DENVER X-RAY CONFERENCE®

# DXC DENVER X-RAY CONFERENCE

71st Annual Conference on Applications of X-ray Analysis

1 - 5 August 2022 • Bethesda North Marriott Hotel & Conference Center, Rockville, Maryland, USA

## — Welcome back! —

# 2022 Program

Sponsored by:

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## 2022 Denver X-ray Conference Organizing Committee

**Tim Fawcett**, Chair, ICDD, Emeritus, USA, DXCfawcett@outlook.com

**Tom Blanton**, ICDD, USA, tblanton@icdd.com

**Lora Brehm**, Dow, Retired, USA, loramoon@sbcglobal.net

**Don Broton**, CTLGroup, USA, dbroton@ctlgroup.com

**Andy Drews**, Ford Motor Company, USA, adrews@ford.com

**Ursula Fittschen**, TU Clausthal, Germany, ursula.fittschen@tu-clausthal.de

**Stephanie Jennings**, ICDD, USA, sjennings@icdd.com

**Scott Misture**, NYS College of Ceramics at Alfred University, USA, misture@alfred.edu

**Conal Murray**, IBM T.J. Watson Research Center, USA, conal@us.ibm.com

**Martina Schmeling**, Loyola University, USA, mschmel@luc.edu

**Brian Toby**, Argonne National Laboratory, Advanced Photon Source, USA, brian.toby@anl.gov

**Thomas Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov

**Mary Ann Zaitz**, IBM, Retired, USA, zaitzmaryann@gmail.com

**Denise Zulli**, ICDD, USA, zulli@icdd.com

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Randolph Barton, Jr., DuPont Co. (ret.), USA
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**Steph Jennings**
**Monika Kottenhahn**
**Denise Zulli**

***ICDD Executive Director:***

**Tom Blanton**

***Future Conference:*** DXC 2023 will be back in Chicago!

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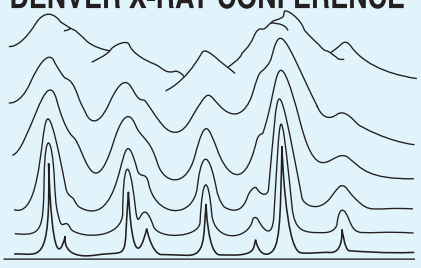

**72nd Annual Denver X-ray Conference**

**7-11 August 2023**

**The Westin Chicago Lombard, Lombard, IL, USA**

# DXC 2022 - Health & Safety Guidelines

**Masks**
At this time, masks will be optional. Local guidelines will be closely monitored and our policy could change. Please see posted signage for the latest updates.

**Onsite Guidelines**
Please do not travel to or attend DXC if you are not feeling well or think you have been exposed to COVID-19. If you become ill onsite, stay in your room and report your illness to Elizabeth Dempsey (dempsey@icdd.com). Seek medical attention to obtain a COVID-19 test, and do not return to the event until you obtain a negative test result.

DXC reserves the right to deny entry to anyone seeking admittance or remove them from the venue should they present any COVID-19-like symptoms or refuse to follow the required guidelines.

**Proof of Vaccination**
All DXC conference attendees must show proof of full vaccination to enter and participate in DXC 2022 workshops, sessions, and exhibits. All attendees must prove vaccination through CrowdPass, a HIPAA compliant service provider. A negative COVID test or exemptions will NOT be accepted.

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**Late Announcements:**

Please download the official DXC Event App – Whova, for the latest program changes.

Visit your App Store on your mobile device, download Whova, the event invitation code is: dxc2022attendee.

Notes:

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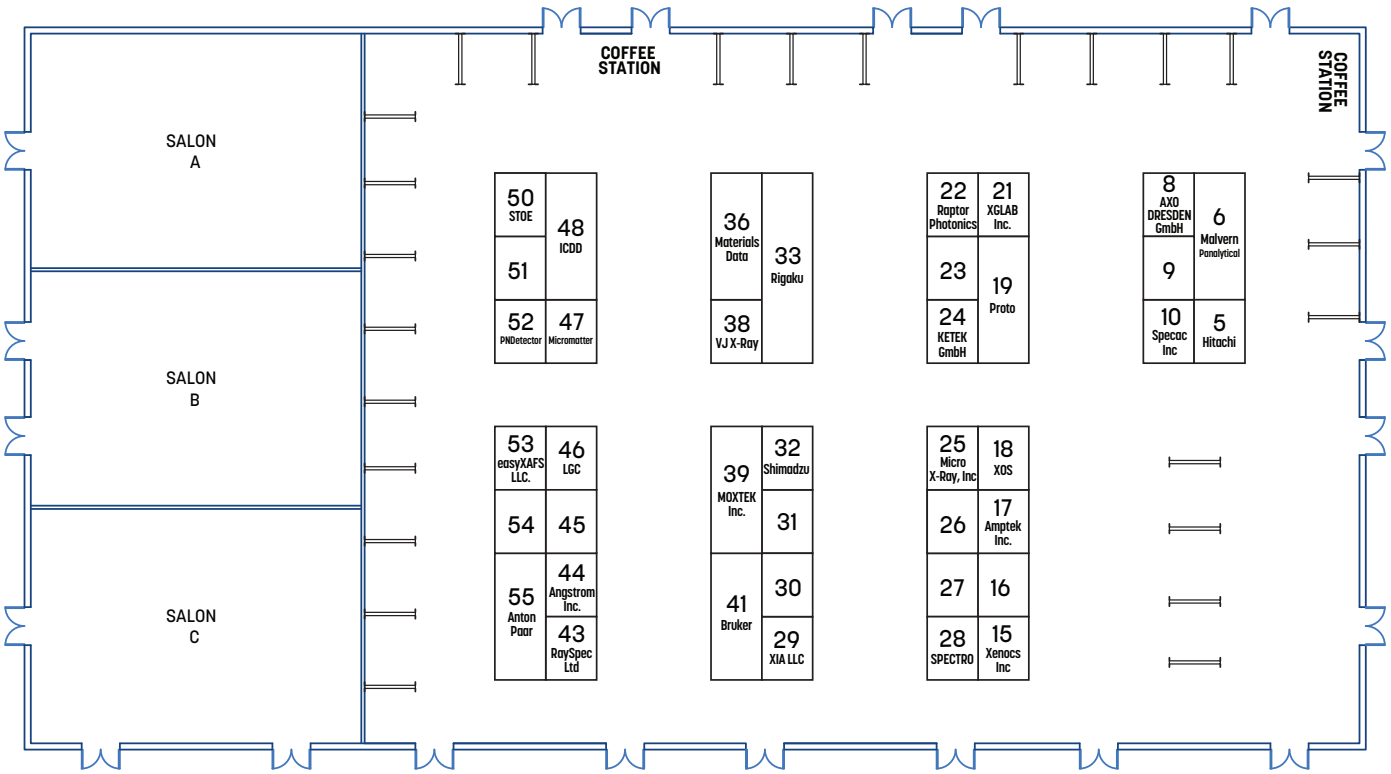


## Exhibit Hours:

Tuesday*, 2 August: 10:00am – 7:00pm
Wednesday*, 3 August: 12:00pm – 7:00pm
Thursday, 4 August: 10:00am – 1:00pm

*Poster sessions and wine & cheese receptions will be held on Tuesday and Wednesday evening from 5:00-7:00pm.

## Exhibitor Booth Numbers

| Exhibitor | Booth Number(s) |
|---|---|
| Amptek, Inc. | 17 |
| Angstrom, Inc. | 44 |
| Anton Paar | 55, 56 |
| AXO DRESDEN / Huber Diffraction | 8 |
| Bruker | 41, 42 |
| easyXAFS, LLC. | 53 |
| Hitachi High Tech Science America, Inc. | 5 |
| ICDD | 48, 49 |
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| LGC Standards \| LGC Industrial | 46 |

| Exhibitor | Booth Number(s) |
|---|---|
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| Materials Data | 36, 37 |
| Micro X-Ray, Inc | 25 |
| Micromatter Technologies / Calmetrics | 47 |
| MOXTEK, Inc. | 39, 40 |
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| Rigaku Americas Corporation | 33, 34, 35 |

| Exhibitor | Booth Number(s) |
|---|---|
| Shimadzu Scientific Instruments, Inc. | 32 |
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| VJ X-Ray | 38 |
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# Exhibitors

**Amptek, Inc.**
**Booth: 17**
Website: www.amptek.com
Email: amptek.sales@ametek.com

Amptek is a high technology company and a recognized world leader in the design and manufacture of state-of-the-art nuclear instrumentation for the satellite, X-ray and gamma ray detection, laboratory, analytical, and portable instrumentation industries. Products for Your Imagination for 45 years!

**Angstrom, Inc.**
**Booth: 44**
Website: www.angstrom-inc.com
Email: sales@angstrom-inc.com

Angstrom is a manufacturer of sample preparation equipment and supplies for XRF analysis. Products on display at DXC include the TE250 Ring & Puck Mill and the 4452 Programmable Pellet Press. Both products are highly regarded in the XRF community and are well suited for laboratories that require high sample throughput. A complete line of aluminum sample cups will also be on display, including a variety of standard depth and deep cup sizes.

**Anton Paar**
**Booths: 55, 56**
Website: www.anton-paar.com
Email: info.us@anton-paar.com

Introducing the revolutionary XRDynamic 500. Driven by 60 years of experience in X-ray diffraction (XRD), small-angle X-ray scattering (SAXS) and advanced X-ray optics, Anton Paar is proud to present the XRDynamic 500. With out-of-box, best-in-class resolution/signal-to-noise ratio, it is the only commercial X-ray diffractometer with a fully evacuated beam path and full automation to combine ease of use and efficiency. Discover Anton Paar's X-ray analysis solutions.

**AXO DRESDEN / Huber Diffraction**
**Booth: 8**
Website: www.axo-dresden.de
Email: contact@axo-dresden.de

AXO DRESDEN is a specialist for high precision deposition and multilayer coatings for multilayer X-ray optics, XRD and XRF applications. In addition to this, the new Primux 50 micro focus X-ray source system will be presented. HUBER DIFFRACTION is a manufacturer of precise positioning and diffraction equipment for laboratory, synchrotron and neutron applications.

**Bruker**
**Booths: 41, 42**
Website: www.bruker.com
Email: info.baxs@bruker.com

Bruker is the worldwide leading supplier of advanced X-ray solutions. Continual innovation in X-ray sources, optics, detectors, software and sample handling ensures that Bruker is able to offer a solution for virtually any X-ray analytical task. Stop by our booth to learn about the latest innovations in diffraction, fluorescence and Microtomography systems, including our D8 DISCOVER, D8 ADVANCE, D8 ENDEAVOR, D2 PHASER, S2 PUMA, S6 JAGUAR, S8 TIGER and the SKYSCAN family of MicroCTs.

