long viral polyprotein into smaller functional units, remarkably carried out in part by an enzyme, M^{pro}, itself contained within the polyprotein. Researchers using the APS have determined crystal structures that capture the moment M^{pro} begins this process. Aside from benefits to basic research, the structures will help guide the researchers in developing small-molecule drugs designed to stop the spread of COVID-19 by inhibiting M^{pro}'s ability to set viral replication in motion. Coronaviruses became a major public health concern in 2002 when severe acute respiratory syndrome coronavirus (SARS-CoV) jumped from animals to humans, in a process known as "spillover", where it caused SARS, a severe respiratory illness. This was followed in 2012 by the emergence of Middle East respiratory syndrome, caused by MERS-CoV, and COVID-19 in 2019, caused by SARS-CoV-2. Far more transmissible than either SARS-CoV or MERS-CoV, SARS-CoV-2 has caused nearly 2.5 million deaths worldwide to date, making it a global priority. These results were published in the journal *Nature Communications.* — Judy Myers

Read the entire *APS Science* article here.

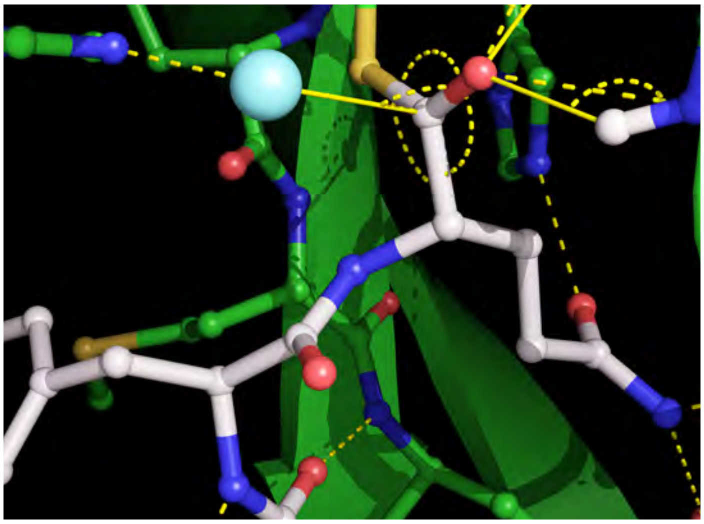
See: Jaeyong Lee[1,2], Liam J. Worrall[1], Marija Vuckovic[1], Federico I. Rosell[1], Francesco Gentile[1], Anh-Tien Ton[1], Nathanael A. Caveney[1], Fuqiang Ban[1], Artem Cherkasov[1], Mark Paetzel[2]*, and Natalie C. J. Strynadka[1]**, "Crystallographic structure of wild-type SARS-CoV-2 main protease acyl-enzyme intermediate with physiological C-terminal autoprocessing site," Nat. Commun. **11**, 5877 (2020). DOI: 10.1038/s41467-020-19662-4

Author affiliations: [1]The University of British Columbia, [2]Simon Fraser University

Correspondence: * mpaetzel@sfu.ca, ** ncjs@mail.ubc.ca

GM/CA-XSD has been funded in whole or in part with Federal funds from the National Cancer Institute (ACB-12002) and the National Institute of General Medical Sciences (AGM-12006); and the Eiger 16M detector by NIH grant S10 OD012289. This work was funded by operating grants from the Canadian Institutes of Health Research to N.C.J.S., M.P., and A.C. N.C.J.S. is a Tier I Canada Research Chair in Antibiotic Discovery. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Extraordinary facility operations were supported in part by the DOE Office of Science through the National Virtual Biotechnology Laboratory, a consortium of DOE national laboratories focused on the response to COVID-19, with funding provided by the Coronavirus CARES Act.

GM/CA-XSD 23-ID-B station



Llama Antibodies Could Block Coronaviruses from Invading Our Cells

Our bodies' immune systems are up against a lot. Harmful bacteria, fungi, parasites, and viruses have a devastating ability to hijack our cells and wreak havoc on the systems that keep us alive and well. Scientists across industries and sectors work tirelessly to engineer vaccines and therapeutics that help us combat these pathogens. With the goal of designing much-needed treatments for deadly coronaviruses like MERS-CoV, SARS-CoV, and SARS-CoV-2, a team of molecular scientists set out to understand the structures of coronavirus spike proteins and how they facilitate viral entry into our cells. While past work focused on applying structural information to the development of therapies for respiratory diseases like RSV, this group more recently—and to great acclaim—designed a stabilized version of the SARS-CoV-2 spike protein, which was used as the basis for the Moderna, Pfizer, and Johnson & Johnson vaccines. The researchers went on to produce the first molecular structure of the novel coronavirus' spike protein. Recently, these researchers developed a potential COVID-19 antibody therapy using antibodies from llamas. This work involved immunizing llamas with prefusion-stabilized coronavirus spikes and subsequently isolating the resulting single-domain antibodies, or VHHs. Working at the APS, the team determined the crystal structures of the isolated VHHs in complex with viral agents and thus revealed their mechanisms of neutralization. These findings, published in the journal *Cell,* add to the growing research highlighting VHHs as desirable therapeutic candidates for viral respiratory diseases. Paired with their high thermo- and chemostability, impressive production yields, and their potential to be administered via inhaler, the antibodies could provide much-needed therapies for those infected with coronaviruses. — Alicia Surrao

Read the entire *APS Science* article here.

See: Daniel Wrapp[1], Dorien De Vlieger[2,3], Kizzmekia S. Corbett[4], Gretel M. Torres[5], Nianshuang Wang[1], Wander Van Breedam[2,3], Kenny Roose[2,3], Loes van Schie[2,3], VIB-CMB COVID-19 Response Team, Markus Hoffmann[6], Stefan Pöhlmann[6,7], Barney S. Graham[4], Nico Callewaert[2,3], Bert Schepens[2,3], Xavier Saelens[2,3], and Jason S. McLellan[1]*, ""Structural Basis for Potent Neutralization of Betacoronaviruses by Single-Domain Camelid Antibodies," Cell **181,** 1004 (May 28, 2020). DOI: 10.1016/j.cell.2020.04.031

Author affiliations: [1]The University of Texas at Austin, [2]VIB-UGent Center for Medical Biotechnology, [3]Ghent University, [4]National Institutes of Health, [5]Geisel School of Medicine at Dartmouth, [6]Leibniz Institute for Primate Research, [7]University Göttingen

Correspondence: * jmclellan@austin.utexas.edu

This work was supported by a National Institutes of Health (NIH)/National Institute of Allergy and Infectious Disease (NIAID) grant R01-AI127521 (to J.S.M.) and in part by intramural NIAID funding (B.S.G.). Research was supported by funding from VIB, Ghent University GOA project to N.C. and X.S., FWO and VLAIO fellowships and research projects to various VIB-CMB COVID-19 response team members. We acknowledge the team of the VIB Nanobody Service Facility for their services. D.D.V. was supported by a FWOsb fellowship, W.V.B. by the FWO-SBO grant "GlycoDelete," S.P. by BMBF (RAPID consortium, 01K11723D), and B.S. by FWO-EOS project VIREOS. We are deeply indebted to the VIB-CMB COVID-19 response team members, who volunteered to offer their expertise and agile work under conditions of almost complete lockdown and societal standstill. We thank the support staff of both VIB-IRC and VIB-CMB centers, the members of VIB Discovery Sciences units' COVID-19 team for rapid and consistent support and input. SBC-XSD is operated by UChicago Argonne, LLC, for the U.S. Department of Energy, Office of Biological and Environmental Research under contract DE-AC02-06CH11357. This research also used resources of the Argonne Leadership Computing Facility, which is a U.S. Department of Energy (DOE) Office of Science User Facility supported under Contract DE-AC02-06CH11357, and of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Extraordinary facility operations were supported in part by the DOE Office of Science through the National Virtual Biotechnology Laboratory, a consortium of DOE national laboratories focused on the response to COVID-19, with funding provided by the Coronavirus CARES Act.

SBC-XSD 19-ID-D station

New Structures of SARS-CoV-2 Lead to Improved Understanding of a Viral Replication Engine

The economic, societal, and personal reverberations from the historic COVID-19 virus will be felt for years to come. As we continue to brace for new variants of SARS-CoV-2 and think about the potential for future pandemics, it is important that we develop a thorough understanding of the structures and reactivities of these deadly viruses so that we can be better prepared for the next global outbreak. To do this, we not only need to know the similarities between different viruses, but also their differences so that we can understand why some viruses only spread to a few thousand people whereas some have the ability to shut down the entire world. A team of researchers from conducting experiments at the APS are making significant strides in understanding the structures, active sites, and reactivity of SARS-CoV-2. At the early stage of the pandemic, the team characterized the reactivity and structure of a new subunit of SARS-CoV-2, a nidoviral RNA endoribonuclease known as NendoU. The insights gained through this research, published in the journal *Protein Science*, may lead to a better understanding of why SARS-CoV-2 is much more transmittable in comparison to other coronaviruses like SARS-CoV and MERS-CoV. – Stephen Taylor

Read the entire *APS Science* article here.

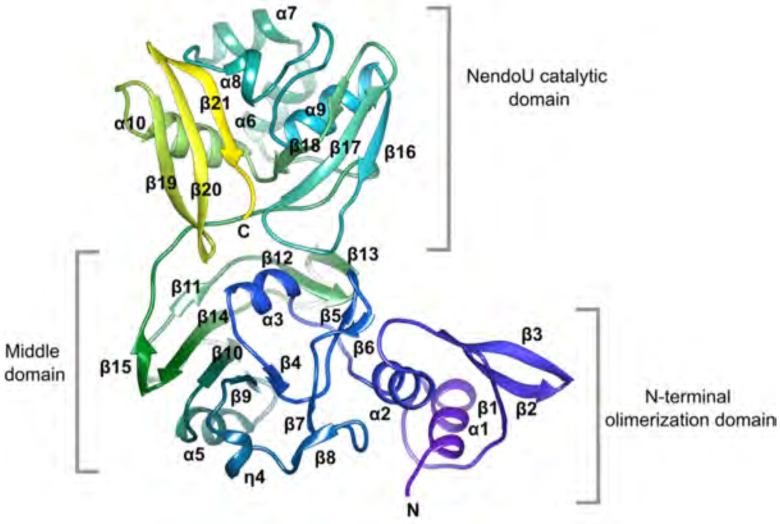
See: Youngchang Kim[1,2], Robert Jedrzejczak[1,2], Natalia I. Maltseva[1,2], Mateusz Wilamowski[1], Michael Endres[2], Adam Godzik[1], Karolina Michalska[1,2], and Andrzej Joachimiak[1,2]*, "Crystal structure of Nsp15 endoribonuclease NendoU from SARS-CoV-2," Prot. Sci. **29**, 1596 (2020). DOI: 10.1002/pro.3873

Author affiliations: [1]The University of Chicago, [2]Argonne National Laboratory, [3]University of California Riverside

Correspondence: * andrzejj@anl.gov

We thank the members of SBC-XSD at Argonne National Laboratory, especially Darren Sherrell and Alex Lavens for their help with setting beamline and data collection. Funding for this project was provided in part by federal funds from the National Institute of Allergy and Infectious Diseases, National Institutes of Health, Department of Health and Human Services, under Contract HHSN272201700060C. The use of SBC-XSD beamlines at the Advanced Photon Source is supported by the U.S. Department of Energy (DOE) Office of Science and operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DEAC02-06CH11357. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility, operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357. Extraordinary facility operations were supported in part by the DOE Office of Science through the National Virtual Biotechnology Laboratory, a consortium of DOE national laboratories focused on the response to COVID-19, with funding provided by the Coronavirus CARES Act.

SBC-XSD 19-ID-D station



Redirecting the Immune System to Kill Cancer Cells More Efficiently

Cancer ranks as one of the greatest causes of death in the United States. Each year, nearly 600,000 Americans die from this tragic disease. While remarkable progress has been made in the field of oncology, many cancers are still presently incurable. One recent anti-cancer approach uses recombinant T cell receptors (TCRs), which are designed to help the immune system kill cancerous cells. Traditionally, TCRs have been unstable and challenging to express. With the goal of improving the efficacy of this approach, a group of researchers performed molecular modeling to discover mutations that improve the stability and expression of TCRs. These mutations reduce the glycosylation of these genetically engineered TCRs, which is an important post-translational protein modification. Importantly, these modified TCRs are able to efficiently kill tumor cells *in vitro*. An integral part of this work, which was published in the journal *Nature Communications*, involved the collection of x-ray diffraction data at the APS. These research endeavors could potentially pave the way for powerful new anti-cancer treatments.

– Stephen Taylor

Read the entire *APS Science* article here.

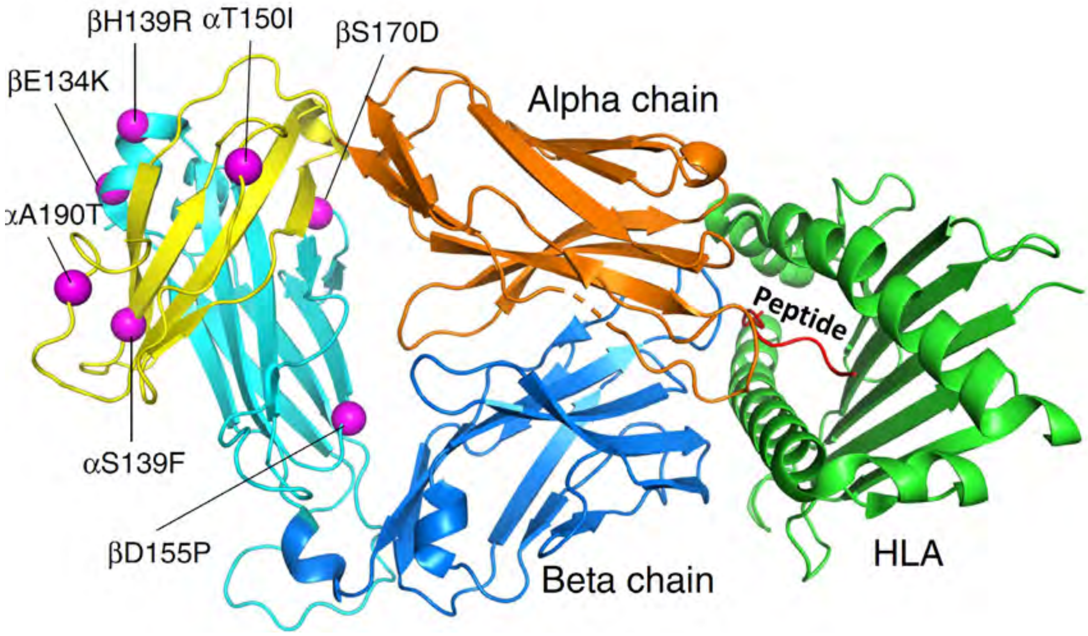
See: Karen Froning[1], Jack Maguire[2], Arlene Sereno[1], Flora Huang[1], Shawn Chang[1], Kenneth Weichert[1], Anton J. Frommelt[1], Jessica Dong[1], Xiufeng Wu[1], Heather Austin[1], Elaine M. Conner[1], Jonathan R. Fitchett[1], Aik Roy Heng[1], Deepa Balasubramaniam[1], Mark T. Hilgers[1], Brian Kuhlman[2]*, and Stephen J. Demarest[1]**, "Computational stabilization of T cell receptors allows pairing with antibodies to form bispecifics," Nat. Commun. **11**, 2330 (2020). DOI: 10.1038/s41467-020-16231-7 Figure © 2021 Springer Nature Limited

Correspondence: * bkuhlman@email.unc.edu, ** demarestsj@lilly.com

Author affiliations: [1]Eli Lilly Biotechnology Center, [2]University of North Carolina at Chapel Hill

Use of the Lilly Research Laboratories Collaborative Access Team (LRL-CAT) beamline at Sector 31 of the Advanced Photon Source was provided by Eli Lilly and Company, which operates the facility. We thank Anton Frommelt, John Koss, Laura Morisco, and Jordi Benach for data collection support at the LRL-CAT beamline. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

LRL-CAT 31-ID-D station



Catching Proteins in the Act of Unfolding

The process by which proteins fold and unfold is vital to most cellular functions. Proteins unexpectedly unfolding play an as-yet unexplained part in diseases such as cancer. To better understand unfolding, scientists need to determine the structure of the protein at each step of that process. Unfortunately, many techniques for imaging an unfolding protein average its structure either over time or spatially within a solution. Recent efforts by an international team of scientists leveraged modeling and genetic algorithms to resolve the spatial structure averaged by the x-ray data they obtained at the APS. Their results, published in the journal *Structural Dynamics*, demonstrate the success of this combination of methods by detailing the structures as a protein unfolds in real time, opening a new avenue for studying this crucial process. — Mary Alexandra Agner

Read the entire *APS Science* article here.