**easyXAFS, LLC.**
**Booth: 53**
Website: www.easyxafs.com
Email: info@easyxafs.com

easyXAFS is the global leader in laboratory XAFS and XES instrumentation. Our proven laboratory X-ray spectrometers give synchrotron-quality spectra and game-changing scientific freedom. Add to your existing research program or launch a new thrust. Imagine what you can do with reliable, easy access to advanced X-ray spectroscopy.

**Hitachi High Tech Science America, Inc.**
**Booth: 5**
Website: www.hitachi-hightech.com/hhs-us
Email: del.redfern@hitachi-hightech.com

Hitachi High Tech Science America Inc. designs and manufactures the Vortex line of Silicon Drift Detectors (SDDs) for applications ranging from benchtop instrumentation to the most demanding synchrotron spectroscopy and mapping installations. We work closely with end-users on design customization. The Vortex sensor is available with thicknesses of 0.5, 1.0 and the 2.0 mm thick SDD sensor which extends the capabilities of the Vortex SDD to higher energies.

**ICDD**
**Booths: 48, 49**
Website: www.icdd.com
Email: info@icdd.com

For over 80 years, we have focused on meeting the needs of the scientific community through the publication of the Powder Diffraction File™ (PDF®) and providing forums for the exchange of ideas and information. ICDD's material identification databases interface with diffractometers and data analysis systems of the world's leading software developers and manufacturers of X-ray equipment. The Powder Diffraction File is available in PDF-2, PDF-4+, PDF-4/Minerals, PDF-4/Organics, and PDF-4/Axiom. Release 2023 of the PDF will feature over 1,100,000 entries.

**KETEK GmbH**
**Booth: 24**
Website: www.ketek.net
Email: info@ketek.net

The leading manufacturer of Silicon Drift Detectors presents the newest VITUS SDD generation with KETEK's proprietary Graphene window. It offers significantly higher X-ray transmission below 3keV and boosts the LOD for lighter elements like fluorine or magnesium. The best-in-class cooling performance allows stable chip temperature down to -60°C at up to +65°C heat sink (Δ T > 125K) at 50% lower power consumption. With energy resolutions <123eV (MnKα), P/B ratios above 25,000 and peaking times down to 50ns the newest VITUS SDD series marks the state-of-the-art.

**LGC Standards | LGC Industrial**
**Booth: 46**
Website: www.lgcstandards.com/industrial
Email: lgcindustrial@lgcgroup.com

You've trusted us for decades to create superior reference materials and innovative measurement tools for petroleum, metals, aqueous inorganic, and geological industrial applications. Leveraging the synergies of the LGC Industrial product lines, we are joining together, VHG, ARMI, MBH, and Paragon Scientific, to deliver you The Material Difference. Building on our collective expertise, LGC Industrial fosters the innovation and the agility necessary to create the measurement tools you rely on when developing, using, and transforming materials to achieve your mission. LGC Industrial – The Material Difference.

**Malvern Panalytical**
**Booths: 6, 7**
Website: www.malvernpanalytical.com
Email: ask@malvernpanalytical.com

At Malvern Panalytical, we are big on small – helping our customers unleash the power of very small things, to make big things happen. Our materials analysis solutions provide highly reliable and robust elemental, morphological and structural information that can help scientists and engineers solve challenges with maximizing productivity, developing better products and getting them to market faster. We will feature X-ray diffraction and X-ray fluorescence systems, fusion sample prep equipment, and will have application scientists available to answer your questions. Visit us in Booths 6 and 7.

**Materials Data**
**Booths: 36, 37**
Website: www.materialsdata.com
Email: mdi@materialsdata.com

Materials Data® (MDI™), now part of the ICDD®, continues creating hardware-independent analysis software for X-ray Powder Diffraction embraced world-wide. Our products for XRD are engineered by a group of PhD Materials Scientists with a vision for better methods to analyze, characterize, quantify and simulate both the complex and routine. Together with the ICDD, we are building scalable products with break-through ideas and methods for the XRD community. Visit our booth at DXC for a current demo of JADE®.

**Micro X-Ray, Inc.**
**Booth: 25**
Website: www.microxray.com
Email: info@microxray.com

Micro X-Ray designs and manufactures X-ray tubes and X-ray sources entirely in our California facility. Our X-ray sources provide best-in-class performance for a wide variety of XRF modalities. We offer packaged tubes in various configurations and geometries, with customizable power levels, target materials, spot geometries, integrated shielding, and integrated cooling options tailored to your application and environment. Whether you are a large OEM, system integrator, repair facility, or university, we welcome the opportunity to discuss your specific X-ray tube requirements.

**Micromatter Technologies / Calmetrics**
**Booth: 47**
Website: www.micromatter.com
Email: sales@micromatter.com

Micromatter / Calmetrics has provided XRF calibration materials for more than 50+ years. We offer the world's largest selection of certified coating thickness and material composition reference XRF standards. We manufacture high accuracy reference standards capable of calibrating virtually any X-ray Fluorescence (XRF) system. Our products include ultra-light standards for air quality monitoring, coating thickness standards - including but not limited to: thin and thick films (single and multi-layer), alloy films, bulk standards including alloys and pure elements, precious metal standards, WEEE/RoHS standards and other custom standards for a broad range of industrial and scientific applications. Micromatter is also a leading manufacturer of beam stripping foils, with specialization on diamond-like carbon, DLC-Boron hybrid, pure boron and graphene based material.

**MOXTEK, Inc.**
**Booths: 39, 40**
Website: www.moxtek.com
Email: xraysales@moxtek.com

MOXTEK is a leading supplier of advanced nano-optical and X-ray components used in display electronics, imaging, and analytical instrumentation. MOXTEK provides innovative, solution-based products and services focused on performance, quality, and value. MOXTEK products enable many new scientific discoveries and improve the quality of everyday life. MOXTEK X-ray products empower compact handheld and benchtop elemental analysis for positive material identification. MOXTEK products are used in various EDXRF, WDXRF, and XRD systems for environmental screening, hazardous substance analysis, and sorting and recycling. MOXTEK optical polarizers and polarizing beamsplitters enable advancements in projection display and analytical instrumentation including: 2-D and 3-D projection display, near-eye display, and optical analysis instrumentation.

**PNDetector**
**Booth: 52**
Website: www.pndetector.de
Email: info@pndetector.de

For more than a decade PNDetector's SDDs are at the forefront of radiation detector technology, as they combine both excellent energy resolution and short processing times. Our key technology is an ultra-pure sensor chip manufacturing, which enables us to develop and produce innovative, advanced silicon radiation detectors used in X-ray fluorescence or microanalysis for applications like materials science and quality assurance. Monolithic multi-element and large-area SDDs including unique geometries with maximum solid angle complement our product portfolio.

**Proto Manufacturing**
**Booth: 19, 20**
Website: www.protoxrd.com
Email: info@protoxrd.com

PROTO is excited to continue growing our X-ray diffraction product offerings with the introduction of the AXRD-LPD High-Resolution Diffractometer. This is now the fourth instrument added to our powder diffraction line-up, in addition to our extensive range of residual stress, single-crystal orientation systems, and X-ray tubes. At PROTO we believe in customizing our products to provide you with the best possible system for your application.

**Raptor Photonics**
**Booth: 22**
Website: www.raptorphotonics.com
Email: sales@raptorphotonics.com

Raptor Photonics is a leading developer and supplier of next generation, high-performance digital camera solutions for the Scientific, Surveillance and Aerospace markets. Raptor offers a range of CCD, EMCCD and InGaAs solutions. As well as standard products, Raptor provides custom solutions to OEM and Instrumentation companies around the World. Raptor offers an extensive range of direct and indirect X-ray camera options for hard high energy applications featuring a choice of sensors and sensor options, fibre optic input plates across a range of interfaces.

**RaySpec, Ltd.**
**Booth: 43**
Website: www.rayspec.co.uk
Email: sales@rayspec.co.uk

RaySpec, Ltd. is a specialist manufacturer of customised Silicon Drift Detectors (SDD) and signal processing electronics for X-ray Fluorescence applications. Previously known as Gresham Scientific, E2V and SGX Sensortech, RaySpec has been supplying X-ray detectors for 24 years. RaySpec supplies original equipment manufacturers and specialist end-users in synchrotrons and research facilities around the world. The unique capabilities of RaySpec satisfy the most demanding of specialised requirements. Detectors

are available with a wide range of active areas in single and multi-sensor designs. With optimisations available for high count rate, high solid angle and 3rd party pulse processing electronics. RaySpec prides itself on building unique solutions to meet the needs of customers. If you have a project requiring an SDD, please come and explain your needs and we will work towards an optimal solution.

**Rigaku Americas Corporation**
**Booths: 33, 34, 35**
Website: www.rigaku.com
Email: info@rigaku.com

Rigaku Corporation is a leading manufacturer and supplier of analytical equipment with diverse groups specializing in X-ray, Electron, Infra-red and Thermal technologies.

The X-ray technologies embrace the primary X-ray applications of: X-ray Diffraction (XRD), Single Crystal Analysis (SCX), Small Angle X-ray Scattering (SAXS), X-ray Fluorescence (XRF) (Wavelength and Energy Dispersive) and X-ray imaging (XCT) including 3D X-ray microscopy. The recent introduction of Electron Diffraction for single crystal analysis completes Rigaku's unprecedented range of diffraction solutions for materials analysis.

For more than seven decades, Rigaku has been providing industry ready and customized solutions for materials characterization, and welcomes an opportunity to consult with you on your materials analysis requirements.

**Shimadzu Scientific Instruments, Inc.**
**Booth: 32**
Website: www.ssi.shimadzu.com
Email: maquaranta@shimadzu.com

Shimadzu offers an array of EDXRF spectrometers and X-ray diffractometers for an array of materials science applications. Advanced EDX-7200/8100 spectrometers incorporate a high-performance, electronically cooled semiconductor detector, a high fluorescent X-ray count per unit time, five primary filters, and a sample observation camera. Software features an intuitive user interface, simplifying operation for all operators. A new one-dimensional detector with 1280 channels for XRD provides high-speed quantitative analysis with three types of measurement modes, high sensitivity, and enhanced operational efficiency.

**Specac, Inc.**
**Booth: 10**
Website: www.specac.com
Email: sales@specac.com

How are you preparing your samples for XRF? Do you have samples that are hard to analyze? Are your laboratory sample presses and dies slowing you down? With the right press and right die, XRF analysis can be simple and easy. Visit Specac at Booth 10 to learn more about the Autotouch Press and Apex Die.