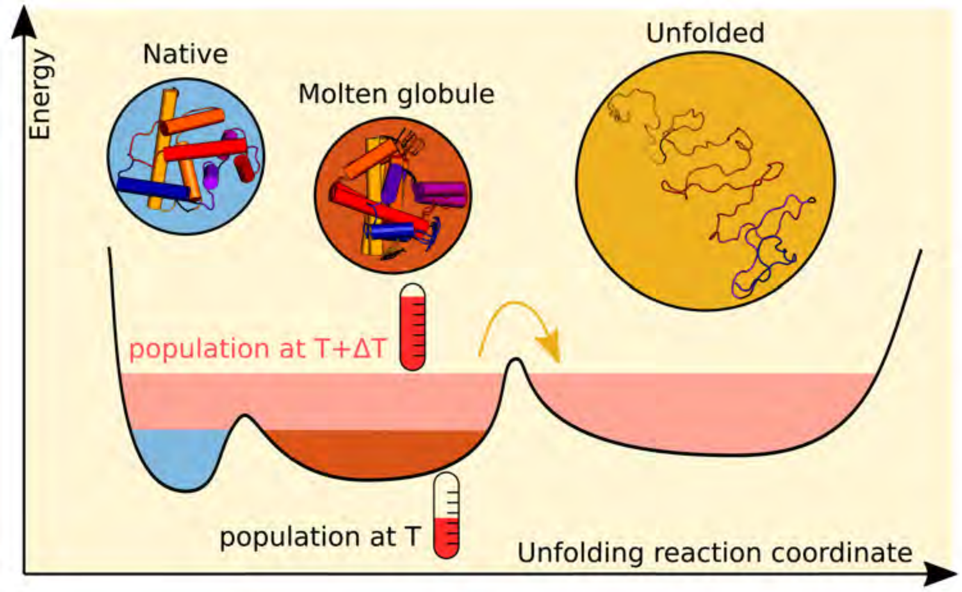
See: L. Henry[1], M. R. Panman[1], L. Isaksson[1], E. Claesson[1], I. Kosheleva[2], R. Henning[2], S. Westenhoff[1]*, and O. Berntsson[1, 3]**, "Real-time tracking of protein unfolding with time-resolved x-ray solution scattering," Struct. Dyn. **7**, 054702 (2020). DOI: 10.1063/4.0000013

Author affiliations: [1]University of Gothenburg, [2]The University of Chicago, [3]Lund University

Correspondence: * westenho@chem.gu.se, ** oskar.berntsson@maxiv.lu.se

This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by the Argonne National Laboratory under Contract No. DE-AC02–06CH11357. The use of BioCARS was also supported by the National Institute of General Medical Sciences of the National Institutes of Health under Grant No. P41 GM118217. The content is solely the responsibility of the authors and does not necessarily represent the official views of the National Institutes of Health. The time-resolved setup at Sector 14 was funded in part through a collaboration with Philip Anfinrud (NIH/NIDDK). The thermostated capillary holder was developed by the group of Lin X. Chen, and we are grateful for their support when setting it up. The simulations were performed on resources provided by the Swedish National Infrastructure for Computing (SNIC) at C3SE.

BioCARS 14-ID-B station



How New Monoclonal Antibodies Neutralize Dangerous Henipaviruses

Hendra and Nipah henipaviruses are emerging pathogens that cause high fatality rates as they spread from animals to humans. There are currently no drugs or vaccines targeting these viruses. To that end, an international team of scientists developed monoclonal antibodies targeting the henipavirus and made crystal structures of two of the most potent antibodies using the APS. The structures show that the two antibodies recognize diverse sites on the viruses' receptor-binding proteins and neutralize the viruses in different ways. When administered to animals that had been infected with a highly lethal strain of the Nipah virus, the antibodies protected the animals from severe disease and death. These results, published in the journal *Cell*, suggest that monoclonal antibodies HENV-26 and HENV-32 can be used cooperatively as a therapeutic "cocktail" against the henipavirus, while the crystal structures can be used to design effective vaccines. — Judy Myers

Read the entire *APS Science* article here.

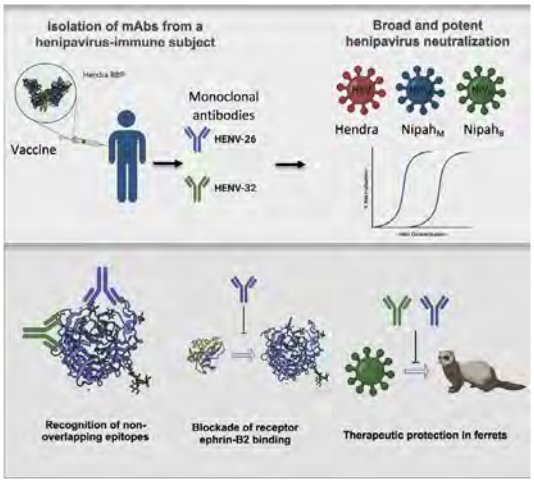
See: Jinhui Dong[1], Robert W. Cross[2], Michael P. Doyle[1], Nurgun Kose[1], Jarrod J. Mousa[1‡], Edward J. Annand[3, 4], Viktoriya Borisevich[2], Krystle N. Agans[2], Rachel Sutton[1], Rachel Nargi[1], Mahsa Majedi[1], Karla A. Fenton[2], Walter Reichard[1], Robin G. Bombardi[1], Thomas W. Geisbert[2], and James E. Crowe, Jr.[1, 2*], "Potent Henipavirus Neutralization by Antibodies Recognizing Diverse Sites on Hendra and Nipah Virus Receptor Binding Protein," Cell **183**, 1536 (December 10, 2020). DOI: 10.1016/j.cell.2020.11.023 Figure ª 2020 Elsevier Inc.

Author affiliations: [1]Vanderbilt University Medical Center, [2]The University of Texas Medical Branch, [3]University of Sydney, [4]Black Mountain Laboratories & Australian Centre for Disease Preparedness, Health and Biosecurity [‡]Present address: University of Georgia

Correspondence: * james.crowe@vumc.org

This work was supported by a grant from the National Institutes of Health (NIH) U19 AI142764 and departmental funds from UTMB to Thomas Geisbert. M.P.D. was supported by NIH fellowship grant F31 AI152332. The project described was supported by CTSA award no. UL1 TR002243 from the National Center for Advancing Translational Sciences (NCATS). Use of the LS-CAT Sector 21 was supported by the Michigan Economic Development Corporation and the Michigan Technology Tri- Corridor (grant 085P1000817). Support for crystallography was provided from the Vanderbilt Center for Structural Biology. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

LS-CAT 21-ID-G station



Engineering New Treatments for Cancer

Trametinib, one example of a class of drugs known as MEK inhibitors, is a drug used to treat specific forms of skin and lung cancer and may be useful for treating several other forms of disease. MEK is an enzyme that controls a protein cascade that can malfunction in cancer, leading to the proliferation of cancer cells. While trametinib's ability to stop MEK's action makes it useful for treating some cancers, exactly how trametinib interacts with MEK was a mystery. A new study, which involved collecting x-ray diffraction data at the APS, solved this mystery by revealing the structure of trametinib and provides new insights into how it interacts with proteins involved in cancer. This study, published in the journal *Nature*, also describes the creation of a new compound called trametiglue, which works even better than trametinib at disrupting the cancer pathway. This discovery may pave the way for a new generation of cancer drugs. – Summer Allen

Read the entire *APS Science* article here.

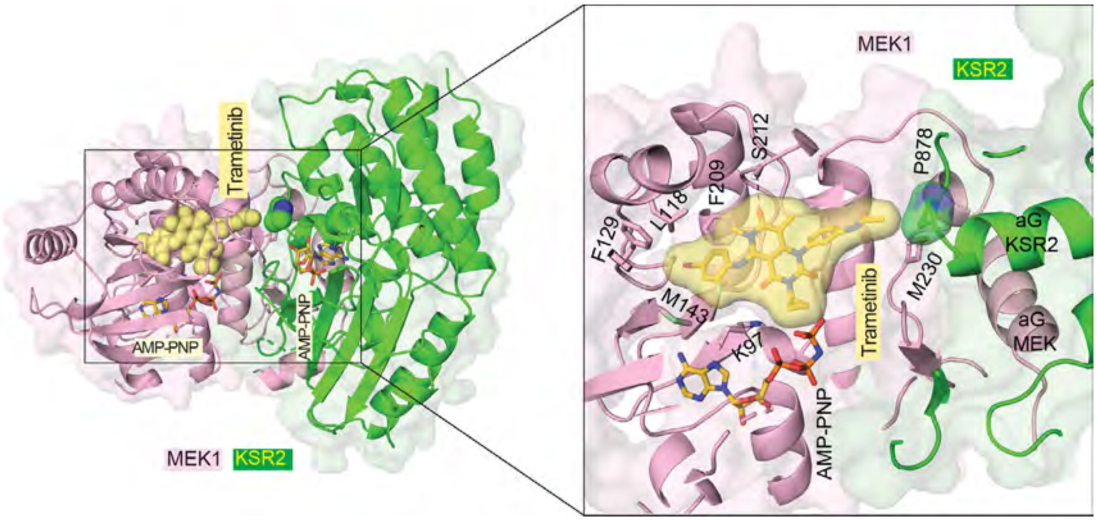
See: Zaigham M. Khan, Alexander M. Real, William M. Marsiglia, Arthur Chow, Mary E. Duffy, Jayasudhan R. Yerabolu, Alex P. Scopton, and Arvin C. Dar*, "Structural basis for the action of the drug trametinib at KSR-bound MEK," Nature **588**, 509 (17 December 2020). DOI: 10.1038/s41586-020-2760-4

Author affiliation: Icahn School of Medicine at Mount Sinai

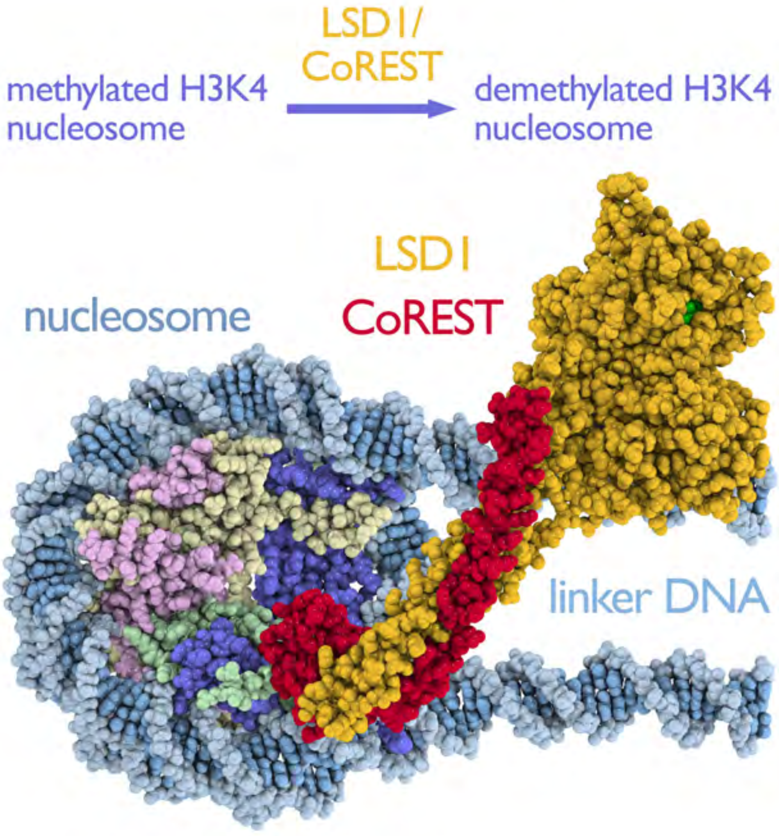
Correspondence: * arvin.dar@mssm.edu

We thank the staff at LS-CAT and the National Synchrotron Light Source II for help with x-ray diffraction experiments. The Dar laboratory has been supported by innovation awards from the NIH (1DP2CA186570-01) and Damon Runyan Rachleff Foundation, as well as National Institutes of Health (NIH) grants 1RO1CA227636 and 5U54OD020353. The authors are also supported by National Cancer Institute grant P30 CA196521 to the Tisch Cancer Institute. A.M.R. and W.M.M. are recipients of NIH F30 (CA232454) and F99/K00 (CA212474) awards, respectively. A.C. and M.E.D. are recipients of T32 fellowships 5T32CA078207 and 5T32GM062754, respectively. A.C.D. has been supported as a Pew-Stewart Scholar in Cancer Research and a Young Investigator of the Pershing-Square Sohn Cancer Research Alliance. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

LS-CAT 21-ID-F station



The Crystal Structure of a Clinically Relevant Enzyme that Regulates Gene Activity



Within a cell's nucleus, an intricate system exists that efficiently packages DNA. Histone proteins form an integral portion of this complex system by packaging DNA into structural units known as nucleosomes. The activity of histones is in part regulated by an important family of gene regulation enzymes known as histone demethylases. As an indicator of how biomedically important such gene regulation enzymes are, the histone deacetylase inhibitor Belinostat is an FDA-approved drug used to treat peripheral T-cell lymphoma. More broadly, histone demethylases have an intimate relationship with cancer. In stellar work published in *Molecular Cell*, researchers from The Pennsylvania State University used the APS to solve the crystal structure of the histone demethylase LSD1 bound to its nucleosome substrate together with its accessory protein known as CoREST. Given that LSD1 is upregulated in various cancers and regulates stem cells, these findings have biomedical relevance. It would be intriguing to see if these major structural findings could be manipulated to generate drugs relevant to oncology and/or regenerative medicine. — Alicia Surrao

Read the entire *APS Science* article here.

See: Sang-Ah Kim, Jiang Zhu, Neela Yennawar, Priit Eek, and Song Tan*, "Crystal Structure of the LSD1/CoREST Histone Demethylase Bound to Its Nucleosome Substrate," Mol. Cell **78**, 903 (June 4, 2020). DOI: 10.1016/j.molcel.2020.04.019

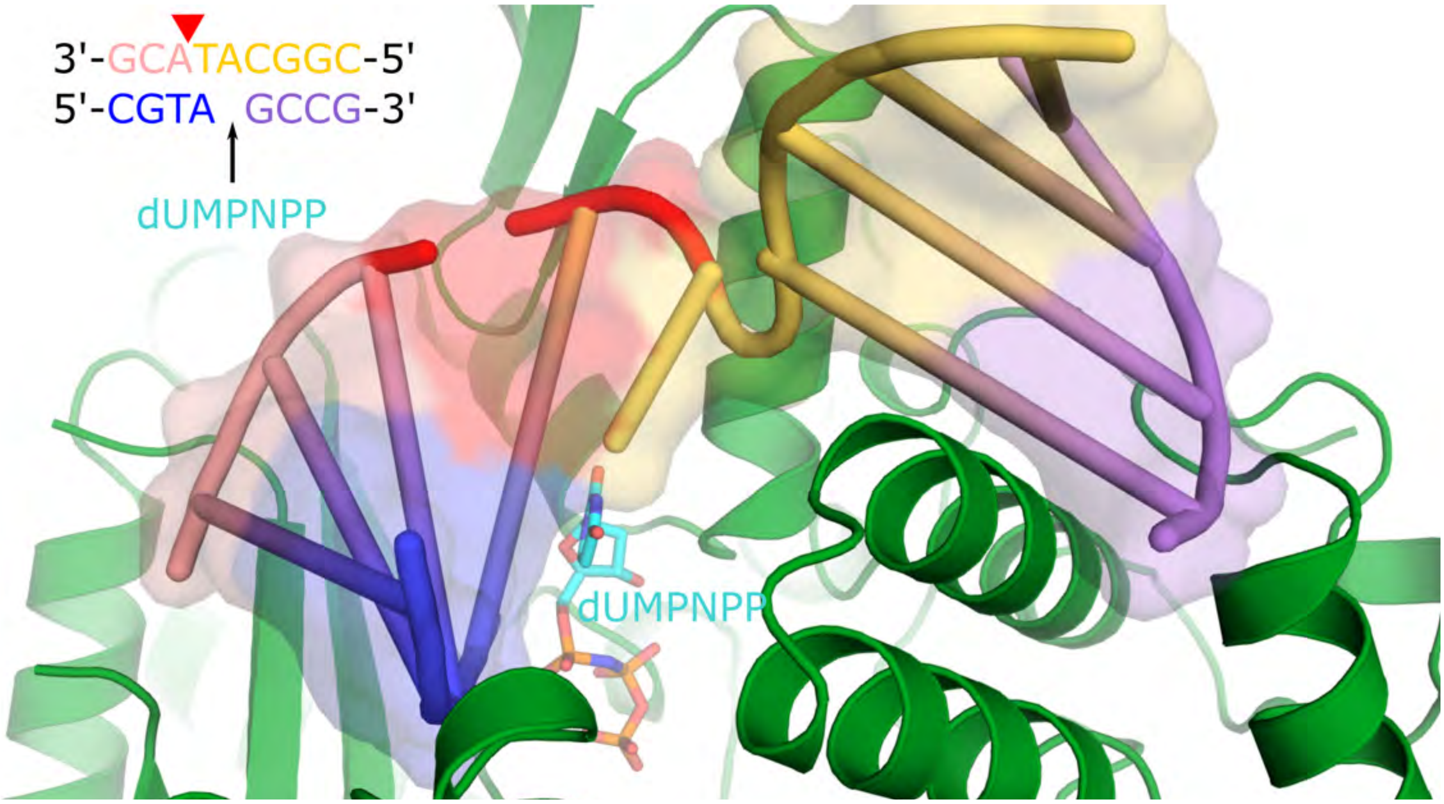
Author affiliation: The Pennsylvania State University

Correspondence: * sxt30@psu.edu

We thank the staff of NE-CAT for their help during synchrotron data collection. NE-CAT is funded by the National Institute of General Medical Sciences from the National Institutes of Health (P30 GM124165). The Eiger 16M detector on the 24-ID-E beamline is funded by a National Institutes of Health-Office of Research Infrastructure Programs High-End Instrumentation Grant (S10OD021527). This work was supported by Estonian Research Council grant PUTJD906 to P.E. and by National Institutes of Health, National Institute of General Medical Sciences grants R01 GM088236, R01 GM111651, and R35 GM127034 to S.T. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

NE-CAT 24-ID-E station

Capturing How DNA-Repair Enzymes Bridge the Gaps



It is well known that DNA is critical to life itself, playing a role in almost everything we do and impacting our health as well as disease. But what happens when this crucial but microscopically-thin double-stranded helix of nucleotides breaks? Researchers seeking to learn more about the answer to this question published results in *Nature Communications* based on work conducted at the APS. The work involved generating crystals that captured pre-catalytic and catalytic snapshots, *in crystallo*, of a DNA repair enzyme, Polμ, at the site of a DNA break, providing insights into the role of Polμ in DNA repair that will enhance our understanding of cancer and other diseases in which DNA breaks may play a role. — Sandy Field

Read the entire *APS Science* article here.

See: Andrea M. Kaminski[1], John M. Pryor[2], Dale A. Ramsden[2], Thomas A. Kunkel[1], Lars C. Pedersen[1]*, and Katarzyna Bebenek[1], "Structural snapshots of human DNA polymerase μ engaged on a DNA double-strand break," Nat. Commun. **11**, 4784 (2020). DOI: 10.1038/s41467-020-18506-5

Author affiliations: [1]National Institutes of Health, [2]University of North Carolina at Chapel Hill

Correspondence: * pederse2@niehs.nih.gov

This work was supported in part by the Division of Intramural Research of the National Institute of Environmental Health Sciences, National Institutes of Health Grants 1ZIA ES102645 (to L.C.P.) and Z01 ES065070 (to T. A.K.), and National Cancer Institute grant CA097096 (to D.A.R). SER-CAT is supported by its member institutions, and equipment grants (S10_RR25528 and S10_RR028976) from the National Institutes of Health. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

SER-CAT 22-ID-D station

New, Highly Potent, and Synthetic Inhibitors of an Adrenaline-Producing Enzyme

The enzyme phenylethanolamine N-methyltransferase (PNMT) is responsible for catalyzing the conversion of norepinephrine to epinephrine. It does this by transferring a methyl chemical group from a compound called S-adenosylmethionine (SAM) to norepinephrine. Evidence indicates that this protein may play a role in the age-related brain disorder Alzheimer's disease. In recent work published in the *Journal of the American Chemical Society*, a new series of synthetic PNMT inhibitors were described. These potent molecules are able to inhibit PNMT in the nanomolar range, and a structural analysis demonstrated how one of these inhibitors mediates this effect. Specifically, inhibitor 3 was shown to fill the catalytic binding pockets of SAM and the binding sites of norepinephrine, thereby preventing the ability of PNMT to work with either its cofactor (i.e., SAM) or its substrate (i.e., norepinephrine). The researchers in this study collected x-ray diffraction at the APS. Future research efforts are warranted to assess the effects of these new inhibitors *in vivo* and to determine whether or not they exacerbate disease symptoms in animal models of Alzheimer's disease. — Stephen Taylor

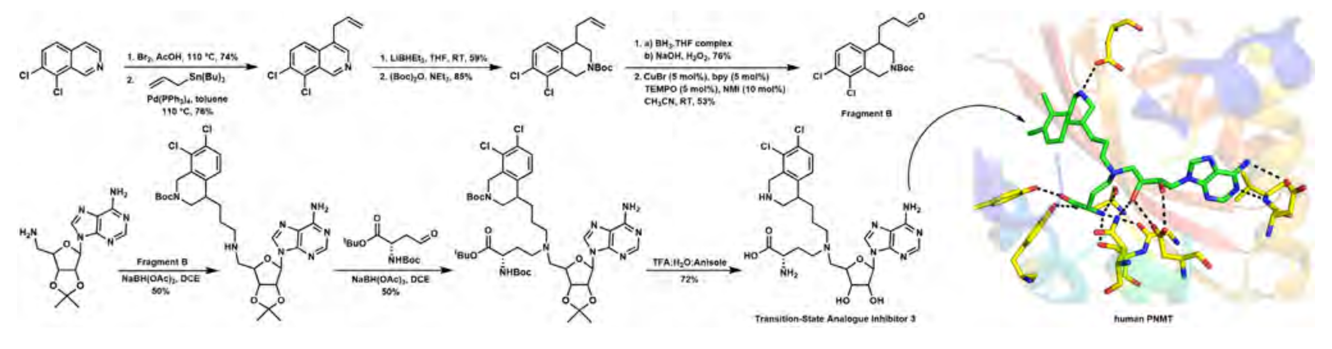
Read the entire *APS Science* article here.

See: Niusha Mahmoodi, Rajesh K. Harijan, and Vern L. Schramm*, "Transition-State Analogues of Phenylethanolamine N-Methyltransferase," J. Am. Chem. Soc. **142**, 14222 (2020).
DOI: 10.1021/jacs.0c05446

Correspondence: * vern.schramm@einsteinmed.org

This work was supported by National Institutes of Health (NIH) research grant GM041916. The Albert Einstein Crystallographic Core X-ray diffraction facility is supported by NIH Shared Instrumentation Grant S10 OD020068. Use of the LRL-CAT beamline was provided by Eli Lilly Co., which operates the facility. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357..

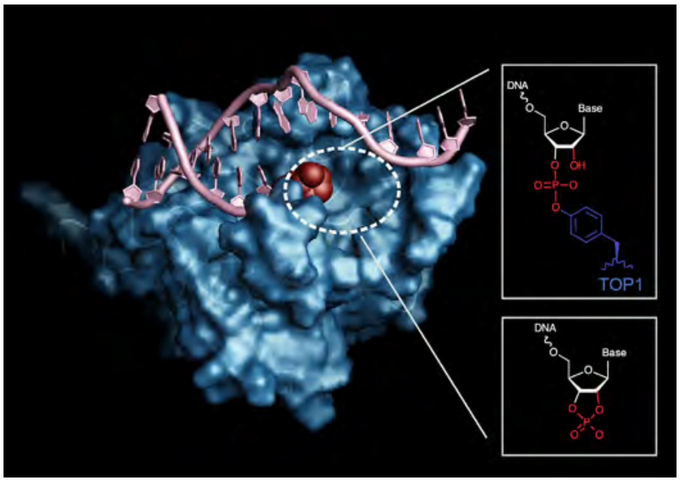
LRL-CAT 31-ID-D station



Stop the Repair, Stop the Cancer

The complex lengths to which many cells will go to replicate themselves is truly astounding. There is an intricate web of DNA repair mechanisms that help keep the cell running and dividing, and scientists continue to discover new threads in the tangle. A key motivation to studying DNA repair mechanisms is the possibility for developing new cancer therapeutics, as kinks in the DNA repair chain often portend uncontrolled growth. But then again, blocking DNA repair may be a useful strategy for targeting cancer cells. Using a slew of biochemical studies as well as a structural model of the catalytic domain of a previously mysterious repair protein called the APE2 nuclease—created using the APS—researchers discovered a new vulnerability for certain tumor cells. APE2 reverses DNA 3' blocks, lesions that preclude DNA synthesis and appear lethal to cells with cancer-causing BRCA 1 and 2 mutations, thereby allowing these cancer cells to divide. The findings, published in the journal *Molecular Cell*, suggest that drugs that inhibit APE2 could represent a new type of cancer treatment.. – Erika Gebel Berg

Read the entire *APS Science* article here.



See: Alejandro Álvarez-Quilón[1], Jessica L. Wojtaszek[2], Marie-Claude Mathieu[3], Tejas Patel[2], C. Denise Appel[2], Nicole Hustedt[1‡], Silvia Emma Rossi[1], Bret D. Wallace[2], Dheva Setiaputra[1], Salomé Adam[1], Yota Ohashi[1], Henrique Melo[1], Tiffany Cho[1, 4], Christian Gervais[5], Ivan M. Muñoz6, Eric Grazzini[5], Jordan T.F. Young[3], John Rouse[6], Michael Zinda[3], R. Scott Williams[2*], and Daniel Durocher[1, 4*], "Endogenous DNA 3' Blocks Are Vulnerabilities for BRCA1 and BRCA2 Deficiency and Are Reversed by the APE2 Nuclease," Mol. Cell **78**, 1152 (June 18, 2020). DOI: 10.1016/j.molcel.2020.05.021

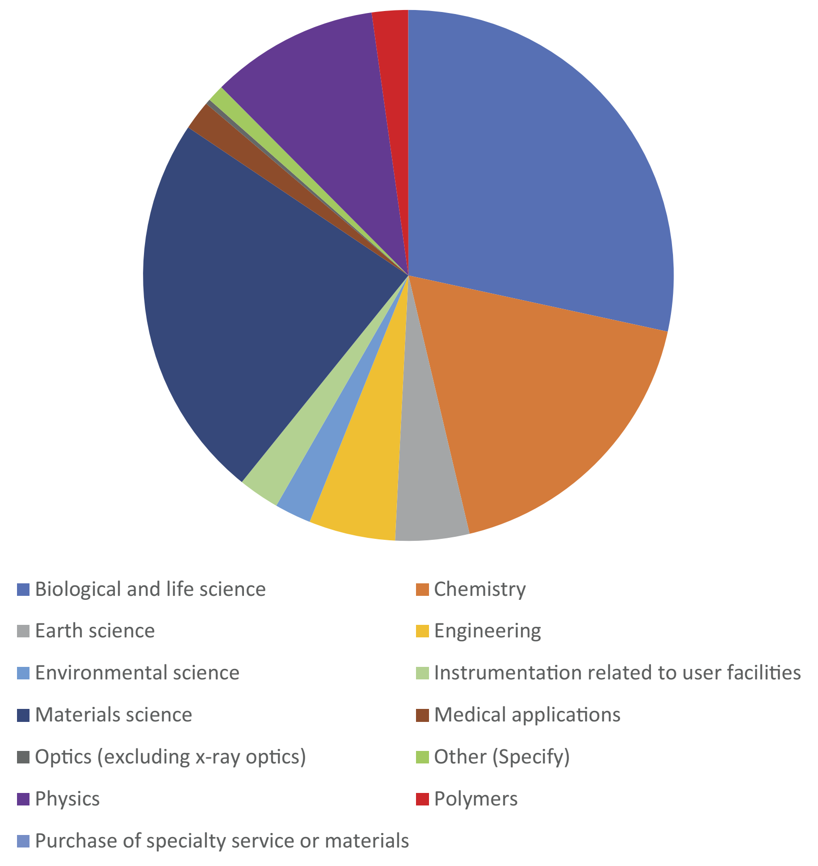
Author affiliations: [1]Mount Sinai Hospital, [2]U.S. Department of Health and Human Services, [3]Repare Therapeutics, [4]University of Toronto, [5]National Research Council Canada Human Health Therapeutics Research Center, [6]University of Dundee [‡]Present address: Ridgeline Therapeutics