**SPECTRO Analytical Instruments**
**Booth: 28**
Website: www.spectro.com
Email: spectro.info@ametek.com

Members of the AMETEK Materials Analysis Division, SPECTRO Analytical Instruments is a worldwide leading supplier of OES and X-ray fluorescence spectrometry technology, used for the elemental analysis of materials in industry, research and academia. SPECTRO will feature the SPECTRO XEPOS and new SPECTROCUBE with breakthrough advances in excitation and detection. They are an excellent choice for R&D, process development, process control, and at-line or field analysis.

**STOE**
**Booth: 50**
Website: www.stoe.com
Email: info@stoe.com

STOE, originally founded in 1887 to manufacture equipment for the optical analysis of crystals, has been a pioneer in powder and single crystal X-ray diffraction since the 1960's. E.g. STOE invented and patented the transmission geometry technique for Powder XRD, as well as for single crystals, produced the first pixel detector XRD system with an open Eulerian cradle. STOE is based in Darmstadt, Germany, and keeps the R&D, software programming, electrical and mechanical engineering and production all in house, allowing STOE to provide customers with standard, as well as individual solutions. Whenever it comes to quality, STOE accepts no compromises. This high-level of detail is what sets STOE apart. STOE is the partner in X-ray Diffraction to crystallographers, chemists, material scientists and pharmacists all over the world.

**VJ X-Ray**
**Booth: 38**
Website: www.vjt.com

Since 2008, VJ X-Ray has designed and manufactured integrated X-ray sources and high voltage generators for OEMs of X-ray Inspection Systems in markets including Security, Food & Pharmceutical, Industrial NDT, Medical, Electronics, and Analytical Instrumentation. The IXS series of integrated X-ray sources incorporates the high voltage power supply, X-ray tube, and control electronics into single compact products. These units have high stability and performance over an extensive range of output power. The small form factor, integrated cooling, and proprietary radiation shielding of IXS products set them apart from their competition. The HVL/HVG series of high voltage x-ray generators are optimized for performance and reliability over a variety of voltage and current outputs. VJ X-Ray serves their global customer base from their two facilities in New York, United States and Suzhou, China. Their technical team has over 20 years of experience in high voltage design and X-ray integration, allowing them to build a solid foundation to support OEM's customized solutions. Their X-ray sources and generators are backed by VJ Technologies, a company that has delivered integrated X-ray system solutions for the past three decades.

**Xenocs, Inc.**
**Booth: 15**
Website: www.xenocs.com
Email: sales.us@xenocs.com

Xenocs is the leader in Small Angle X-ray Scattering (SAXS) for Nanoscale Metrology. We offer a wide range of versatile tools for molecular structure analysis of soft matter, polymers, nanomaterials, proteins, surfaces and nanoelectronics. Our innovative portfolio includes SAXS/WAXS instruments with capabilities from specific measurements to state-of-the-art research tools. All our products are backed by the most experienced worldwide team of specialist scientists and engineers. Stop by and see our new Xeuss 3.0 scattering platform, now with imaging.

**XGLAB**
**Booth: 21**
Website: www.xglab.it
Email: info.xglab@bruker.com

XGLab is a leading provider of innovative readout electronics for radiation detectors and instrumentation for X- and Gamma-ray application. The strong focus on Research and Development and the numerous active collaborations with research institutions, synchrotrons and academies makes XGLab the best partner for high quality and technology based product innovation. The main areas of expertise of XGLab are: Charge Sensitive Amplifiers for radiation sensors, Digital Pulse Processors for X-ray spectroscopy, ASIC design, test and long term supply, X-ray Spectrometers. XGLab is part of Bruker Nano Analytics (BNA), a division of the Bruker Corporation, a global leader in scientific instruments and solutions for life sciences and materials research, as well as industrial process and quality control. XGLab is headquartered in Milan, Italy.

**XIA LLC**
**Booth: 29**
Website: www.xia.com
Email: sales@xia.com

XIA LLC invents, develops and markets advanced digital pulse processing and data acquisition electronics for use with X-ray and gamma-ray detectors in industry, university research and National Labs. We are technology leaders in high-rate spectroscopy electronics at synchrotron facilities around the world, as well as a major OEM supplier for compact low power handheld and benchtop spectroscopy instruments. Please visit the XIA Booth (#29) for more information.

**XOS**
**Booth: 18**
Website: www.xos.com
Email: info@xos.com

XOS is a leading global provider of advanced optics and OEM sub-systems that greatly improve the measurement speed, precision, and sensitivity of X-ray analytical instrumentation. XOS' polycapillary optics can be used in many applications, including plating thickness, forensics, cultural heritage, and elemental mapping— such as on the Mars 2020 rover, where an XOS polycapillary optic has a critical role in the search for past life on Mars after landing in February 2021. XOS also offers a range of compact and customizable X-ray generator solutions, including fleX-Beam™, which combines a low-powered X-ray source and precisely aligned polycapillary optic to deliver a bright X-ray beam for advanced material analysis. We've also recently released the brand-new Mini-Beam, our latest and most pocket-sized solution capable of many of the same functions as fleX-Beam, its big sister. The innovative optic mounting and alignment designs of the new Mini-Beam enable easy X-ray tube and/or optic replacements, making both Beams user-friendly tools for both OEMs and end users. Learn more: www.xos.com/oem

# DXC 2022 EXHIBIT PASSPORT

**New! – Two ways to participate. Have your QR code scanned in the Whova event app, or have exhibitors sign this card!**

| | | | | | |
|---|---|---|---|---|---|
| AMPTEK | Angstrom | Anton Paar | AXO DRESDEN & Huber Diffraction | Bruker | easyXAFS |
| Hitachi | ICDD | KETEK | LGC | Malvern Panalytical | Materials Data |
| Micro X-Ray | Micromatter | MOXTEK | PNDectector | PROTO | Raptor Photonics |
| | RaySpec | Rigaku Americas | Shimadzu | Specac | Spectro |
| | | | STOE | VJ X-Ray | Xenocs |
| | | | XGLab | XIA | XOS |

**VISIT TO WIN!**
**Visit: Get:**
**10 companies = 1 chance**
**20 companies = 2 chances**
**All companies = 3 chances**
**VISIT TO WIN!**

**Win one of <u>four</u> $100 Amazon gift cards! The more exhibit companies you visit, the more chances you have to win!** For every exhibit company you visit, you'll be given a "stamp" for your passport. Participate by using this card or your Whova event app Passport. Collect stamps by visiting each exhibitor booth and having an exhibitor sign your program book passport card or ask to have your QR Code scanned. **Participation will only count from one passport source - the Whova App or the Onsite Program**. Please "turn in" your stamped passport by Thursday, 1:00pm at the Conference Registration Desk. A member of the Conference Services team will give you chance tickets and you will be entered into a drawing to win. Remember: the more companies you visit the more chances you have to win! The winners will be announced by 3:00pm on Thursday, via Whova and a posting at the Conference Registration Desk. You must be able to pick up your gift card by Friday morning at 10am, or the prize will be forfeited.

**Only registered attendees are eligible to enter the drawing. Exhibit Hall Only attendees, employees of an exhibiting vendor, guests, and members of the DXC Organizing Committee may not participate.*

**Return to Conference Registration Desk by Thursday at 1:00 pm for your chance to win one of four $100 Amazon gift cards!**

# 2022 Denver X-ray Conference Workshops

Morning Workshops – 9:00 AM – 12:00 Noon
Afternoon Workshops – 1:30 PM – 4:30 PM

## Monday Morning Workshops 9:00 AM – 12:00 Noon

### Machine Learning Techniques in X-ray Analysis — White Oak A

**Organizers & Instructors:**
**M. Cherukara,** Argonne National Laboratory, USA, mcherukara@anl.gov
**A. Mehta,** SLAC National Accelerator Laboratory, USA, mehta@slac.stanford.edu

The capabilities provided by next generation light sources along with the development of new characterization techniques and detector advances are expected to dramatically increase the complexity and volume of data generated by instruments at the new light sources. Traditional techniques of data reduction and analysis will not be able to keep pace. Machine learning methods applied to a variety of X-ray characterization techniques have shown promise in accelerating, and in some cases improving the accuracy of X-ray data inversion, abstraction and inference. This workshop is being organized to discuss the current state and potential of machine learning methods applied to synchrotron and XFEL data.

### XRD Sample Preparation — White Oak B

**Organizer & Instructors:**
**T. Fawcett,** ICDD, Emeritus, USA, dxcfawcett@outlook.com
**S. Quick**, The Pennsylvania State University, USA, quick@cse.psu.edu
**M. Rodriguez**, Sandia National Laboratories, USA, marodri@sandia.gov

Specimen preparation is often the limiting step for obtaining good results in a diffraction experiment. Preparation methods can influence the accuracy and precision of peak positions, intensities and profiles. These are the basic measurements required for qualitative and quantitative analysis. The presentation will focus on crystallite and particle effects, orientation and texture, particle statistics, and how various preparation methods can reduce or eliminate these influences.

We will also discuss “tricks of the trade” and various techniques that experts use to analyze odd shaped parts, limited samples, and air and moisture sensitive specimens.

### Sample Preparation of XRF — Glen Echo

**Organizer & Instructors:**
**M.A. Zaitz**, IBM, Retired, USA, zaitzmaryann@gmail.com
**Y. Hernandez**, Malvern Panalytical, USA, Yusniel.hernandez@malvernpanalytical.com

This workshop will focus on the different aspects of fusion and powder preparation for XRF analysis of both simple and difficult samples. It will begin with borate fusion preparation, and then include the basic chemistry of peroxide fusion preparations, and their applications. The general physics of XRF sample preparation will also be discussed. Finally, the interconnection between sample preparation methods, calibration range, standard selection, and accuracy will be discussed. These techniques and methods are essential tools in today's modern XRF/ICP laboratory.

### Layered Structures — Forest Glen

**Organizers & Instructors:**
**K. Hradil**, TU Wien X-ray Center, Austria, klaudia.hradil@tuwien.ac.at
**P. Wobrauschek**, Vienna University of Technology, Austria, wobi@ati.ac.at
**D. Ingerle**, TU Wien Atominstitut, Austria, dieter.ingerle@tuwien.ac.at
**C. Streli**, TU Wien, Atominstitut, Austria, streli@ati.ac.at

The characterization of layered structures from the nanometer range to the 10 µm range is of increasing importance, especially if the analytical methods are non-destructive.

In the first part Confocal micro-XRF (X-ray fluorescence analysis) is introduced by Christina Streli. This technique allows the characterization of layers in the range of some 10 µm. The principle, some experimental setups (synchrotron radiation as well as lab instruments) will be described and some showcases presented.