Correspondence: * williamsrs@niehs.nih.gov, ** durocher@lunenfeld.ca

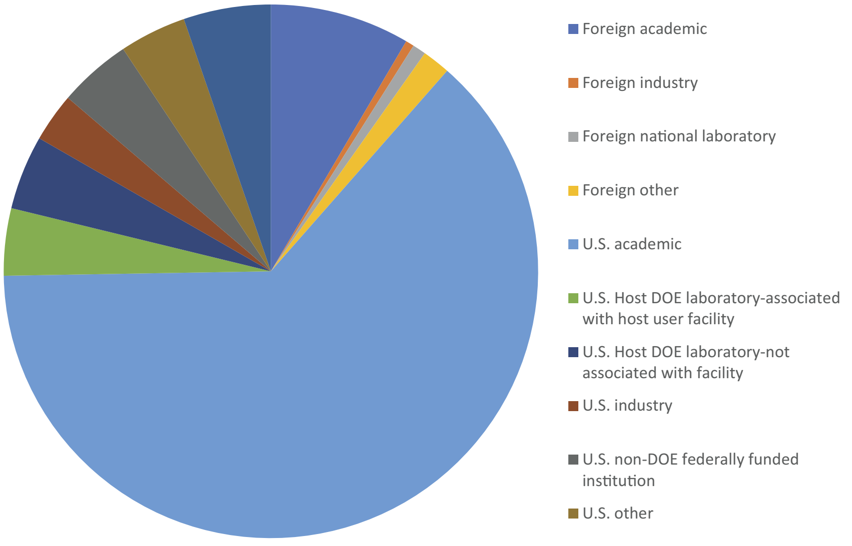
A.A.-Q. is a recipient of a long-term EMBO fellowship, D.S. was supported by a CIHR fellowship, and S.A. was a Banting postdoctoral fellow. Research in the R.S.W. laboratory was supported by National Institutes of Health Intramural Program, National Institute of Environmental Health Sciences (NIEHS) 1Z01ES102765. We thank L. Pedersen of the NIEHS Collaborative crystallography group for data collection support. SER-CAT is supported by its member institution equipment grants (S10_RR25528 and S10_RR028976) from the National Institutes of Health. D.D. is a Canada Research Chair (Tier I), and work in the D.D. lab was supported by grants from the CIHR (FDN143343) and Canadian Cancer Society (705644) with additional support from the Krembil Foundation and Repare Therapeutics. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

SER-CAT 22-ID-D station

APS USERS BY EXPERIMENT SUBJECT

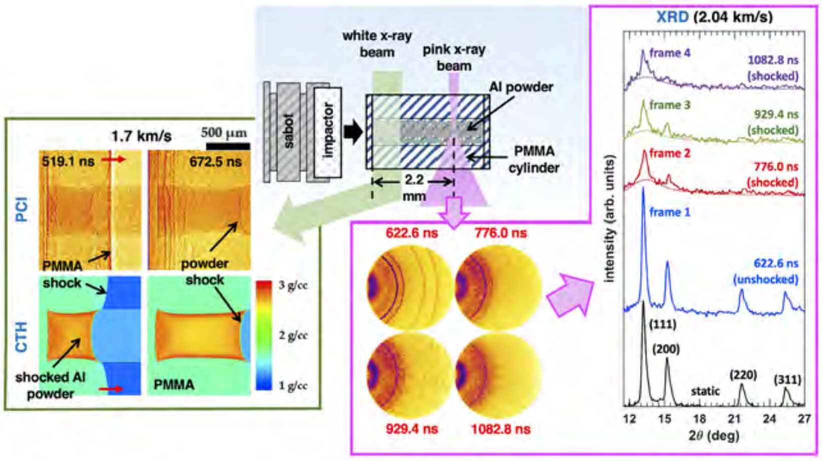


APS USERS BY EMPLOYER



Environmental, Geological, and Planetary Science

Shock-Induced Melting of a Porous Solid



When materials experience sudden, impulsive loading via impact, shock waves travel through those materials compressing them and often causing rapid structural changes, such as melting. Scientists using the APS have now directly observed, for the first time, such shock-induced melting in a porous solid. The insights these results provide into the mechanisms behind such melting could be valuable for materials scientists. They could also improve our understanding of high-impact collisions between planetesimals (small celestial bodies formed during the creation of planets) and crater formation, which are widespread in the solar system and involve shock-induced melting of porous solids such as regolith, rock, or ice. It could even help us figure out how to safely deflect potentially hazardous asteroids. The results were published in *Physical Review Materials*. – Michael Allen

Read the entire *APS Science* article here.

See: A. Mandal[1]*, B. J. Jensen[1], M. C. Hudspeth[2‡], S. Root[2], R. S. Crum[3], and M. C. Akin[3], "Direct observations of shock-induced melting in a porous solid using time-resolved x-ray diffraction," Phys. Rev. Mat. **4**, 063604 (2020).
DOI: 10.1103/PhysRevMaterials.4.063604

Author affiliations: [1]Los Alamos National Laboratory. [2]Sandia National Laboratories, [3]Lawrence Livermore National Laboratory ‡Present Address: XTD-NTA, Los Alamos National Laboratory

Correspondence: * anirban_mandal@lanl.gov

All PCI data shown here were obtained using LANL's novel multiframe x-ray phase contrast imaging (MPCI) system developed on the IMPULSE (IMPact System for ULtrafast Synchrotron Experiments) capability at APS. Nick Sinclair, Adam Schuman, Drew Rickerson, Brendan Williams, Yuelin Li, and other DCS team members are thanked for their assistance with the XRD and PCI experiments. A.M. and B.J.J. acknowledge the financial support from LANL's Science Campaigns, Joint Munitions Program, and MaRIE concept, and National Security Technologies Shock Wave Physics Related Diagnostic programs. LANL is operated by Triad National Security, LLC, for the National Nuclear Security Administration (NNSA) of the U.S. Department of Energy (DOE) under Contract No. 89233218CNA000001. M.C.H. and S.R. acknowledge financial support provided by the Truman fellowship (LDRD) and Science Campaigns within SNL. SNL is a multi-mission Laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's NNSA under Contract DENA0003525. R.S.C. and M.C.A.'s work was performed under the auspices of the U.S. DOE by LLNL under Contract No. DE-AC52-07NA27344 and was supported by LLNL Laboratory Directed R&D Program (tracking No. 16-ERD-010). The Dynamic Compression Sector is operated by Washington State University under the U.S. DOE/NNSA Award No. DENA0003957. This research used resources of the APS, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357..

DCS 35-ID-B,C,D,E station

Carbonate-induced Melting in the Deep Upper Mantle

Carbon is crucial in life, energy, climate, and other Earth systems. The Earth's upper mantle stores carbon, and carbonate-rich melts are important in regulating the deep carbon cycle where surficial carbon is subducted into Earth's mantle at convergent plate boundaries and is recycled to the atmosphere by partial melting and degassing at volcanoes. However, experimental challenges have kept researchers from determining the elastic properties of carbonate melts, which are important in seismic detection of such melts and decipher their stability in the Earth's mantle. This research, carried out at the APS, revealed the first sound velocity and density data of dolomite melt under upper mantle conditions. The results, published in the journal *Proceedings of the National Academy of Science of the United States of America*, will foster a better understanding of the role of carbon in the Earth's geochemical and geophysical systems.

— Dana Desonie

Read the entire *APS Science* article here.

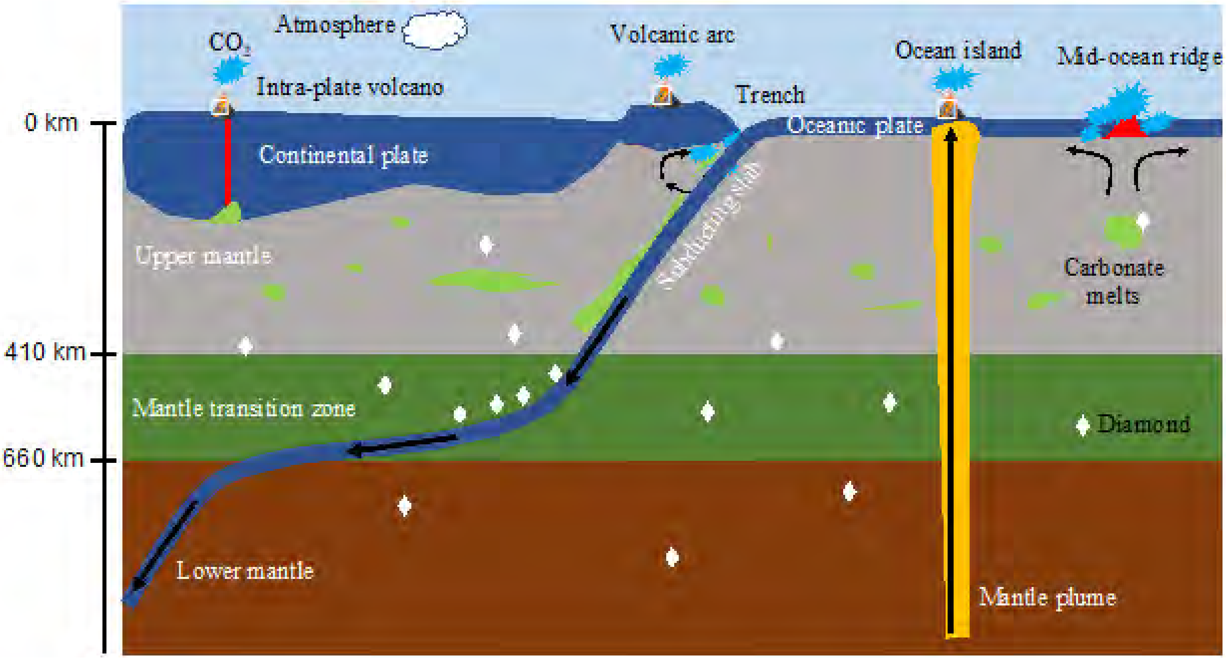
See: Man Xu[1,2], Zhicheng Jing[2]*, Suraj K. Bajgain[3], Mainak Mookherjee[3], James A. Van Orman[1], Tony Yu[4], and Yanbin Wang[4], "High-pressure elastic properties of dolomite melt supporting carbonate-induced melting in deep upper mantle," Proc. Natl. Acad. Sci. U.S.A. **117**(31), 18285 (August 4, 2020). DOI: 10.1073/pnas.2004347117

Author affiliations: [1]Case Western Reserve University, [2]Southern University of Science and Technology, [3]Florida State University, [4]The University of Chicago

Correspondence: * jingzc@sustech.edu.cn

This study was partly supported by the National Natural Science Foundation (NSF) (EAR-1619964 and 1620548) and the National Natural Science Foundation of China (41974098). S.K.B. and M.M. acknowledge funding from the NSF (EAR-1763215 and EAR-1753125) and XSEDE resources (TG-GEO170003). GSECARS is supported by the National Science Foundation-Earth Sciences (EAR-1634415). This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357.

GSECARS 13-ID-C,D station



Earth's Early Toxic Atmosphere

Venus is supremely uninhabitable due to its toxic carbon dioxide (CO_2)-rich atmosphere and runaway greenhouse effect. In research conducted in part at the APS, scientists revealed that Earth's early atmosphere resembled that found on Venus today (97% CO_2, 3% nitrogen [N2], and some water vapor), but then evolved differently due to its larger mass and greater distance from the Sun. This work, published in the journal Science Advances, provides a better understanding of the early evolution of Earth's atmosphere, and may help scientists identify planets elsewhere in the galaxy that may host living organisms. — Dana Desonie

Read the entire *APS Science* article here.

See: Paolo A. Sossi[1,2]*, Antony D. Burnham[3], James Badro[2], Antonio Lanzirotti[4], Matt Newville[4], and Hugh St.C. O'Neill[3], "Redox state of Earth's magma ocean and its Venus-like early atmosphere," Sci. Adv. **6**(48), eabd1387 (25 November 2020). DOI: 10.1126/sciadv.abd1387

Author affiliations: [1]Institute of Geochemistry and Petrology, [2]Institut de Physique du Globe de Paris, [3]Australian National University, [4]The University of Chicago

Correspondence: * paolo.sossi@erdw.ethz.ch

P.A.S. acknowledges support from SNSF Ambizione Fellowship grant no. 180025 and H.S.O. on IPGP visiting professorship in September 2017. A.D.B. and H.S.O. acknowledge support from ARC Laureate Fellowship no. FL130100066. Parts of this work were supported by the UnivEarthS Labex program (ANR-10-LABX-0023 and ANR-11-IDEX-0005-02) and IPGP multidisciplinary program PARI (Paris–IdF region SESAME Grant no. 12015908). GeoSoilEnviroCARS is supported by the National Science Foundation–Earth Sciences (EAR: 1634415). This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357

GSECARS 13-ID-E station

Image credit: Tobias Stierli/NCCR PlanetS.

Altering the Fate of Phosphorous Fertilizer in Mildly Calcareous Soils

Crops treated with phosphorous (P) fertilizer raise crop yields and return-on-investment. But phosphorous, a crucial plant nutrient, is sometimes the limiting factor in crop growth. Phosphorous management in P-limited, highly weathered acidic soils or soils containing calcium carbonate (i.e., calcareous) is challenging due to rapid P sorption reactions known as "P-fixation." Added P fertilizers are not always effective in calcareous soils, as the P precipitates out as calcium phosphate or adsorbs onto calcium carbonate. So, applying the right amount of P in the right form is challenging. The source of the phosphorous has been thought to be irrelevant, leaving the growers' choice to price and application method preference. Often excess phosphorous is applied, resulting in environmental degradation. A better understanding of the behavior of P in soils could lead growers to select the right form of fertilizer or researchers to develop new fertilizers that could increase profits and be better for the environment. This work, carried out at the APS and published in the S*oil Science Society of America Journal,* studied P partitioning in various liquid fertilizers, with different dilutions, and the presence or absence of a gelling agent in two mildly calcareous soils from Kansas. Results from controlled laboratory incubation studies in combination with synchrotron-based x-ray techniques, will help researchers and industries to re-visit the use of soil-test P methods and develop new fertilizers. — Dana Desonie

Read the entire *APS Science* article here.

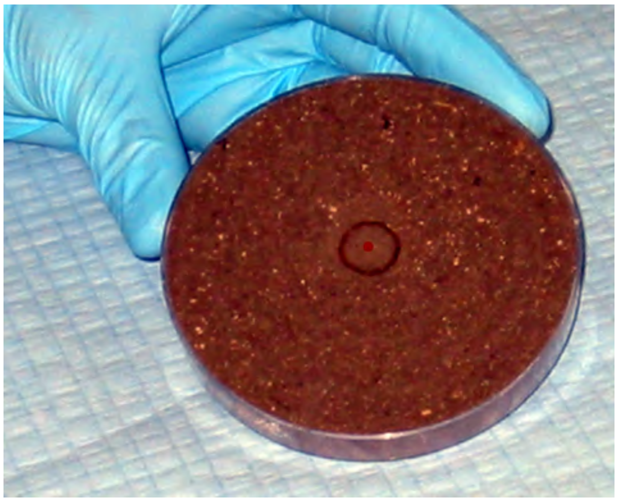
See: Joseph J. Weeks, Jr., and Ganga M. Hettiarachchi*, "Source and formulation matter: New insights into phosphorus fertilizer fate and transport in mildly calcareous soils," Soil Sci. Soc. Am. J. **84**,731 (2020). DOI: 10.1002/saj2.20054

Author affiliation: Kansas State University

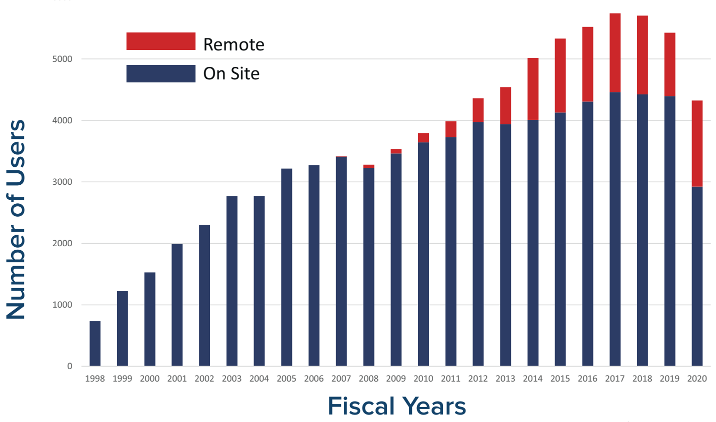
Correspondence: * ganga@ksu.edu

This work was supported by the Kansas State Research and Extension, The Fluid Fertilizer Foundation, Bio Huma Netics, Inc., and the USDA National Institute of Food and Agriculture NC-1187 Multistate Research Project. The authors thank Advanced Photon Source and the Canadian Light Source Incorporated for providing the opportunity to use their synchrotron facilities; the beamline scientists Tianpin Wu, George Sterbinsky, and Lu Ma at beamline 9 BM-B of Advanced Photon Source; and Yongfeng Hu and Qunfeng Xiao at SXRMB 06B1-1 of the Canadian Light Source. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

XSD Spectroscopy Group 9-BM-B,C station

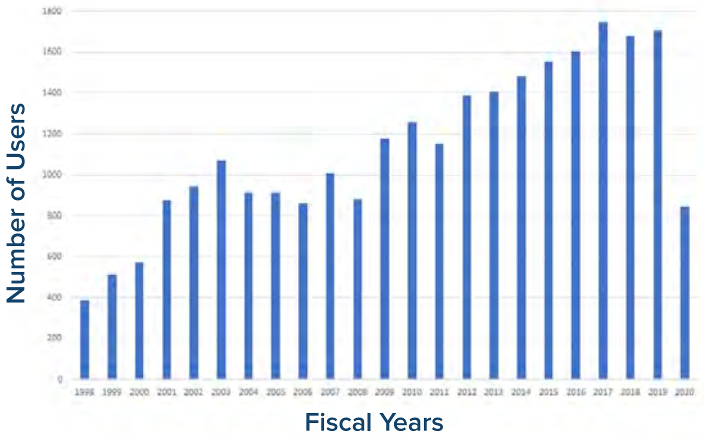


APS USERS, ON SITE AND REMOTE

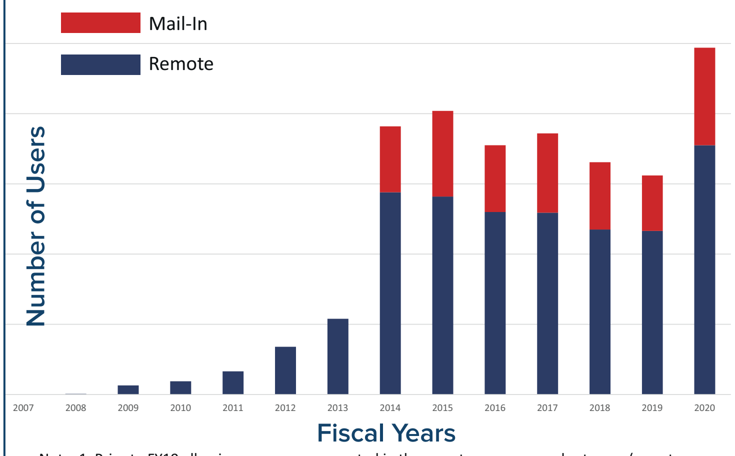


Note: 1. Prior to FY19 all unique users were counted in the remote user proposal category (remote access and mail-in) 2. In FY19 BES requested that only one unique user be counted for each remote user proposal (remote access and mail-in) 3. In FY20 BES requested that all unique users be counted for each remote access proposal and one unique user be counted for each mail-in proposal.

FIRST-TIME ON-SITE APS USERS



FIRST-TIME REMOTE APS USERS



Note: 1. Prior to FY19 all unique users were counted in the remote user proposal category (remote access and mail-in) 2. In FY19 BES requested that only one unique user be counted for each remote user proposal (remote access and mail-in) 3. In FY20 BES requested that all unique users be counted for each remote access proposal and one unique user be counted for each mail-in proposal.

Nanoscience

Broadening the Scope of Fluid Phase Transition Studies

The nanoscale structures that develop near the critical point of a phase transition are particularly fascinating in complex fluids. As a critical point is approached, large fluctuations emerge, driving many anomalous static and dynamic properties. Because the fluctuations extend over regions much larger than nearest-neighbor interactions, the details of these interactions become less important near a critical point, providing for a great deal of similarity in the critical behavior of diverse fluid systems. As a result, the divergent behavior of correlation lengths, susceptibilities, and fluctuation relaxation times can be described by scaling laws having universal features for a given class of transition. Researchers using the APS investigated the extent to which static and dynamic scaling laws apply to a larger region of study than had been investigated before in a complex fluid typical of those used in liquid-liquid extractions. The results were published in *Physical Review Letters*. — Vic Comello

Read the entire *APS Science* article here.

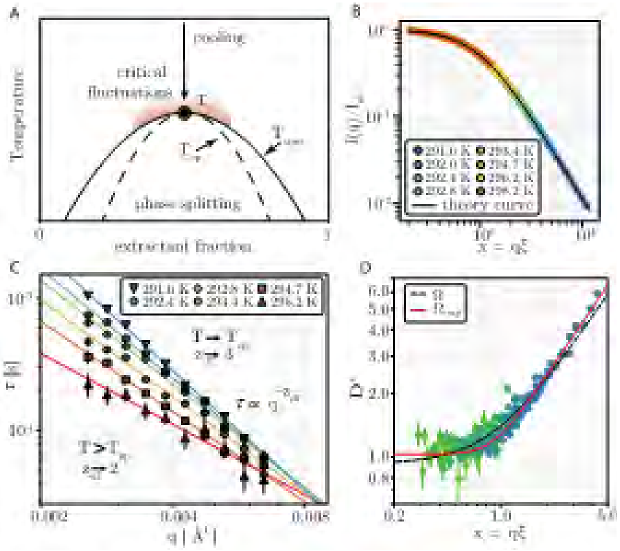
See: D. Sheyfer[1*], Qingteng Zhang[1], J. Lal[1,2], T. Loeffler[1], E. M. Dufresne[1], A. R. Sandy[1], S. Narayanan[1], S.K.R.S. Sankaranarayanan[1,3], R. Szczygiel[4], P. Maj[4], L. Soderholm[1], M. R. Antonio[1], and G. B. Stephenson[1**], "Nanoscale Critical Phenomena in a Complex Fluid Studied by X-ray Photon Correlation Spectroscopy," Phys. Rev. Lett. **125**, 125504 (2020).
DOI: 10.1103/PhysRevLett.125.125504

Author affiliations: [1]Argonne National Laboratory, [2]Northern Illinois University, [3]University of Illinois at Chicago, [4]AGH University of Science and Technology

Correspondence: * dsheyfer@anl.gov, ** gbs@anl.gov

The researchers acknowledge the expert technical assistance of R. Ziegler. Studies of critical phenomena in LLE systems were supported by LDRD funding from Argonne National Laboratory, provided by the Office of Science (OS) of the U.S. Department of Energy (DOE) under Contract No. DE-AC02-06CH11357. The authors acknowledge support from DOE OS-Basic Energy Sciences, Materials Science and Engineering Division (XPCS method and analysis development) and Chemical Sciences, Geosciences, and Biosciences Division (separation science). The detector development was supported by the National Centre for Research and Development, Poland (PBS1/A3/12/2012) and by the Polish National Agency for Academic Exchange (NAWA), under Contract No. PPI/APM/2018/1/00049/ U/001. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Dynamics & Structure Group 8-ID-I station



Seeking the Right Recipe for Better All-Solid-State Batteries

All-solid-state batteries are a promising next-generation power source for electric vehicles and consumer electronics. Replacing the liquid electrolyte with a solid could let battery makers use electrodes that hold more energy, potentially doubling the distance an electric car could drive on a single charge. At the same time, solid electrolytes should be less flammable, and therefore less potentially dangerous than existing lithium-ion batteries. The trick will be in designing solid-state batteries that are sufficiently robust to last the lifetime of an electric vehicle. Scientists using the APS have uncovered some of the properties that could help build a better battery. Their research was published in the journal *Joule.* — Neil Savage

Read the entire *APS Science* article here.

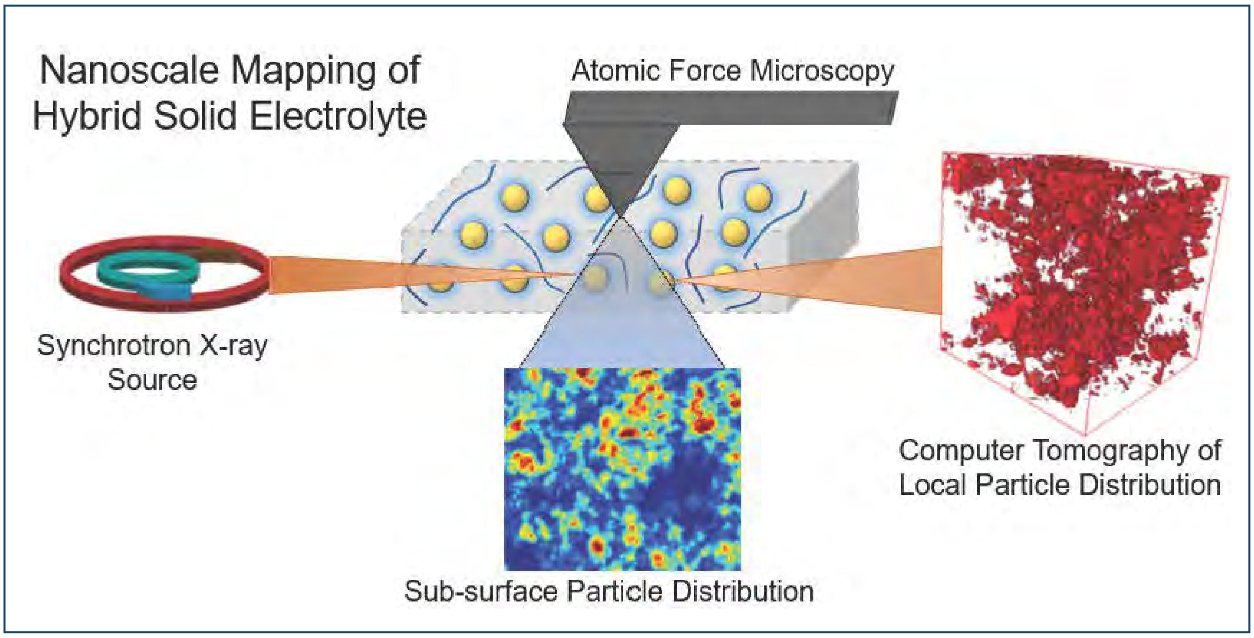
See: Marm B. Dixit[1], Wahid Zaman[1], Nicholas Hortance[1], Stella Vujic[1], Brice Harkey[1], Fengyu Shen[1], Wan-Yu Tsai[2], Vincent De Andrade[3], X. Chelsea Chen[2], Nina Balke[2], and Kelsey B. Hatzell[1]*, "Nanoscale Mapping of Extrinsic Interfaces in Hybrid Solid Electrolytes," Joule **4**, 207 (January 15, 2020). DOI: 10.1016/j.joule.2019.11.015

Author affiliations: [1]Vanderbilt University, [2]Oak Ridge National Laboratory, [3]Argonne National Laboratory

Correspondence: * kelsey.b.hatzell@vanderbilt.edu

The authors were supported by the National Science Foundation under grant nos. 1727863 and 1847029. AFM measurements were supported by the Fluid Interface Reactions, Structures and Transport (FIRST) Center, an Energy Frontier Research Center (EFRC) funded by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences (W.-Y.T. and N.B.). The experiments and sample preparation in this work were performed and supported at the Center for Nanophase Materials Sciences in Oak Ridge National Lab, which is a DOE Office of Science user facility. Part of the electrochemical and materials characterization was supported by the U.S. DOE Office of Science-Basic Energy Sciences, Materials Science and Engineering Division (X.C.C.). This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science user facility operated for the DOE Office of Science by the Argonne National Laboratory under contract no. DE-AC02-06CH11357.

XSD Imaging Group 32-ID-B,C station



Controlling the Rheology of Toxic Wastes

The fragmentation and aggregation of anisotropic nanoparticles under flow is governed by the interplay of hydrodynamic and colloidal forces. For this work, these multi-institution researchers developed a technique in which they measured boehmite nanoparticle clusters as they recirculated through a capillary rheometer at the APS. Understanding the behavior of nanoparticles under flow is important for applications in engineering, materials science, and chemistry. The ability to control the rheology (deformation and flow) of toxic wastes, including high-level nuclear wastes, is essential for their long-term storage. This research, published in the *Journal of Colloid and Interface Science*, will help workers control rheology in the transfer and treatment of Hanford wastes and in many other applications. — Dana Desonie

Read the entire *APS Science* article here.

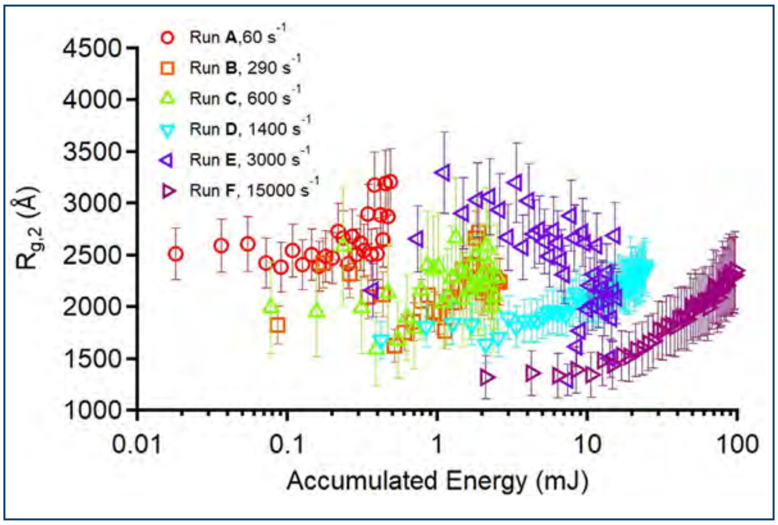
See: Anthony J. Krzysko[1,2], Elias Nakouzi[2], Xin Zhang[2], Trent R. Graham[2], Kevin M. Rosso[2], Gregory K. Schenter[2], Jan Ilavsky[3], Ivan Kuzmenko[3], Matthew G. Frith[3], Cornelius F. Ivory[1], Sue B. Clark[1,2], Javen S. Weston[4], Katie M. Weigandt[5], James J. De Yoreo[1, 6], Jaehun Chun[2]*, and Lawrence M. Anovitz[7]**, "Correlating inter-particle forces and particle shape to shear-induced aggregation/fragmentation and rheology for dilute anisotropic particle suspensions: A complementary study via capillary rheometry and *in-situ* small and ultra-small angle X-ray scattering," J. Colloid Interf. Sci. **576**, 47 (September 2020). DOI: 10.1016/j.jcis.2020.04.016 Figure © 2021 Elsevier B.V. or its licensors or contributors.