In the second part GIXA, Dieter Ingerle will present the combination of Grazing incidence XRF (GIXRF) and X-ray reflectivity (XRR). GIXA allows the characterization of nanometer layers, the determination of the elemental composition, density and thickness. Setups, data evaluation software and showcases are presented.

The third part of the workshop, presented by Klaudia Hradil, will include the theoretical background and experimental techniques of thin film analysis by X-ray diffraction methods. This will include the experimental techniques and the analysis of data for grazing incidence diffraction. The possibilities for the microstructure properties analysis of thin films like stress/strain and texture analysis, classical phase analysis and thin film crystallinity properties with lab methods will be introduced for selected examples.

# Monday Afternoon Workshops 1:30 PM – 4:30 PM

## 2D Detectors — White Oak A

**Organizers & Instructors:**
**T. Blanton**, ICDD, USA, tblanton@icdd.com
**B. He**, Bruker AXS Inc., USA, bob.he@bruker.com
**M. Mueller**, DECTRIS Ltd., Switzerland, marcus.mueller@dectris.com
**Y. Nakaye**, Rigaku, Japan, nakaye@rigaku.co.jp
**S. Speakman**, Malvern Panalytical, USA, scott.speakman@panalytical.com

Two-dimensional diffraction data contain abundant information about the atomic arrangement, microstructure, and defects of a solid or liquid material. In recent years, the use of two-dimensional detectors has dramatically increased in academic, government and industrial laboratories. This workshop covers recent progress in two-dimensional X-ray diffraction in terms of detector technology, geometry and configuration of the two-dimensional diffractometer. Various applications such as phase ID, texture, stress, crystallinity, combinational screening and thin film analysis will be discussed.

## X-ray Absorption Spectroscopy (XAS) — White Oak B

**Organizer & Instructors:**
**S. Seshadri**, Sigray, Inc., USA, srivatsan.seshadri@sigray.com
**Y. Tian**, Sigray, USA, ytian@sigray.com
**A. Hoffman**, SLAC National Accelerator Laboratory, USA, ashoff@slac.stanford.edu

This introductory hands-on workshop brings together a group of scientists active in the field of X-ray Absorption Spectroscopy (XAS). They will share their expertise with other scientists and students interested in learning about laboratory and synchrotron based XANES and EXAFS methods. These methods include introduction to laboratory based XAS instrumentation and their differences with synchrotron-based instruments, acquisition of experimental data, and analyses.

The workshop will be divided into two sessions. The first session of the workshop includes lectures on the instrumentation, acquisition of XAS data and good practices, and Q&A sessions on these subjects. The second session of the workshop is devoted entirely to the hands-on analyses of XAS data using Athena and Artemis. The attendees are encouraged to bring their laptops with Athena and Artemis installed. Data from several samples will be analyzed. Participants are also encouraged to bring data they acquired from their samples.

## Basic XRF — Glen Echo

**Organizer & Instructors:**
**M.A. Zaitz**, IBM, Retired, USA, zaitzmaryann@gmail.com
**P. Wobrauschek**, Vienna University of Technology, Austria, wobi@ati.ac.at

This workshop provides a basic introduction to the principles of XRF and is specifically aimed at those new to the field. It begins with a general overview of the technique and the various instrumentation configurations including their main applications. This is followed by more specific details of XRF Physics. Basic WDX instrumentation will be described with its use and applications. In the second half of the workshop, basic EDX instrumentation including general purpose bulk analyzers (benchtop EDX), TXRF, Micro analyzers, and Handheld analyzers will be reviewed. Capabilities and applications in actual practice will be described.

## Handheld XRF — Forest Glen

**Organizer & Instructors:**
**M. Loubser**, University of Pretoria, South Africa, maggi.loubser@up.ac.za
**M. Hinds**, MHinds Analytical Consulting, Inc., Canada, mike@mhindsanalyticalconsulting.com

Handheld XRF spectrometers have increased market share 100-fold in the past ten years. Since these spectrometers are relatively inexpensive compared to laboratory-based spectrometers, they are more affordable and more companies acquire them, often without the necessary trained people to operate them. Different to laboratory-based spectrometers, the handheld spectrometers mostly come with factory calibrations, eliminating the need for a qualified analytical chemist to operate them. Herein lies the biggest danger, because people with very little insight into the theory behind XRF spectrometry can generate huge quantities of totally meaningless data.

In this workshop, we really want to share the good, the bad and the ugly. Firstly, demonstrate the amazing opportunities suddenly possible because as spectroscopists we now have a tool we can take into the field, to the artifact, or wherever we need in-situ analyses. We also want to demonstrate that the physics of XRF spectroscopy has not changed, and if you operate in a point and shoot mode, the data will reflect that! The difference between in-situ and laboratory analyses would be explained and the fact that the representativeness of the sample remains the biggest challenge, as in any analytical technique.

Safe operation and quality control protocols will also be discussed.

Mike Hinds is adding his unique insights after years of working with mostly gold samples at the Canadian Mint, but most of his experience is equally applicable to all other metal analyses. The analysis of metals by handheld XRF is generally a good application. However, one must understand the limitations of both the XRF spectrometer and the metal materials to achieve the best results possible. This section will cover the structure of metals, sampling, metal identification, and quantitative determination using a handheld XRF. There will also be some discussion on the manufacture and use of metal reference materials.

## Tuesday Morning Workshops 9:00 AM – 12:00 Noon

### X-ray CT in Laboratory Settings — White Oak A

**Organizer & Instructors:**
**E. Cakmak**, Oak Ridge National Laboratory, USA, cakmake@ornl.gov
**C. Frazer**, Covalent Metrology, USA, colleen@covalentmetrology.com
**A. Takase**, Rigaku, USA, aya.takase@rigaku.com

Laboratory scale X-ray computed tomography (XCT) has advanced significantly over the years with spatial resolutions reaching those available at a synchrotron. With state-of-the-art laboratory scale XCT instruments, micron to sub-micron voxel resolutions are achievable. This has enabled researchers and industry to have rapid access to high resolution 3D imaging at their home institutions, except for when kinetic studies are required.

This workshop is intended as an introduction to laboratory scale XCT. Within this context, we will begin the course with a brief introduction to the technique, go over the basic components of a system, and talk about its general capabilities (including in-situ loading). This will be followed by examples covering a broad range of materials from ceramics to composites to metals, including engineering components, as well as limitations.

Post-processing and data analyses are important parts of XCT experiments. The workshop will cover aspects of data reconstruction and analyses (including image processing, segmentation, and metrology). An interactive demonstration on data analyses will be performed with ImageJ and the attendees will have a chance to follow along on their **own laptops**.

The workshop will conclude with examples of industrial applications with an emphasis on semiconductors.

### Stress Analysis — Glen Echo

**Organizers & Instructors:**
**C. Murray**, IBM T.J. Watson Research Center, USA, conal@us.ibm.com
**T. Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov
**J. Bunn**, Oak Ridge National Laboratory, USA, bunnjr@ornl.gov

This workshop is intended to introduce novice users to the basic techniques used in X-ray and neutron diffraction-based residual stress determinations. Sin2(psi) and other stress determination techniques will be introduced and instrumental errors associated with the measurement will be discussed. Examples will be provided that use laboratory X-ray, synchrotron-based techniques, including microbeam measurements, and neutrons. At the end of the seminar, the attendees should be able to evaluate the validity of a diffraction-based stress determination experiment. One aim is for the practitioner to be able to evaluate the validity of an experiment and understand the advantages and disadvantages of each technique.

### Micro XRF — Forest Glen

**Organizers & Instructors:**
**K. Tsuji**, Osaka City University, Japan, tsuji@a-chem.eng.osaka-cu.ac.jp
**M.A. Zaitz**, IBM, Retired, USA, zaitzmaryann@gmail.com
**D. Matsunaga**, Horiba Ltd., Japan, daisuke.matsunaga@horiba.com

The workshop will cover the basic principles of Energy Dispersive X-ray Fluorescence analysis including theory, instrumentation, software, spectral processing, qualitative and quantitative analysis. Advances in ED-XRF instrumentation have made the technique one of the most versatile spectrometers available for elemental analysis. EDXRF instruments have been applied for planetary and deep-sea exploration with high tech manufacturing for process control and are a mainstay in any well-equipped laboratory. Micro-XRF analysis is one of the variations in EDXRF spectrometers and provides information on samples that are difficult to analyze by more traditional EDXRF spectrometers such as small particles or small features, odd size samples, or localized contaminated areas. We will discuss the state of the art instruments (X-ray source, X-ray optics for micro beam, and detectors) and applications including elemental mapping. An update on applications of micro XRF analyzers in various files such as industry, environmental science and artwork will also be discussed.

# Tuesday Afternoon Workshops 1:30 pm – 4:30 pm

## Rietveld Analysis for Phase Quantification — White Oak A

**Organizers & Instructors:**
**J. Kaduk**, Poly Crystallography, Inc., USA, kaduk@polycrystallography.com
**S. Misture**, Alfred University, USA, misture@alfred.edu

This workshop will cover the application of Rietveld analysis to quantitative phase analysis, both the theoretical background and things that can go wrong. We will also cover structure-less full-pattern techniques for quantitative phase analysis, such as PONKCS (partial or no known crystal structure).

## Small-angle X-ray Scattering (SAXS) — White Oak B

**Organizer & Instructors:**
**T. Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov
**Y. Mao**, NIST, USA, ymmao@umd.edu
**J. Skov Pederen**, Aarhus University, Denmark, jsp@chem.au.dk
**C. Zhu**, Lawrence Berkeley National Laboratory, USA, chenhuizhu@lbl.gov

This workshop will consist of three sections: fundamentals, data analysis and in situ measurements. In the first section, the basics of the experimental set-up, scattering from various particle shapes and calibration will be covered. Next, data reduction, analysis, and interpretation will be discussed with the aim of guiding the user to obtain useful structural information after quality data has been collected. Finally, in situ or operando measurements of advanced functional materials in various sample environments will be presented. Examples and case studies will be given in all three sections including battery materials and proteins.

## Multimodal XRF Microscopy Fitting Tools — Glen Echo

**Organizers & Instructors:**
**O. Antipova**, Argonne National Laboratory, USA, oantipova@anl.gov
**A. Glowacki**, Argonne National Laboratory, USA, aglowacki@anl.gov
**A. Pattammattel**, Brookhaven National Laboratory, USA, pattammattel@bnl.gov

Synchrotrons are notorious for facility specific analysis software. M-BLANK is very powerful for blank correction and fitting of thin samples; GeoPIXE has lots of very nice capabilities for analyzing X-ray data; and the X-ray Sciences Division (XSD) at the Advanced Photon Source (APS) is currently writing a new GUI, based on MAPS, with the aim of it being more easily distributable and open source. We would like to bring together individuals in the field to strategize a multi-platform code capable of handling data from any synchrotron around the world. Such software would need to account for many different sample types from thin biological samples to archaeological samples and rocks.