Author affiliations: [1]Washington State University, [2]Pacific Northwest National Laboratory, [3]Argonne National Laboratory, [4]University of Tulsa, [5]National Institute of Standards and Technology, [6]University of Washington, [7]Oak Ridge National Laboratory

Correspondence: * jaehun.chun@pnnl.gov, ** anovitzlm@ornl.gov

This research was supported by the Interfacial Dynamics in Radioactive Environments and Materials (IDREAM), an Energy Frontier Research Center funded by the U.S. Department of Energy (DOE) Office of Science-Basic Energy Sciences. PNNL is a multiprogram national laboratory operated for DOE by Battelle Memorial Institute under Contract No. DE-AC05-76RL0-1830. A.J.K. is grateful for the support from the PNNL-WSU DGRP and the DOE-SCGSR. This material is based upon work supported by the U.S. DOE Office of Science Graduate Student Research (SCGSR) program. The SCGSR program is administered by the Oak Ridge Institute for Science and Education (ORISE) for the DOE. ORISE is managed by ORAU under contract number DE-SC0014664. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract DE-AC02-06CH11357.

XSD Chemical & Materials Science 9-ID-B,C station



Giving RNA the Golden Touch by Adding to its Alphabet

Ribonucleic acid, or RNA, is a molecule that is essential in a variety of cellular processes centered on protein synthesis and gene expression. Consequently, being able to study its structure and function is key to developing a better understanding of various disease processes and to developing therapeutics. Toward that end, researchers have sought to develop labels to attach to both natural and synthetic RNAs to elucidate their structure, locate them in cells, and visualize their interactions with other molecules. The majority of RNA labeling thus far has relied on solid-phase synthesis, a technique in which researchers incorporate chemical tags into synthetic RNA. Though this method has proven useful for smaller RNAs under 100 nucleotides, the units that make up nucleic acids, it doesn't work for larger pieces of RNA. Looking for a better way to label large RNAs, scientists in this study developed a new method that involves creating synthetic RNA strands that incorporate an unnatural nucleotide modified with chemical groups that can bind gold nanoparticles. Using the APS, the researchers performed a proof-of-principle study showing that attaching one or two gold nanoparticles onto large RNAs from the dengue virus genome can function as a molecular ruler, allowing them to collect data that supports a conformational change this viral genome needs to alternate between creating proteins and replicating itself. Their results were published in the *Proceedings of the National Academy of Sciences of the United States of America*. — Christy Brownlee

Read the entire *APS Science* article here.

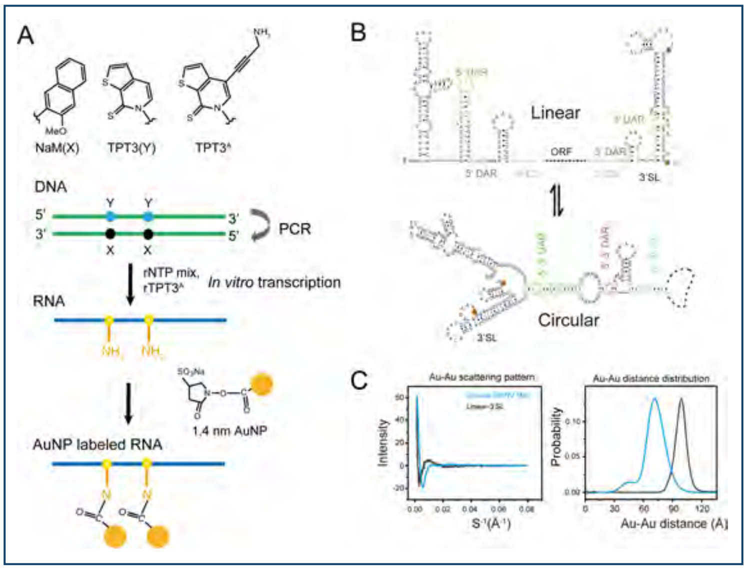
See: Yan Wang, Yaoyi Chen, Yanping Hu, and Xianyang Fang*, "Site-specific covalent labeling of large RNAs with nanoparticles empowered by expanded genetic alphabet transcription," Proc. Natl. Acad. Sci. U.S.A. **117**(37), 22823 (September 15, 2020). DOI: 10.1073/pnas.2005217117

Author affiliation: Tsinghua University

Correspondence: * fangxy@tsinghua.edu.cn

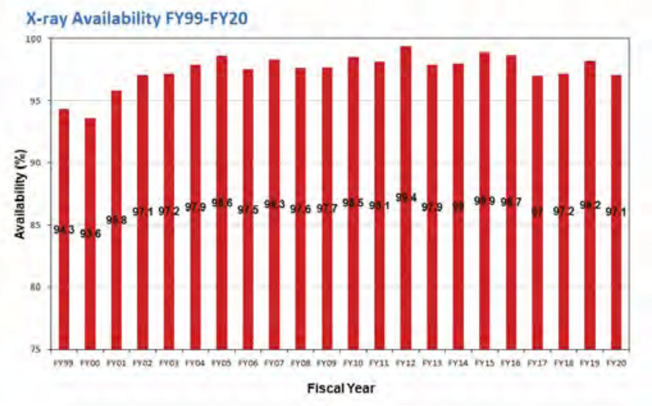
The authors thank Xiaobing Zuo at the beamline 12-ID-B, Advanced Photon Source, Argonne National Laboratory for assistance during data collection. This work was supported by grants from the National Natural Science Foundation of China (U1832215), the Beijing Advanced Innovation Center for Structural Biology, and the Tsinghua-Peking Joint Center for Life Sciences to X.F. This research used resources of the Advanced Photon Source, a U.S. Department of Energy (DOE) Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357.

XSD Chemical & Materials Science 12-ID-B station

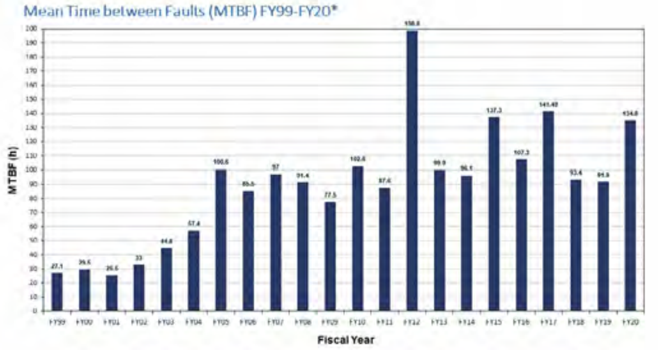


APS X-ray Availability and Reliability

In fiscal year 2020*, the APS x-ray source continued to function as a highly reliable delivery system for synchrotron x-ray beams for research. Several factors support the overall growth in both the APS user community and the number of experiments carried out by that community. But there is a direct correlation between the number of x-ray hours available to users; the success of the APS experiment program; and the physicists, engineers, and technicians responsible for achieving and maintaining optimum x-ray source performance. Below are definitions of important measures for the delivery of x-ray beam to users (latest data shown graphically).



X-ray Availability: The number of hours that beam is available to users divided by the number of hours of scheduled beam delivery prior to the beginning of a run. The specific definition of available beam is that the APS main control room has granted permission to users to open shutters, and there is more than 50-mA stored beam in the storage ring.



Storage Ring Reliability: A measure of the mean time between beam losses (faults), or MTBF, calculated by taking the delivered beam and dividing by the total number of faults. The APS targets, and routinely exceeds, 70 h MTBF. A fault is defined as complete unavailability of beam either via beam loss or removal of shutter permit not related to weather. A fault also occurs when beam has decayed to the point where stability and orbit can no longer be considered reliable (50 mA).

* While the highlights in, and title of, this report cover calendar year 2020, data on accelerator performance and user statistics are measured on the basis of fiscal years.

Typical APS Machine Parameters

Linac

Output energy	425 MeV
Output beam charge	0.3–3 nC
Normalized emittance	5–20 mm-mrad
Frequency	2.856 GHz
Modulator pulse rep rate	30 Hz
Gun rep rate	2–26 Hz
(1-13 pulses, 33.3 ms apart every 0.5 s)	
Beam pulse length	8–15 ns
Bunch length	1–10 ps FWHM

Particle Accumulator Ring

Nominal energy	425 MeV
Circumference	30.66 m
Cycle time	0.5 s or 1 s
Fundamental radio frequency (RF1)	9.77 MHz
12th harmonic RF frequency (RF12)	117.3 MHz
RMS bunch length (after compression)	0.34 ns

Injector Synchrotron (Booster)

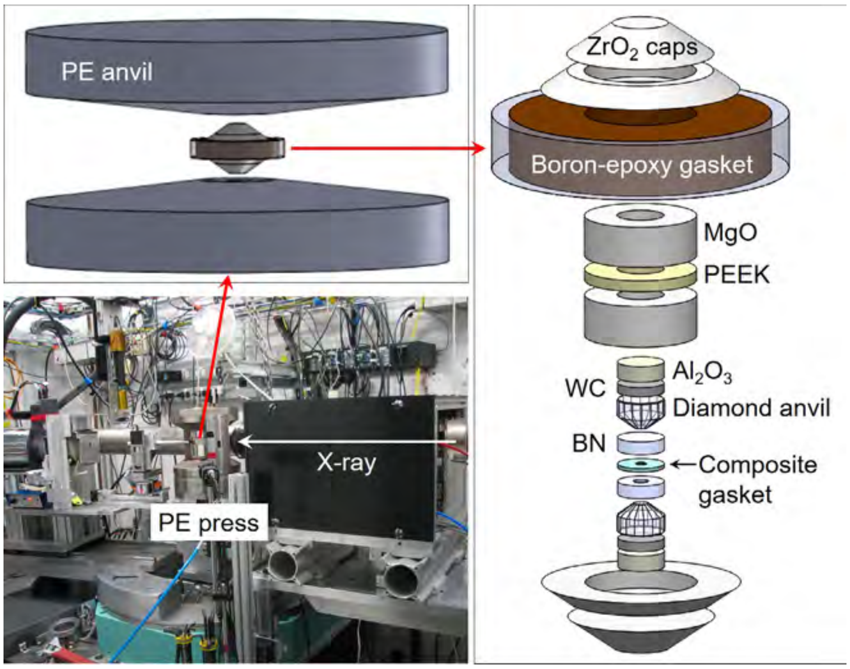
Nominal extraction energy	7.0 GeV
Injection energy	425 MeV
Circumference	368.0 m
Ramping rep rate	2 Hz or 1 Hz
Natural emittance	132 nm-rad (nominal) 87 nm-rad (actual)
Booster RMS bunch length	100 ps
Radio frequency	351.935 MHz

Storage Ring System

Nominal energy	7.0 GeV
Circumference	1104 m
Number of sectors	40
Length available for insertion device	5.0 m
Nominal circulating current, multibunch	100 mA
Natural emittance	2.5 nm-rad
RMS momentum spread	0.096%
Effective emittance	3.1 nm-rad
Vertical emittance	0.040 nm-rad
Coupling (operating)	1.5%
Revolution frequency	271.555 kHz
Radio frequency	351.935 MHz
Operating number of bunches	24 to 324
RMS bunch lengths	33 ps to 25 ps
RMS bunch length of 16 mA in hybrid mode	50 ps

Novel Accelerator and X-ray Techniques and Instrumentation

New Technique Traces the Structural Evolution of SiO_2 Glass at Ultrahigh Pressures



The ultrahigh-pressure behavior of silicon dioxide (SiO_2) glass has attracted considerable attention because of its importance not only in high-pressure physics and materials science but also in geophysics. The physical properties of silicate melts and glasses at ultrahigh pressures and temperatures play fundamental roles in present-day magmatic processes in the Earth's interior and are key to understanding the evolution of the early Earth. Although the structural development of SiO_2 glass at moderate pressures (below 50 GPa) is well-known, its evolution in the ultrahigh-pressure (Mbar) regime remains controversial partly due to conflicting values of the Si coordination number (CSi) (number of ions bonded to Si). Even though many structural properties of network-forming glasses like SiO_2 can be obtained from the structure factor S(Q), its determination in x-ray diffraction experiments has proved problematic at ultrahigh pressures. Such experiments are usually conducted using diamond anvil cells that permit only small sample sizes and very limited momentum transfer (Q) ranges, which are serious limitations in studying SiO_2 glass due to the inherently low scattering signal. To overcome these difficulties, a group of researchers using the APS conducted ultrahigh-pressure measurements of S(Q) using their recently developed opposed-anvil-type double-stage large-volume cell press. These results, published in *Physical Review Letters*, provide important implications for understanding the mechanisms underlying the pressure-induced structural evolution of network-forming glasses in physics and materials sciences, and also for investigating the nature of silicate magmas in geophysics. — Vic Comello

Read the entire *APS Science* article here.

See: Yoshio Kono[1,2*‡], Yu Shu[3], Curtis Kenney-Benson[3], Yanbin Wang[4], and Guoyin Shen[3], "Structural Evolution of SiO_2 Glass with Si Coordination Number Greater than 6," Phys. Rev. Lett. **125**, 205701 (2020).
DOI: https://doi.org/10.1103/PhysRevLett.125.205701

Author affiliations: [1]Carnegie Institution of Washington, [2]Ehime University, [3]Argonne National Laboratory, [4]The University of Chicago, ‡Present address: Ehime University

Correspondence: * kono.yoshio.rj@ehime-u.ac.jp

This research was supported by the National Science Foundation under Grant No. EAR-1722495. HPCAT-XSD operations are supported by the U.S. Department of Energy (DOE-NNSA) National Nuclear Security Administration's Office of Experimental Sciences. Y. K. acknowledges support by JSPS KAKENHI Grants No. 19KK0093 and No. 20H00201, and by JSPS Bilateral Program Grant No. JPJSBP120209926. Y. W. acknowledges NSF support EAR-1620548. This research used resources of the Advanced Photon Source, a U.S. DOE Office of Science User Facility operated for the DOE Office of Science by Argonne National Laboratory under Contract No. DE-AC02-06CH11357

HPCAT-XSD 16-BM-B station

Capturing Protein Motions from Thousands of Fragile Protein Crystals

To understand how proteins participate in physiological processes, scientists probe crystallized proteins using x-ray diffraction to determine their structures and how those structures change during physiological activities. However, proteins are fragile (compared with other carbon-based materials) and data collection conditions for investigating them don't always correspond to the protein's physiological temperature. A team of collaborators made changes to the basic diffractometer design to address these issues and using the APS demonstrated how their new diffractometer platform automatically conducts large-scale, serial Laue diffraction at room temperature directly from the devices where the crystals were grown. The results were published in *IUCrJ*.

Read the entire *APS Science* article here.