## Trace Analysis — Forest Glen

**Organizer & Instructors:**
**P. Wobrauschek**, TU Wien, Atominstitut, Austria, wobi@ati.ac.at
**N. Kawahara**, Rigaku Corporation, Japan, kawahara@rigaku.co.jp
**C. Streli**, TU Wien, Atominstitut, Austria, streli@ati.ac.at
**K. Tsuji**, Osaka City University, Japan, tsuji@a-chem.eng.osaka-cu.ac.jp

Both beginners and experienced X-ray scientists and applicants, physicists and chemists, will gain information by attending the trace analysis workshop. Presentations of most modern techniques and instrumentation for trace element analysis using EDXRS will be given. Physical methods to improve minimum detection limits in XRF by background reduction will be discussed; special emphasis will be on synchrotron radiation as excitation source. Introduction to total reflection XRF (TXRF) and actual instrumentation will show achievable advantages and results in terms of detection limits, sensitivities and detectable elemental range down to light elements (e.g. Carbon). Micro-XRF and Confocal µ-XRF will be presented as methods for 2D and 3D spatial resolved elemental imaging. Applications from fields as environment, microelectronics, forensic, and life science will show the successful use of the various XRF spectrometric techniques. The possibilities of trace analysis using wavelength dispersive XRF will also be covered, showing the benefits and limitations of the technique. A comparison of achievable detection limits with the various techniques on some specific samples will be discussed.

# XRD Poster Session – Tuesday Evening
## Grand Ballroom D-H

**Signifies presenting author, when noted*

The Tuesday evening XRD poster session will be held 5:00 pm – 7:00 pm in the Grand Ballroom D-H, in conjunction with a wine and cheese reception. Three "Best Poster" awards will be given at the end of the session, including "Best Student Poster".

Chairs:
**E. Cakmak**, Oak Ridge National Laboratory, USA, cakmake@ornl.gov
**T.R. Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov

**D-2** **Crystal Structures of Large-Volume Commercial Pharmaceuticals**
**J.A. Kaduk, E.L. Markun, N.C. Boaz**, North Central College, USA
**Y. Lee, Y. Wangf, P.G. Khalifah, P.W. Stephens**, Stony Brook University, USA
**S. Gates-Rector, A.M. Gindhart, T.N. Blanton**, ICDD, USA

**D-3** **XRDynamic 500: The Automated Multipurpose Powder X-ray Diffractometer from Anton Paar**
**A.O.F. Jones*, M. Kremer, T. Müller, B. Puhr, B. Schrode, P. Vir**, Anton Paar GmbH, Austria

**D-4** **Deposition and Structural Characterization of Ag/Au Films**
**Q. Lin**, University of California Irvine, USA

**D-6** **Non-Ambient XRD: New Developments and Possibilities from Anton Paar**
**B. Puhr*, A.O.F. Jones, M. Kremer, T. Müller, B. Schrode, P. Vir**, Anton Paar GmbH, Austria

**D-7** **Investigation on X-ray Photoelectron Spectroscopy, Structural, Optical and Magnetic Properties of Transition Metal Doped ZnO Nanostructures**
**A.M. Alsmadi, B. Salameh**, Kuwait University, Kuwait

**D-10** **Depth Distribution Analysis of Residual Stress and Dislocation Density for Grit-Blasted Hot-Rolled Low Carbon Steel**
**M. Imafuku*, K. Kamada, A. Itoh, Y. Aoki, Y. Narita**, Tokyo City University, Japan

**D-12** **Microstructural Characterization of Ball Python Urates**
**A. Thornton, J. Swift**, Georgetown University, USA
**T. Fawcett**, ICDD, USA
**G. Schuett**, Chiricahua Desert Museum, USA

**D-17** **Surface Strain, Residual Stress and Textures of CVD $Al_2O_3$ Coatings on Metal Cutting Tools**
**T. Shibata**, Kennametal, USA

**D-21** **Analysis of Blue and Green Sphere K2 Granite Using X-ray Microdiffraction Analysis**
**T. Blanton***, ICDD, USA
**S. Zdzieszynski, S. Misture**, Alfred University, USA

**D-26** **Hierarchical Structure Characterization Using SAXS/USAXS**
**M. Kasari*, T. Iwata, K. Omoto, K. Ito, K. Omote**, Rigaku Corporation, Japan
**A. Ohbuchi**, Rigaku Americas Corporation, USA

**D-30** **Challenge of Quantitative Phase Analysis of Slags: A Look at Sample Complexity**
**J. Lyza, S. Page,** Edward C. Levy, Co., USA
**T. Fawcett**, ICDD, USA

**D-33** **A Critical Examination and Re-determination of the Literature Ibuprofen-II Crystal Structure**
**P. Whitfield***, Excelsus Structural Solutions, Switzerland
**C. Smalley**, Bruker UK Ltd, United Kingdom

**D-35** **X-ray Characterization of Crystal Packing in Molecular Co-Crystals Based on $C_{60}$ Fullerene**
**L. Cook, G. Brewer**, The Catholic University of America, USA
**W. Wong-Ng**, NIST, USA

**D-38** **Exploring the Effects of Time and Temperature through Dynamically Heated Bone**
**H. Cross, C. Greenwood**, Keele University, United Kingdom
**G. Harrison**, Manchester University, United Kingdom

**D-41** **Manipulation of Structure-Property Relationships of the Crystallographic Phases of Cytosine Using Molecular Dyes**
**M. Fleming, J. Swift**, Georgetown University, USA

**D-42** **Desolvation Pathways of Variable Composition Solvates**
**J. Werner, J. Swift**, Georgetown University, USA

**D-44** **Inversion Degree and Microstructure Evaluation of $ZnFe_2O_4$ Ferrispinel**
**F.F. Contreras-Torres*, A.C. Murrieta, C. Flores-Jauregui**, Tecnologico de Monterrey, Mexico

**D-47** **Operando PDF Studies of High-Entropy Oxides in Li-ion Batteries**
**O. Jovino Marques, E. Timofeeva, C. Segre**, Illinois Institute of Technology, USA
**K. Wiaderek**, Argonne National Laboratory, USA

**D-48** **PDF Refinement for Local Structure Analysis of Ceramic Oxides**
**N. Henderson*, B. Jones**, Bruker, USA
**M. Evans**, Bruker, Germany

**D-50** **Evolution of the Microstructure of Laser Powder Bed Fusion Ti-6Al-4V during Post-Build Heat Treatment**
**L. Ravkov*, L. Balogh**, Queen's University, Canada
**D. Brown, V. Anghel, B. Clausen, N. Johnson, R. Martinez, E. Zepeda-Alarcon**, Los Alamos National Laboratory, USA
**D. Pagan**, Penn State University, USA
**M. Strantza**, Lawrence Livermore National Laboratory, USA
**G. Rafailov**, Nuclear Research Center of the Negev, Israel

**D-51** **Improving the Precision in Quantitative Analysis of Trace Components by the Rietveld Method Using a Partial Accumulation Measurement**
**T. Kuzumaki, M. Kasari, T. Ozawa**, Rigaku Corporation, Japan
**A. Ohbuchi**, Rigaku Americas Corporation, USA

**D-53** **Structural Characterization by X-ray Powder Diffraction of Two 3-aryl-thiazolo[3,4-α]Pyrazine-5, 8- Diones Compounds**
**C.G. Albarracin, J.A. Henao, R.A. Toro, A.R. Romero**, Universidad Industrial de Santander, Colombia
**J.M. Delgado**, Universidad de Los Andes, Venezuela

**D-54** **Structure Solution of the Bioactive Substances 18-Hydroxyoctadecanenitril and 17-Bromheptadecan-1-ol**
**S.T. Witzleben**, Bonn-Rhein-Sieg University of Applied Sciences, Germany

**D-55** **HPC Detector with 56,000 FPS Full Frame, 100,000 FPS for 100 rows ROI**
**Y. Nakaye*, Y. Sakuma, S. Mukusu, T. Sakumura**, Rigaku Corporation, Japan

**D-61** **Design, Synthesis, and Structu[illegible]dotellurate Salts**
**F. Sarbessa, R. Laitinen**, Univer[illegible]
WITHDRAWN

**D-66** **The Challenge of Grain Size for X-ray Powder Diffraction Analysis of Additively Manufactured Parts**
**S.A. Speakman**, Malvern Panalytical, USA

**D-67** **Real-Time Streaming Bragg Peak Analysis Using Deep Learning**
**D. Trujillo*, Z. Liu, P. Kenesei, M. Engbretson, H. Sharma, J.S. Park, A. Miceli, A. Ali**, Argonne National Laboratory, USA

**D-69** **NIST Standard Reference Materials for X-ray Metrology**
**J. Cline, M. Mendenhall, D. Black, D. Windover, A. Henins**, NIST, USA

**D-71** **Method of Temperature Calibration for Non-Ambient X-ray Diffraction Furnaces Using a Highly Anisotropic Thermal Expansion Material**
**D. Schmuckler*, B. Wheaton**, Corning Research and Development Corporation, USA

**D-74** **Gracing Incidence X-ray Diffraction Analysis of Picoliter Derived Specimen**
**S. Hampel*, D.A. Murcia Gonzalez, Y. Pu, U.E.A. Fittschen, G. Helsch, T. Schirmer**, Clausthal University of Technology, Germany

**D-75** **Use of X-ray Optics to Manufacture a Synthetic Retina**
**J. Maj,** University of Chicago, USA

**D-76** **Sample Displacement Correction for X-ray Diffraction in Debye-Scherrer Geometry with a Flat Area Detector**
**B.S. Hulbert*, W.M. Kriven**, University of Illinois at Urbana Champaign, USA

## XRF Poster Session – Wednesday Evening
Grand Ballroom D-H

**Signifies presenting author, when noted*

The Wednesday evening XRF poster session will be held 5:00 pm – 7:00 pm in the Grand Ballroom D-H, in conjunction with a wine and cheese reception. Three "Best Poster" awards will be given at the end of the session, including "Best Student Poster".

Chair: **M. Schmeling**, Loyola University Chicago, USA, mschmel@luc.edu

**F-1** **ENFORCE TXRF: A European Network for Chemical Elemental Analysis by Total Reflection X-ray Fluorescence**
**D. Eichert***, ELETTRA – Sincrotrone Trieste, Italy
**L. Borgese**, University of Brescia, Italy

**F-8** **X-ray Tomography as a 3D Metrology Technique for AM Materials**
**B. Hunter, E. Jacobson, I. Cummings, A. Wachtor, B. Patterson**, Los Alamos National Laboratory, USA

**F-10** **Quantification and Mathematical Modeling of Gold Nanoparticle Uptake in PC-3 Prostate Cancer Cell Line**
**G. Traplin*, A. Pejović-Milić**, Ryerson University, Canada
**R. Karshafian**, Ryerson University; Institute for Biomedical Engineering, Science and Technology; Keenan Research Centre for Biomedical Science of St. Michael's Hospital, Canada

**F-14** **Chemical State Analysis of 3d- and 4f-transition Metals Using High-resolution XRF System Xspecia™**
**T. Yoneda, S. Mitamura, T. Nyu, H. Motoki, K. Suzuki**, Shimadzu Corporation, Japan

**F-22** **In Situ EXAFS Studies of Pd@Ni(OH)$_2$&C Catalyst for Ethanol Oxidation**
**N. Su*, E.V. Timofeeva, C. Segre**, Illinois Institute of Technology, USA

**F-23** **Investigating the Integrity of a Claimed 1900's Piece of Art Using Portable X-ray Fluorescence Technique**
**S. Mcheik, N. Hedden, A. Pejović-Milić**, Ryerson University, Canada
**M. Bakovic**, Guelph University, Canada

**F-25** **Compact Silicon Drift Detector for High Energy X-ray Applications**
**M. Zhang*, E. Tikhomirov, Y. Tomimatsu, E.V. Damron, D. Redfern**, Hitachi High-Tech Science America, Inc., USA

**F-31** **Analysis of Low Levels of S and Cl in Fuel Samples**
**J. Sedlmair**, Bruker AXS LLC, USA

**F-33** **Evaluation of X-ray Beam Size in Micro-XRF Analysis and Excitation Volume in TXRF Analysis**
**M. Nakae, T. Matsuyama, K. Tsuji**, Osaka Metropolitan University, Japan

**F-40** **Glass Composition Control by Micro-XRF**
**J. Vargeson*, E. Fanning, A. Nached**, Corning RDC, USA

**F-41** **Picoliter Derived Micro Deposits as Tool to Understand Thin Film Sample Preparation**
**S. Hampel*, H.S. Till, U.E.A. Fittschen**, Clausthal University of Technology, Germany
**G. Pepponi**, Fondazione Bruno Kessler, Micro Nano Facility, Italy

**F-42** **3D Printing of Metal Containing Polymer Layers as Reference Samples in Micro XRF Analysis**
**S. Hampel*, U.E.A. Fittschen**, Clausthal University of Technology, Germany
**M. Iro, D. Ingerle, C. Streli**, Vienna University of Technology, Atominstitut, Austria
**I. Carlomagno, G. Aquilanti**, Elettra - Sincrotrone Trieste, Italy
**O.J.L. Fox, K.J. Sawhney**, Diamond Light Source, United Kingdom

# Plenary Session - Wednesday Morning, 3 August
# 8:30 am – 11:45 am
**Signifies presenting author, when noted*
# Grand Ballroom/Salon B & C

## Geology In & Out of This World

Chair: **T. Blanton**, ICDD, USA, tblanton@icdd.com

| | | |
|---|---|---|
| 8:30 | | Welcoming Remarks and Awards<br>**T. Fawcett**, Chairman of the Denver X-ray Conference, Emeritus, ICDD, USA |
| | | 2022 Birks Award presented to Kouichi Tsuji, Osaka Metropolitan University, Japan.<br>Presented by **M.A. Zaitz**, IBM, Retired, USA, Chairman of the Birks Award Selection Committee. |
| | | 2022 Robert L. Snyder Student Awards to be announced by **T. Blanton**, Executive Director, ICDD, USA. |
| | | Remarks by the Plenary Session Chair, **T. Blanton**. |
| 9:00 | P-1 | Unlocking How Biomineral Crystals Record Their Environments<br>**G.A. Farfan***, Smithsonian Institution, USA |
| 9:45 | P-2 | From Western Australia to the Atacama Desert: Lessons about the Past from Modern Microbialites<br>**E.P. Suosaari*, I. Lascu**, Smithsonian Institution, USA<br>**R.P. Reid, A.M. Oehlert, B.E. Vitek**, University of Miami, RSMAS, USA<br>**P. Parlanti**, Istituto Italiano di Tecnologia, Italy |
| 10:30 | | Break |
| 11:00 | P-3 | PIXL's Recent X-ray Data and Findings from the Red Planet<br>**C. Heirwegh***, Jet Propulsion Laboratory, California Institute of Technology, USA |

# Oral Sessions, Wednesday Afternoon, 3 August

## New Developments in XRD & XRF Instrumentation

**Grand Ballroom/Salon B**

Chairs: **T. Fawcett**, Emeritus, ICDD, USA, dxcfawcett@outlook.com
**A. Drews,** Ford Motor Company, USA, adrews@ford.com

| | | |
|---|---|---|
| 1:30 | S-1 | Silicon Drift Detectors with Improved Spectroscopic Performance<br>**A. Pahlke*, R. Fojt, M. Fraczek, L. Hoellt, M. Hofmann, P. Iskra, J. Knobloch**, KETEK GmbH, Germany |
| 1:45 | S-2 | Innovations in End Window X-ray Tube Design for XRF Analysis<br>**M. Maroney**, Micro X-Ray, Inc, USA |
| 2:00 | S-3 | Development of the New Compact X-ray Diffractometer, MiniFlex XpC<br>**A. Tripathi*, A. Ohbuchi, K. Saito**, Rigaku Americas Corporation, USA<br>**T. Kuzumaki, T. Ozawa**, Rigaku Corporation, Japan |
| 2:15 | F-44 | X-ray Detector Technology at Amptek<br>**R. Redus, A. Huber, P. Bennett, M. Fontanella**, Amptek Inc, USA |
| 2:30 | S-6 | Innovative Packaging of SDD Modules For Multi-Element Assemblies<br>**M. Morelle*, J. Elseviers, S. Put**, Mirion Technologies (Canberra Olen) NV, Belgium<br>**M. Kocsis, S. Benichou, C. Cohen**, European Synchrotron Radiation Facility, Grenoble, France |
| 2:45 | S-4 | A Clean PDF Solution – HighScore(Plus) Next<br>**T. Degen*, M. Sadki, E. Bron, M. Gateshki, V. Kogan**, Malvern Panalycal B.V., The Netherlands |
| 3:00 | | Break |
| 3:30 | S-8 | Improvements in the Precision of Real-Time Pulse Height Analysis in Microcalorimeter X-ray Detectors<br>**S. Thurgate**, Murdoch University; NIST, Australia<br>**T. Jach**, NIST, USA |

| | | |
|---|---|---|
| 3:45 | S-23 | Operando XRD and Total Scattering Measurements with SmartLab System for Lithium-Ion Battery Research<br>**E. Vinogradova*, A. Ohbuchi, K. Saito**, Rigaku Americas Corporation, USA<br>**Y. Shiramata, T. Konya**, Rigaku Corporation, Japan |
| 4:00 | S-24 | Active X-ray Optics for Synchrotrons<br>**D. Schmidt, P. Gaal**, TXproducts, Germany |
| 4:15 | S-9 | Versatile Compact Systems with Large Area Silicon Drift Detectors for EDX and XRF Applications<br>**M. Kopetzki, D. Schlosser, M. Bornschlegl, S. Aschauer, A. Niculae**, PNDetector GmbH, Germany |
| 4:30 | S-18 | TOPAS V7: Most Important New Features<br>**K. Knoor*, A. Kern**, Bruker AXS, Germany<br>**B. Jones, N. Henderson**, Bruker AXS, USA |
| 4:45 | S-33 | TruBeam for XRDynamic 500: A Novel Evacuated and Automated Beam Concept for XRD<br>**A.O.F. Jones*, M. Kremer, T. Müller, B. Schrode, P. Vir**, Anton Paar GmbH, Austria |

+ The previously advertised talk, *Highly Flexible Inner-Coated Hollow Capillaries for X-ray Radiation*, J. Wochnowski, Germany Autonomous Research Systems, was withdrawn from the Program.

## General XRD — Grand Ballroom/Salon C

Chair: **C. Murray**, IBM T.J. Watson Research Center, USA, conal@us.ibm.com

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| 1:40 | D-23 | Synchrotron X-ray Characterization of Pillared Cyanonickelates (PICNICs) for $CO_2$ Capture Applications<br>**W. Wong-Ng*, D. Siderius***, NIST, USA<br>**J. Culp**, NETL Support Contractor, USA<br>**Y. Chen**, ChemMatCARS, University of Chicago, USA<br>**L. Li**, Boise State University, USA |
| 2:00 | D-52 | The Use of Adaptable Cloud-based Virtual X-ray Laboratories and Online Real-time Collaborative Environment<br>**Y. Cherner**, ATeL - Advanced Tools for e-Learning, USA<br>**Y. He**, City University of New York, USA<br>**O. Coreño**, Universidad de Guanajuato, México<br>**P.Y. Cherner**, Microsoft Corp., USA |
| 2:20 | D-22 | Characterization of Polymers Used in Pharmaceutical and Biomedical Applications<br>**T. Blanton*, S. Gates-Rector, M. Rost**, ICDD, USA |
| 2:40 | D-62 | Certification of NIST Standard Reference Material 1976c<br>**J. Cline*, M. Mendenhall, D. Black, A. Henins, J. Filliben**, NIST, USA |
| 3:00 | | Break |
| 3:30 | D-20 | Effect of Finite Width of Specimen on Sample Transparency Aberration in Bragg-Brentano Geometry<br>**T. Ida**, Nagoya Institute of Technology, Japan |
| 3:50 | D-11 | Measurement of Coating Thickness with X-ray Diffraction<br>**M. Witte*, R. Beusse**, Salzgitter Mannesmann Forschung GmbH, Germany |
| 4:10 | D-27 | Identifying Disease Biomarkers through X-ray Diffraction of Breast Calcifications<br>**S. Gosling*, E. Arnold, S. Davies, I. Lyburn, K. Rogers**, Cranfield University, United Kingdom<br>**D. Calabrese, J. Nallala, N. Stone**, University of Exeter, United Kingdom<br>**C. Greenwood**, Keele University, United Kingdom<br>**I. Boubayone, S. Pinder**, Kings College London, United Kingdom<br>**L. King, E. Hwang**, Duke University Medical Center, USA |
| 4:30 | D-72 | The Crystal Structure of (S)-Dapoxetine Hydrochloride and (RS)-Trichlormethiazide from Laboratory X-ray Powder Diffraction Data<br>**G. Díaz de Delgado*, A. Dugarte-Dugarte, J.M. Delgado**, Universidad de los Andes, Venezuela<br>**R.A. Toro, J.A. Henao**, Universidad Industrial de Santander, Colombia<br>**J. van de Streek**, Avant-garde Materials Simulation, Germany |