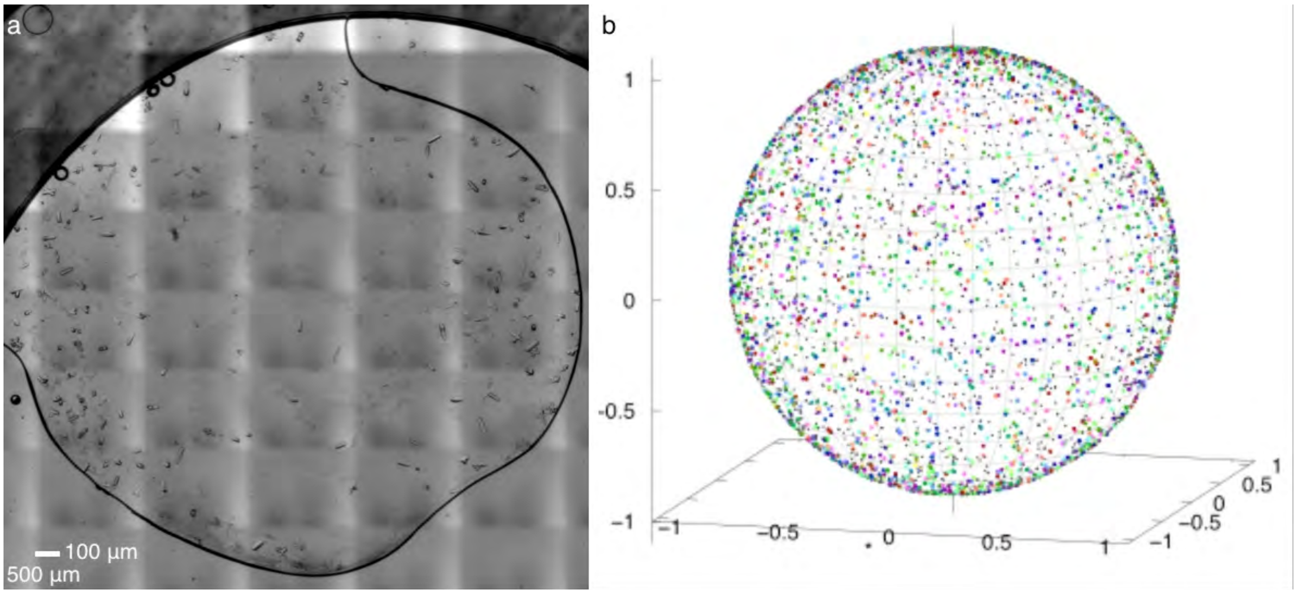
See: Zhong Ren[1,2]* Cong Wang[1], Heewhan Shin[1], Sepalika Bandara[1], Indika Kumarapperuma[1], Michael Y. Ren[3], Weijia Kang[1], and Xiaojing Yang[1]**, “An automated platform for *in situ* serial crystallography at room temperature,” IUCrJ **7**(6), 1009 (November 2020). DOI: 10.1107/S2052252520011288

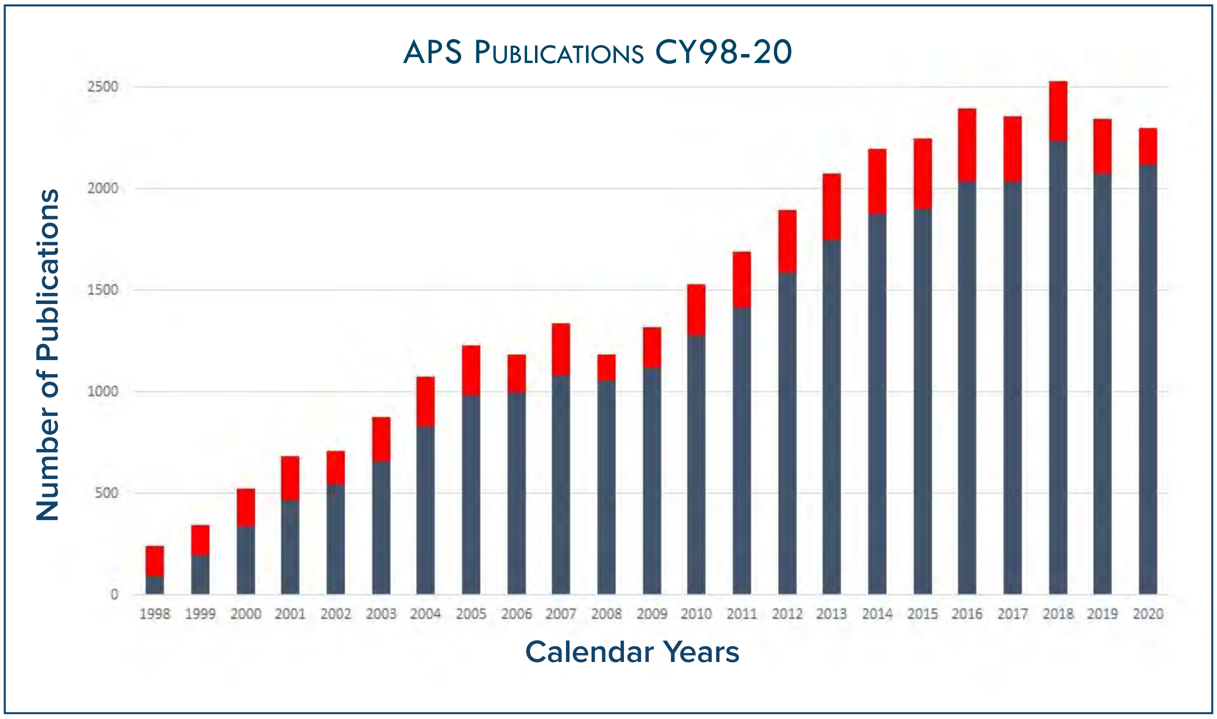
Author affiliations: [1]University of Illinois at Chicago, [2]Renz Research, Inc., [3]University of Maryland,

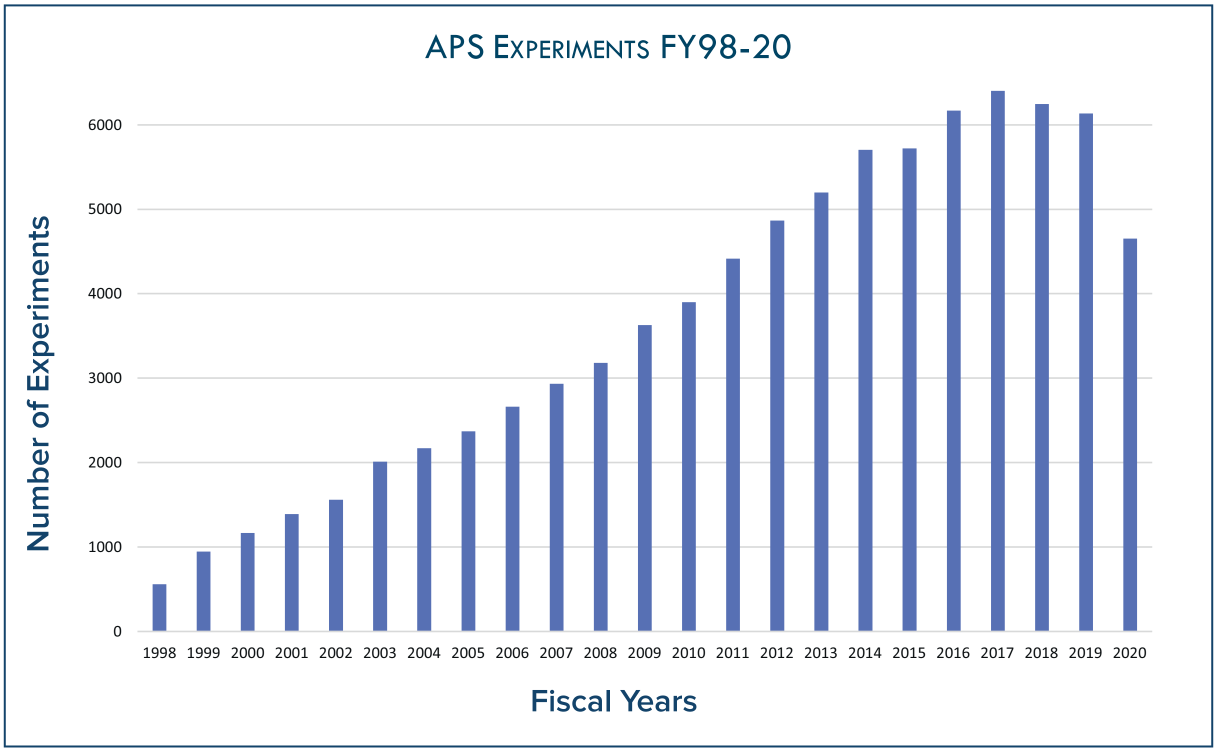
Correspondence: * zren@uic.edu, ** xiaojing@uic.edu

This work is supported by grants from the University of Illinois at Chicago, the National Institutes of Health (grant No. R01EY024363 awarded to X.Y.), and the National Science Foundation (grant No. MCB2017274 awarded to X.Y.). Use of BioCARS was supported by the National Institute of General Medical Sciences of the National Institutes of Health (grant No. P41 GM118217). Use of the Life Sciences Collaborative Access Team was supported by the Michigan Economic Development Corporation and the Michigan Technology Tri- Corridor (grant No. 085P1000817).

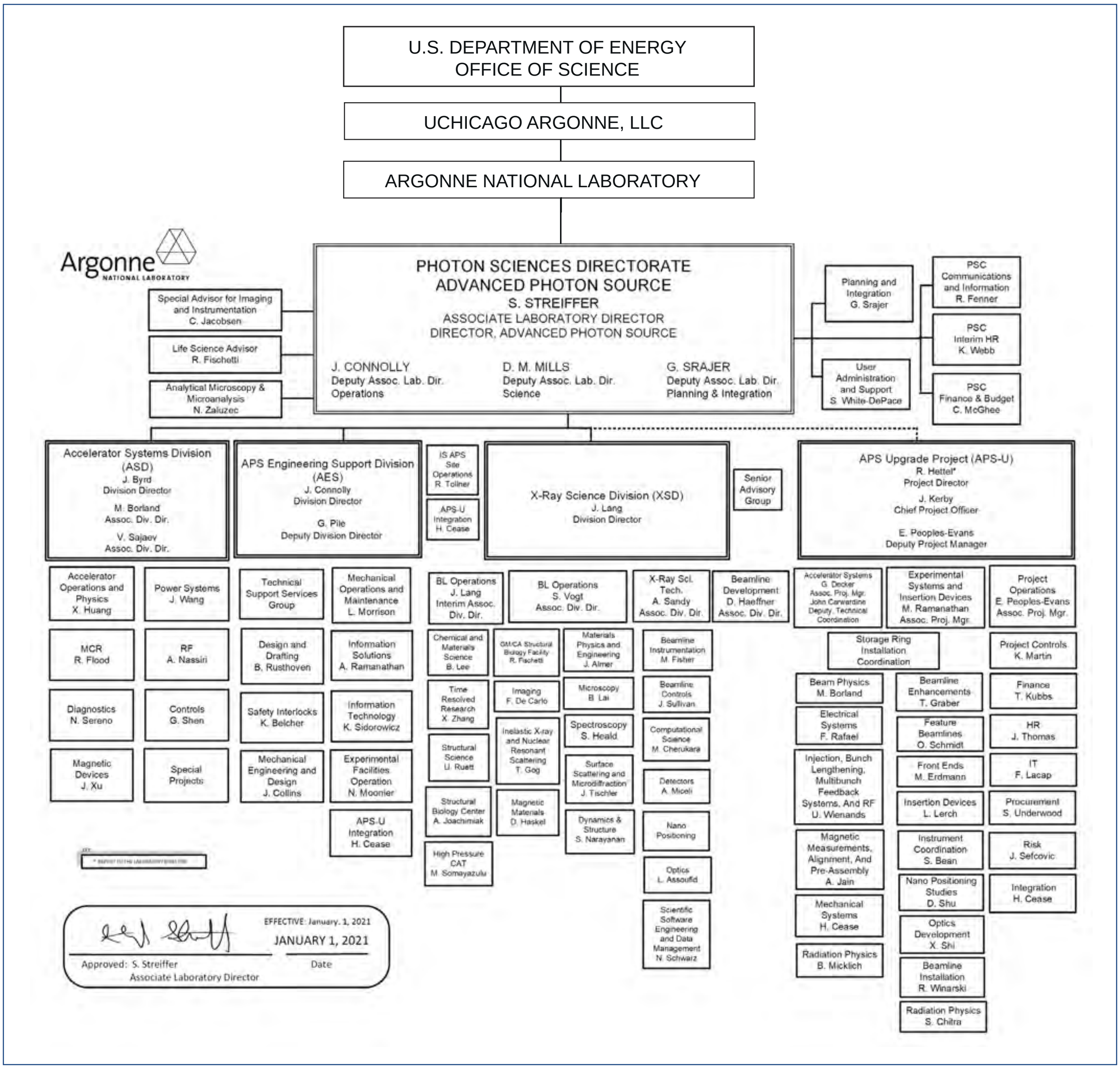
BioCARS 14-ID-B & LS-CAT 21-ID-D stations




APS Publications CY98-20
Number of Publications
0
500
1000
1500
2000
2500
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018
2019
2020
Calendar Years


APS Experiments FY98-20
Number of Experiments
0
1000
2000
3000
4000
5000
6000
1998
1999
2000
2001
2002
2003
2004
2005
2006
2007
2008
2009
2010
2011
2012
2013
2014
2015
2016
2017
2018
2019
2020
Fiscal Years

Photon Sciences Directorate Organization Chart



APS Source Parameters

Undulator A (33 insertion devices [IDs] in 26 sectors)

Period: 3.30 cm
Length: 2.1 m in sectors 16, 21, 23, 24, 25, 28, 34; 2.3 m in Sector 6; 2.4 m in sectors 1, 2, 5, 7, 8, 9, 10, 11, 15, 17, 18, 19, 20, 22, 26, 28, 31, 32, 33
Minimum gap: 10.5 mm
B_{max}/K_{max}: 0.892 T/2.75 (effective; at minimum gap)
Tuning range: 3.0–13.0 keV (1st harmonic)
3.0–45.0 keV (1st–5th harmonic)
On-axis brilliance at 7 keV (ph/s/mrad^2/mm^2/0.1%bw):
4.1 x 10^{19} (2.4 m), 4.0 x 10^{19} (2.3 m), 3.3 x 10^{19} (2.1 m)
Source size and divergence at 8 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 12.7 μrad (2.4 m), 12.8 μrad (2.3 m), 12.9 μrad (2.1 m)
$\Sigma_{y'}$: 6.7 μrad (2.4 m), 6.8 μrad (2.3 m), 7.1 μrad (2.1 m)

2.30-cm Undulator (2 IDs in sectors 11, 14)

Period: 2.30 cm Length: 2.4 m
Minimum gap: 10.5 mm
B_{max}/K_{max}: 0.558 T/1.20 (effective; at minimum gap)
Tuning range: 11.8–20.0 keV (1st harmonic)
11.8–70.0 keV (1st-5th harmonic, non-contiguous)
On-axis brilliance at 12 keV (ph/s/mrad^2/mm^2/0.1%bw): 6.9 x 10^{19}
Source size and divergence at 12 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 12.3 μrad $\Sigma_{y'}$: 5.9 μrad

2.70-cm Undulator (5 IDs in sectors 3, 12, 14, 35)