## X-ray Absorption Spectroscopy (XAS)

**Glen Echo**

Chair: **Y. Tian**, Sigray, USA, ytian@sigray.com

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| 2:00 | S-12 | X-ray Characterization of a Metal-organic Framework during Dehydration and CO2 Adsorption<br>**E.P. Jahrman*, H.G.T. Nguyen, B. Kalanyan,** NIST, USA |
| 2:20 | S-14 | High-Entropy Oxide Bronzes as Tunable Li-ion and Na-ion Anode Materials<br>**S. Shadman*, O. Jovino Marques, C. Segre**, Illinois Institute of Technology, USA |
| 2:40 | S-16 | Operando XAS Studies of High-Entropy Oxides in Li-ion Batteries<br>**O. Jovino Marques*, E. Timofeeva, C. Segre**, Illinois Institute of Technology, USA |
| 3:00 | | Break |
| 3:30 | S-22 | Effect of Initial Structure on High Entropy Oxide Li-ion Anode Materials<br>**C. Segre*, O. Jovino Marques, M. Walter, E. Timofeeva**, Illinois Institute of Technology, USA |
| 3:50 | S-29 | A Laboratory-based High-Energy X-ray Absorption System<br>**Y. Tian*, Y. Liu, R. Qiao, S. Lewis, S.H. Lau, W. Yun, S. Seshadri**, Sigray, Inc., USA |
| 4:10 | S-34 | Identification of Chromium Oxide Species in Cr/Al2O3 Propane Dehydrogenation Catalysts<br>**A.S. Hoffman*, S.R. Bare**, SLAC National Accelerator Laboratory, USA<br>**M. Greaney, C. Lugmair, V.Z. Fridman, R. Xing**, Clariant Corp., USA |

# Oral Sessions, Thursday Morning, 4 August

**Signifies presenting author, when noted*

## Industrial Applications of XRD

**White Oak A**

Chair: **T. Fawcett**, Emeritus, ICDD, USA, dxcfawcett@outlook.com

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| 9:00 | D-39 | Invited - Industrial Applications of Materials Property Understanding via Phase and Microstructure Characterization<br>**B. Wheaton,** Corning Incorporated, USA |
| 9:30 | D-19 | Use of Well-Characterized Nano-Sized ZSM-5 Zeolite Catalyst for Plastic Waste Pyrolysis Feedstock to Produce High-Value Carbons<br>**R. Alghamdi, G. Manos**, University College London, United Kingdom<br>**H. Sitepu, L. Ding**, Saudi Aramco, Saudi Arabia |
| 9:50 | D-28 | Insight into Pharmaceutical Drug Products Using XRD-DSC-HUM<br>**T. Yamamoto*, J. Kim, A. Sasaki**, Rigaku Corporation, Japan<br>**A. Ohbuchi, S. Bates**, Rigaku Americas Corporation, USA |
| 10:10 | | Break |
| 10:40 | D-29 | A Complimentary Discussion of Two Different Thin Film Methods: X-ray Diffraction and X-ray Fluorescence<br>**J. Langford, J. Peters**, Shimadzu Scientific Instruments, USA |
| 11:00 | D-60 | Laboratory Case Study of Identifying Trapped Materials in a Choke Valve<br>**W. Alkhashram, N. Alyami, M. Leoni, A. Al-Asseel, I. Zahrani, H. Muhanna, M. Alotaibi**, Saudi Aramco, Saudi Arabia |
| 11:20 | D-5 | Amorphous Phase Quantification by a Standard-Less Quantification Method<br>**A. Ohbuchi*, S. Bates**, Rigaku Americas Corporation, USA<br>**T. Kuzumaki, T. Ozawa, T. Konya**, Rigaku Corporation, Japan |
| 11:40 | D-64 | X-ray Powder Diffraction Made Easy for Industry Users<br>**K. Knorr**, Bruker AXS GmbH, Germany<br>**N. Henderson, B. Jones**, Bruker AXS LLC, USA |

## Cultural Heritage — White Oak B

Chair: **M. Schmeling**, Loyola University Chicago, USA, mschmel@luc.edu

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| 9:00 | S-15 | Invited - X-ray View on Prehistoric Cave Art. Insights about the Decoration of the Lascaux, Rouffignac and Font-De-Gaume Caves, Dordogne, France<br>**I. Reiche,** PSL Université; Fédération de recherche NewAGLAE, France |
| 9:30 | F-5 | Analysis of Coronado State Historic Site Artifacts using X-rays<br>**S.G. Young, J. Valdez, M. Espy, A. Edgar, J. Brett, A. Chov, B.M. Patterson**, Los Alamos National Laboratory, USA<br>**C. Mathers**, Archeological Analysis and Graphics, USA<br>**M. Barbour**, Coronado and Jemez Historic Sites, USA |
| 9:50 | F-21 | Fragments of History: A Material Elemental Study on Mayapán Ceramics<br>**O.G. de Lucio, M. Pérez**, LANCIC, Instituto de Física, Mexico<br>**S. Ortiz**, Instituto de Geofísica, Unidad Michoacán, Mexico<br>**C. Peraza Lope, W. Cruz Alvarado**, Centro INAH-Yucatan, Mexico |
| 10:10 | | Break |
| 10:40 | S-13 | Invited - MA-XRF Imaging for Historical Paintings – Developments in Data Evaluation and Instrumentation<br>**M. Alfeld**, TU Delft, The Netherlands |
| 11:10 | F-17 | X-ray Investigations of Lawrence University's Wriston Collection<br>**M. Koker, J. McShan, M. Schefchik**, Lawrence University, USA<br>**M. Newville**, GSECARS, APS, USA |
| 11:30 | S-32 | The Use of Handheld XRF Effectively To Learn More about the Materiality of Heritage Objects<br>**M. Loubser**, University of Pretoria, South Africa |

+ The previously advertised talk, Physics and Art: *Use of X-rays Instruments and Techniques for CT Analysis in the Cultural Heritage Field*, L. Vigorelli*, et al., Polytechnic of Torino; Istituto Nazionale di Fisica Nucleare, Italy, was withdrawn from the Program.

## Quantitative Analysis of XRF — Glen Echo

Chairs: **B. Ganly**, CSIRO, Australia, brianna.ganly@csiro.au
**C. Heirwegh**, Jet Propulsion Laboratory, California Institute of Technology, USA, christopher.m.heirwegh@jpl.nasa.gov

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| 9:00 | F-19 | Invited - Quantitative Analysis of Valence Electron Transitions in High Resolution X-ray Fluorescence Spectra<br>**B. Ganly*, J. McIlquham,** CSIRO, Australia<br>**J. Webster, M. Kirkpatrick,** CSIRO & University of Wollongong, Australia |
| 9:30 | F-20 | Invited - Traceability of X-ray Fundamental Parameters<br>**C.I. Szabo**, NIST, USA |
| 10:00 | F-35 | Dwell Time-Specific Errors in Quantitation When Background Correcting X-ray Fluorescence Spectra Using Per-Pixel Baselines<br>**A.M. Crawford*, J. Balough**, Northwestern University, USA<br>**J. Penner-Hahn**, University of Michigan, USA<br>**A. Glowacki, O. Antipova, E. Maxey**, Advanced Photon Source, ANL, USA<br>**Y. Chen**, Feinberg School of Medicine, USA<br>**T. O'Halloran, T. Woodruff**, Michigan State University, USA |
| 10:20 | | Break |
| 10:50 | F-6 | Invited - Scanning-Free Grazing Emission X-ray Fluorescence in the Laboratory<br>**J. Baumann**, Technical University of Berlin, Germany |
| 11:20 | F-39 | Quantification of Calcium Stearate Additive in Polymers Using Benchtop XRF<br>**Y. Yang*, N. Petzetakis, T. Hasan, T. Stewart, S. Wu**, The Dow Chemical Company, USA |

11:40 F-13 X-ray Energy Dependence of Beam Diameter Produced by Polycapillary X-ray Optics
**A. Das, L. Wade, C. Heirwegh**, Jet Propulsion Laboratory, California Institute of Technology, USA
**B. Clark**, Space Science Institute, USA
**T. Elam**, University of Washington, USA

# Oral Sessions, Thursday Afternoon, 4 August

**Signifies presenting author, when noted*

## Machine Learning Techniques in X-ray Analysis — White Oak A

Chairs: **M. Cherukara**, Argonne National Laboratory, USA, mcherukara@anl.gov
**A. Mehta**, SLAC, SSRL, USA, mehta@slac.stanford.edu

1:30 S-11 Invited - DL-Accelerated Nanoscale Coherent Diffraction Imaging
**Y. Yao*, B.B. Frosik, R.J. Harder, M.J. Cherukara, H. Chan,** Argonne National Laboratory, USA

2:00 S-21 Invited - Semi-Mechanistic Probabilistic Generative Models for High Throughput X-ray Diffraction Analysis
**B. DeCost*, H. Joress**, NIST, USA
**E. Holcombe**, Naval Surface Warface Center, Carderock; JHU; NIST, USA
**P. Sreeramagiri**, Ames Laboratory, USA

2:30 S-28 Real-Time Ptychography Data Analysis Using Machine Learning At The Edge
**A.V. Babu, T. Zhou, S. Kandel, Y. Jiang, Y. Yao, S. Veselli, Z. Liu, T. Bicer, M.V. Holt, A. Micelli, M.J. Cherukara**, Argonne National Laboratory, USA
**E. Sirazitdinova, G. Gupta**, NVIDIA, USA

2:50 S-30 Deep-Learning Accelerated X-ray Diffraction Data Analysis
**H. Sharma*, Z. Liu, J.S. Park, P. Kenesei, J. Almer, A. Miceli**, Argonne National Laboratory, USA

3:10 S-17 Complex-valued Convolutional Networks for Efficient Ptychographic Imaging
**S. Kandel*, Y. Yao, J. Deng, R. Harder, Y. Jiang, C. Phatak, A. Tripathi, T. Zhou, Z. Di, M. Cherukara**, Argonne National Laboratory, USA
**J. Reinhardt**, Lawrence Berkeley National Laboratory, USA

3:30 Break

4:00 S-19 Synthesis Sparse Dictionary Learning for Ptychographic Probe Recovery
**A. Tripathi**, Argonne National Laboratory, USA

4:20 S-20 Automating and Accelerating EXAFS Data Collection and Analysis Using Machine Learning Methods
**H. Joress*, B. DeCost, B. Ravel**, NIST, USA
**E. Anber, J. Hollenbach, E. Holcombe, M. Taheri**, Johns Hopkins University, USA
**J. Hattrick-Simpers**, University of Toronto, Canada