Period: 2.70 cm
Length: 2.1 m in Sector 12; 2.4 m in sectors 3, 14, and 35
Minimum gap: 10.5 mm
B_{max}/K_{max}: 0.698 T/1.76 (effective; at minimum gap)
Tuning range: 6.7–16.0 keV (1st harmonic)
6.7–60.0 keV (1st-5th harmonic, non-contiguous)
On-axis brilliance at 8.5 keV (ph/s/mrad^2/mm^2/0.1%bw):
5.7 x 10^{19} (2.4 m), 4.7 x 10^{19} (2.1 m)
Source size and divergence at 8 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 12.7 μrad (2.4 m), 12.9 μrad (2.1 m)
$\Sigma_{y'}$: 6.7 μrad (2.4 m), 7.1 μrad (2.1 m)

3.00-cm Undulator (8 IDs in sectors 12, 13, 16, 21, 23, 27, 34)

Period: 3.00 cm
Length: 2.1 m in sectors 12, 13, 16, 21, 23, 34; 2.4 m in Sector 27
Minimum gap: 10.5 mm
B_{max}/K_{max}: 0.787 T/2.20 (effective; at minimum gap)
Tuning range: 4.6–14.5 keV (1st harmonic)
4.6–50.0 keV (1st-5th harmonic)
On-axis brilliance at 8 keV (ph/s/mrad^2/mm^2/0.1%bw):
4.8 x 10^{19} (2.4 m), 3.9 x 10^{19} (2.1 m)
Source size and divergence at 8 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 12.7 μrad (2.4 m), 12.9 μrad (2.1 m)
$\Sigma_{y'}$: 6.7 μrad (2.4 m), 7.1 μrad (2.1 m)

3.50-cm SmCo Undulator (Sector 4)

Period: 3.50 cm Length: 2.4 m
Minimum gap: 9.75 mm
B_{max}/K_{max}: 0.918 T/3.00 (effective; at minimum gap)
Tuning range: 2.4–12.5 keV (1st harmonic)
2.4–42.0 keV (1st-5th harmonic)
On-axis brilliance at 7 keV (ph/s/mrad^2/mm^2/0.1%bw): 3.7 x 10^{19}
Source size and divergence at 8 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 12.7 μrad $\Sigma_{y'}$: 6.7 μrad

3.60-cm Undulator (Sector 13)

Period: 3.60 cm
Length: 2.1 m
Minimum gap: 11.0 mm
B_{max}/K_{max}: 0.936 T/3.15 (effective; at minimum gap)
Tuning range: 2.2–11.8 keV (1st harmonic)
2.2–40.0 keV (1st-5th harmonic)
On-axis brilliance at 6.5 keV (ph/s/mrad^2/mm^2/0.1%bw): 2.8 x 10^{19}
Source size and divergence at 8 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 12.9 μrad $\Sigma_{y'}$: 7.1 μrad

1.72-cm Undulator (3 IDs in sectors 30, 35)

Period: 1.72 cm
Length: 4.8 m (2 x 2.4 m) in Sector 30; 2.4 m in Sector 35
Minimum gap: 10.6 mm
B_{max}/K_{max}: 0.330 T/0.53 (effective; at minimum gap)
Tuning range: 23.7–26.3 keV (1st harmonic)
On-axis brilliance at 23.7 keV (ph/s/mrad^2/mm^2/0.1%bw):
1.0 x 10^{20} (4.8 m), 4.4 x 10^{19} (2.4 m)
Source size and divergence at 23.7 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 11.6 μrad (4.8 m) 11.9 μrad (2.4 m)
$\Sigma_{y'}$: 4.3 μrad (4.8 m), 4.9 μrad (2.4 m)

1.80-cm Undulator (Sector 32)

Period: 1.80 cm
Length: 2.4 m
Minimum gap: 11.0 mm
B_{max}/K_{max}: 0.244 T/0.41 (effective; at minimum gap)
Tuning range: 23.8 - 25.3 keV (1st harmonic)
71.4 - 75.9 keV (3rd harmonic)
On-axis brilliance at 23.8 keV (ph/s/mrad^2/mm^2/0.1%bw): 2.8 x 10^{19}
Source size and divergence at 23.8 keV:
Σ_x: 276 um Σ_y: 11 um
$\Sigma_{x'}$: 11.9 urad $\Sigma_{y'}$: 4.9 urad

IEX 12.5-cm Quasi-Periodic Polarizing Undulator (Sector 29)

Period: 12.5 cm
Length: 4.8 m

Circular polarization mode:
Max. currents: horizontal coils 34.4 A, vertical coils 20.7 A
K_{max}: 2.73 (effective; at max. currents)
B_{max}: 0.27 T (peak; at max. currents)
Tuning range: 0.44–3.5 keV (1st harmonic)
On-axis brilliance at 1.8 keV (ph/s/mrad^2/mm^2/0.1%bw): 1.4 x 10^{19}

Linear horizontal polarization mode:
Max. current: vertical coils 47.6 A
K_{max}: 5.39 (effective; at max. current
B_{max}: 0.54 T (peak; at max. current)
Tuning range: 0.24–3.5 keV (1st harmonic)
0.24–11.0 keV (1st–5th harmonic)
On-axis brilliance at 2.1 keV (ph/s/mrad^2/mm^2/0.1%bw): 1.1 x 10^{19}

Linear vertical polarization mode:
Max. current: horizontal coils 50.3 A
K_{max}: 3.86 (effective; at max. current)
B_{max}: 0.37 T (peak; at max. current)
Tuning range: 0.44–3.5 keV (1st harmonic)
0.44–11.0 keV (1st–5th harmonic)
On-axis brilliance at 2.1 keV (ph/s/mrad^2/mm^2/0.1%bw): 1.1 x 10^{19}

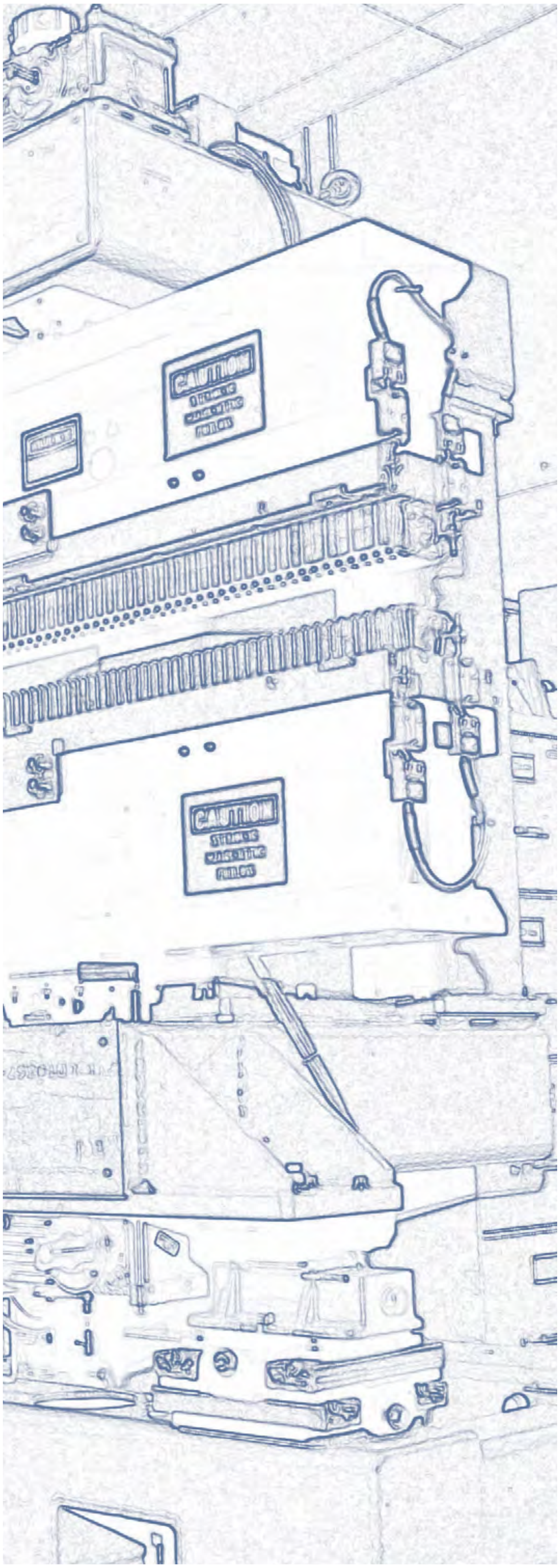
Fast polarization switching not required
Source size and divergence at 2 keV:
Σ_x: 276 μm Σ_y: 13 μm
$\Sigma_{x'}$: 13.9 μrad $\Sigma_{y'}$: 8.8 μrad

12.8-cm Circularly Polarizing Undulator (Sector 4)
Period: 12.8 cm
Length: 2.1 m
Circular polarization mode:
Max. currents: horizontal coils 1.34 kA, vertical coils 0.40 kA
K_{max}: 2.85 (effective; at max. currents)
B_{max}: 0.30 T (peak; at max. currents)
Tuning range: 0.4–3.0 keV (1st harmonic)
On-axis brilliance at 1.8 keV (ph/s/mrad^2/mm^2/0.1%bw): 3.1 x 10^{18}
Linear horizontal polarization mode:
Max. current: vertical coils 0.40 kA
K_{max}: 2.85 (effective; at max. current)
B_{max}: 0.30 T (peak; at max. current)
Tuning range: 0.72–3.0 keV (1st harmonic)
0.72–10.0 keV (1st–5th harmonic)
On-axis brilliance at 2.1 keV (ph/s/mrad^2/mm^2/0.1%bw): 2.3 x 10^{18}
Linear vertical polarization mode:
Max. current: horizontal coils 1.60 kA
K_{max}: 3.23 (effective; at max. current)
B_{max}: 0.34 T (peak; at max. current)
Tuning range: 0.58–3.0 keV (1st harmonic)
0.58–10.0 keV (1st–5th harmonic)
On-axis brilliance at 2.1 keV (ph/s/mrad^2/mm^2/0.1%bw): 2.3 x 10^{18}
Switching frequency (limited by storage ring operation): 0–0.5 Hz
Switching rise time: 50 ms
Source size and divergence at 2 keV:
Σ_x: 276 μm Σ_y: 12 μm
$\Sigma_{x'}$: 16.7 μrad $\Sigma_{y'}$: 12.7 μrad

1.80-cm Superconducting Undulator (2 IDs in sectors 1, 6)
Period: 1.80 cm
Length: 1.1 m
Gap: 9.5 mm (fixed)
Max. current: 450 A
B_{max}/K_{max}: 0.962 T/1.61 (effective; at maximum current)
Tuning range: 11.2–24.7 keV (1st harmonic)
11.2–150.0 keV (1st-13th harmonic, non-contiguous)
On-axis brilliance at 13 keV (ph/s/mrad^2/mm^2/0.1%bw): 3.2 x 10^{19}
Source size and divergence at 13 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 13.2 μrad $\Sigma_{y'}$: 7.5 μrad

3.15-cm Helical Superconducting Undulator (Sector 7)
Period: 3.15 cm
Length: 1.2 m
Coil winding diameter: 31.0 mm
Max. current: 450 A
B_{max}/K_{max}: 0.413 T/1.213 (B_x=B_y effective; at maximum current)
Tuning range: 6.0-13.0 keV (1st harmonic)
On-axis brilliance at 6.0 keV (ph/s/mrad^2/mm^2/0.1%bw): 2.2 x 10^{19}
Source size and divergence at 6 keV:
Σ_x: 276 μm Σ_y: 11 μm
$\Sigma_{x'}$: 14.7 μrad $\Sigma_{y'}$: 10.0 μrad

APS Bending Magnet
Critical energy: 19.51 keV
Energy range: 1–100 keV
On-axis brilliance at 16 keV (ph/s/mrad^2/mm^2/0.1%bw): 5.4 x 10^{15}
On-axis angular flux density at 16 keV (ph/s/mrad^2/0.1%bw): 9.6 x 10^{13}
Horizontal angular flux density at 6 keV (ph/s/mradh/0.1%bw): 1.6 x 10^{13}
Source size and divergence at the critical energy:
Σ_x: 92 μm Σ_y: 31 μm
$\Sigma_{x'}$: 6 mrad $\Sigma_{y'}$: 47 μrad



Acknowledgments

APS Science 2020 Editorial Board:

John Byrd (ANL-ASD), John Connolly (ANL-AES), Robert Fischetti (ANL-PSC), Robert Hettel (ANL-PSC), Jim Kerby (ANL-PSC), Jonathan Lang (ANL-XSD), Dennis Mills, (ANL-PSC), Stephen Streiffer (ANL-PSC), Stefan Vogt (ANL-XSD)

Reviewers:

Vukica Srajer (BioCARS); Thomas Irving (Bio-CAT); Binhau Lin (ChemMatCARS); Yogendra Gupta, Sheila Heyns, and Paulo Rigg (DCS), Denis Keane (DND-CAT); Michael Becker, Robert Fischetti, and Janet Smith (GMCA-XSD); Mark Rivers, and Steve Sutton (GSECARS); Maddury (Zulu) Somayazulu (HPCAT-XSD); Lisa Keefe (IMCA-CAT); Jordi Benach (LRL-CAT); Keith Brister (LS-CAT); Carlo Segre (MR-CAT); Kay Perry (NE-CAT); Andrzej Joachimiak (SBC-XSD); John Patrick Rose and Bi-Cheng Wang (SER-CAT); Ahmet Alatas, Jonathan Almer, Francesco De Carlo, Paul Fenter, Thomas Gog, Daniel Haskel, Steve Heald, Barry Lai, Byeongdu Lee, Suresh Narayanan, Uta Ruett, Jon Tischler, Alec Sandy, Shastri and Xiaoyi Zhang (XSD)

Unless otherwise noted, the research highlights in this report were written by:

Mary Alexandra Agner (marymary@alum.mit.edu)
Summer Alen (summer.e.allen@gmail.com)
Christen Brownlee (christenbrownlee@gmail.com)
Erika Gebel Berg (erikagebel@gmail.com)
Vic Comello (ANL-CPA - retired) (vcomello@anl.gov)
Dana Desonie (desonie@cox.net)
Sandy Field (sfield@fieldscientific.com)
Philip Koth (philkoth@comcast.net)
Kim Krieger (mskrieger@gmail.com)
Judy Myers (myers.judy@gmail.com)
Chris Palmer (crpalmer2009@gmail.com)
Neil Savage (neil@stefan.com)
Alicia Surrao (alicia@untoldcontent.com)
Stephen Taylor (stephen@untoldcontent.com)
Mark Wolverton (exetermw@earthlink.net)

Aerial photograph of the APS: John Hill (Tigerhill Studio, http://www.tigerhillstudio.com)
Publications, contracts, rights and permissions, circulation: Jessie L. Skwarek (ANL-PSC)
Editorial, project coordination, design, photography: Richard B. Fenner (ANL-PSC)

Our thanks to the corresponding authors and others who assisted in the preparation of the research highlights, to the users and APS personnel who wrote articles for the report, and our apologies to anyone inadvertently left off this list. To all: your contributions are appreciated.

Advanced Photon Source
Argonne National Laboratory
9700 S. Cass Ave.
Lemont, IL 60439 USA
www.anl.gov • www.aps.anl.gov