4:40 S-7 Non-Scanning Grazing-Exit XANES Analysis of Stratified Samples and the Optimization of the Data Collection Process
**C.T. Cakir*, A. Buzanich, U. Reinholz, M. Radtke** Federal Institute for Materials Research and Testing, Germany
**C. Streli**, Technical University Wien, Austria

5:00 S-10 A Critical Review of Neural Networks for the Identification of X-ray Diffraction Spectra
**J. Schuetzke*, M. Reischl**, Karlsruhe Institute for Technology, Germany
**N.J. Szymanski, G. Ceder**, Lawrence Berkeley National Laboratory, USA

## Non-ambient Analysis — White Oak B

Chair: **S. Misture**, NYS College of Ceramics at Alfred University, USA, misture@alfred.edu

2:00 D-68 Invited - Evaluating the Temperature Dependence of PZT Structures Using a Virtual Reality Environment
**M.A. Rodriguez*, J. Krukar, N.R. Valdez, J.Z. Harris, K.A. Perkins, C. DiAntonio, P. Yang,** Sandia National Laboratories, USA

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| 2:30 | D-15 | MetalJet X-ray sources for Experiments at Non-ambient Pressures and Temperatures<br>**A. Adibhatla**, Excillum, USA<br>**J. Hallstedt**, Excillum, Sweden |
| 2:50 | D-63 | Dynamics of the A-site Modulation in the Hollandite Phase<br>**J. Schaeperkoetter*, S. Misture**, Alfred University, USA |
| 3:10 | D-73 | High Temperature X-ray Diffraction of Thermite Reactive Nanolaminates<br>**C. Skidmore, J.-P. Maria**, Pennsylvania State University, USA |
| 3:30 | | Break |
| 4:00 | D-43 | Invited - Investigation of the Phase Stability of Yttrium Titanium Oxide Using Correlative in situ High-Temperature X-ray Diffraction and Transmission Electron Microscopy<br>**X. Pu, L. He**, Idaho National Laboratory, USA<br>**H. Kim**, University of Florida, USA |
| 4:30 | D-32 | Low Temperature Crystal Structures of the Solvent Dimethyl Carbonate<br>**P. Whitfield**, Excelsus Structural Solutions, Switzerland |
| 4:50 | D-37 | It's Been a Long Time Coming - Temperature Dependent Structure Solution of Rb[SCN]<br>**L.C. Folkers***, STOE & Cie GmbH, Germany<br>**F. Tambornino**, Philipps-Universität Marburg, Germany |

## Stress Analysis — Glen Echo

Chair: **T.R. Watkins**, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov

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| 2:30 | D-70 | Invited - Utilizing the Upgraded HIDRA Neutron Diffractometer to Characterize Residual Stress in Friction Stir Welds<br>**J. Bunn*, P. Cornwell, A. Payzant,** Oak Ridge National Laboratory, USA<br>**B. Wing,** University of Tennessee, USA<br>**P. Lyda**, Ohio State University, USA |
| 3:00 | D-16 | Defining Residual Stresses Measured by Diffraction<br>**M.H. Seren***, Cornell High Energy Synchrotron Source, USA<br>**I.C. Noyan**, Columbia University, USA |
| 3:20 | | Break |
| 3:50 | D-9 | Evaluation of Non-Joulian Magnetostriction in Giant Magnetostrictive Alloys, Terfenol-D and Galfenol<br>**M. Imafuku*, K. Sato, K. Kawasaki, T. Otsubo**, Tokyo City University, Japan |
| 4:10 | D-24 | Microstructure Parameters, Residual Stresses, and Preferred Orientation of Laser Additive Manufactured H13 Tool Steel<br>**K. Trojan*, J. Capek, J. Cech, N. Ganev, K. Kolarík**, Czech Technical University in Prague, Czech Republic<br>**V. Ocelík**, University of Groningen, The Netherlands |

## Trace Analysis — Forest Glen

Chair: **D. Eichert**, Elettra – Sincrotrone Trieste, Italy, diane.eichert@elettra.eu

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| 1:00 | F-30 | Invited - Dimensional and Analytical Metrology for Semiconductor Nanostructures Using Grazing X-ray Fluorescence Techniques<br>**P. Hönicke, Physikalisch-Technische Bundesanstalt, Germany** |
| 1:30 | F-34 | Invited - How Can XRF-Based Trace Element Analysis Help to Solve Pressing Global Problems?<br>**H. Stosnach**, Bruker Nano Analytics, Germany |
| 2:00 | F-11 | Analyses of Trace Metals in Biological Materials by TXRF and GFAAS<br>**M. Schmeling*, M. Gende**, Loyola University Chicago, USA |
| 2:20 | F-26 | Analytical Characterization of the Benchtop TXRF Spectrometric Analysis of Two Se Metabolites in Simulated Human Urine<br>**N. Dasgupta-Schubert*, J. Rodriguez, I. Serrato**, University of Michoacán, Mexico |

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| 2:40 | F-36 | Towards Developing an In-Vivo Bone Tungsten K X-ray Fluorescence Detection System: Monte Carlo Simulations<br>**S. Mcheik, A. Pejović-Milić**, Ryerson University, Canada |
| 3:00 | | Break |
| 3:30 | F-38 | Invited – Synchrotron Microprobe Analyses of Thorium- and Uranium-bearing Mineral Allanite from Palawan, Philippines – a Micro-XRF and Micro-XRD Study<br>**V.I. Samson*, C.M. Dingle, R.R. Diwa, F.C. Hila, J.M. Jecong, G.E. Lopez, N.R.D. Guillermo**, Philippine Nuclear Research Institute, Philippines<br>**D. Sanchez, D. Grolimund**, Paul Scherrer Institut, Switzerland |
| 4:00 | F-18 | X-ray Fluorescence under Grazing Incidence Analysis of Particulate Matter Filters: Understanding the Effect of Beam Footprint<br>**P. Cirelli*, F. Bilo, L.E. Depero, L. Borgese**, University of Brescia, Italy<br>**G. Siviero**, GNR srl, Italy<br>**D. Eichert**, Elettra-Sincrotrone Trieste, Italy<br>**T. Hase**, University of Warwick, United Kingdom<br>**D. Wermeille**, European Synchrotron Radiation Facility, France |

## Micro XRF using Imaging — Forest Glen

Chairs: **P. Wobrauschek**, Atominstitut – TU Wien, Vienna, Austria, wobi@ati.ac.at
**M.A. Zaitz**, IBM, Retired, USA, zaitzmaryann@gmail.com

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| 4:20 | F-15 | Invited - Steps Towards the Quantitative Interpretation of Confocal Micro-X-ray Fluorescence Measurements (QCMXRF)<br>**M. Iro*, D. Ingerle, P. Kregsamer, C. Streli,** Atominstitut, TU Wien, Austria |
| 4:50 | F-9 | Application of Micro XRF for Determining Homogeneity of Calibration Standards Prepared for Bulk XRF Analysis of Trace Elements<br>**P. Dutta**, Dow Inc., USA |
| 5:10 | F-7 | A Compact High Solid Angle Four Segmented Annular Silicon Drift Detector System for Synchrotron and Particle Beam Applications<br>**D.M. Schlosser*, A. Bechteler, M. Bornschlegl, R. Lackner, D. Steigenhöfer, S. Aschauer, A. Niculae, H. Soltau**, PNDetector GmbH, Germany |

# Oral Sessions, Friday Morning, 5 August

**Signifies presenting author, when noted*

## Small-angle X-ray Scattering (SAXS)

**White Oak A**

Chairs: **W. Bras**, Oak Ridge National Laboratory, USA, brasw@ornl.gov
**L. Yang**, Brookhaven National Laboratory, USA, lyang@bnl.gov

8:30 D-58 Invited - Time-Resolved Small-angle X-ray Scattering Analysis of Reaction Kinetics during Polymerization-Induced Self-Assembly of Block Copolymers
**O.O. Mykhaylyk*, G. Liao, S.P. Armes,** The University of Sheffield, United Kingdom

9:00 D-40 Invited - Investigating Advanced Manufacturing Processes of Polymeric Materials with X-ray Scattering Techniques
**L. Wiegart**, Brookhaven National Laboratory, USA

9:30 D-36 Coherent Surface Scattering Imaging (CSSI) at Grazing Incidence Small Angle X-ray Scattering (GISAXS) Geometry
**P. Myint*, J. Zhang, M. Chu, A. Tripathi, J. Wang, S. Narayanan**, Argonne National Laboratory, USA

9:50 Break

10:10 D-46 Invited - Small Angle X-ray Scattering Applications in Structural Biology
**L. Fan***, Frederick National Laboratory for Cancer Research; National Cancer Institute, USA
**Y.-X. Wang**, National Cancer Institute, USA

10:40 D-59 Imaging Biological Tissues Using X-ray Scattering as a Contrast Mechanism
**L. Yang**, Brookhaven National Laboratory, USA

11:00 D-25 MetalJet X-ray Source for Time Resolved and in-situ SAXS
**J. Hållstedt, E. Espes**, Excillum, Sweden
**A. Adibhatla**, Excillum, USA

11:20 D-13 Anomalous Small Angle X-ray Scattering Study of Counterion Distribution Around Nanoparticles and Polyelectrolytes
**J. Chen**, Argonne National Laboratory, USA
**M. Bera**, NSF's ChemMatCARS, University of Chicago, USA
**T. Liu**, University of Akron, USA

## Applications of Rietveld Analysis

**White Oak B**

Chairs: **J. Kaduk**, Poly Crystallography, Inc., USA, kaduk@polycrystallography.com
**S. Misture**, NYS College of Ceramics at Alfred University, USA, misture@alfred.edu

8:30 D-1 Psilocybin: Crystal Structure Solutions Enable Phase Analysis of Prior Art and Recently Patented Examples
**J.A. Kaduk**, North Central College; Illinois Institute of Technology; Poly Crystallography Inc., USA
**A.M. Sherwood, R.B. Kargbo, K.W. Kaylo, P. Meisenheimer**, Usona Institute, USA
**N.V. Cozzi**, University of Wisconsin, USA

8:50 D-31 Structural and Cocrystal Formation Studies of Pyridinedicarboxylic Acid Regioisomers by Synchrotron Powder Diffraction in Idealized and Multiplexed Sample Formats and at Variable Temperatures
**J. Chen*, A.Yakovenko, U. Ruett**, Argonne National Laboratory, USA
**H. Patel, Y.Ma, K. Schaab**, DeNovX, USA
**J.A. Kaduk**, North Central College; Illinois Institute of Technology, USA
**A. Bond**, DeNovX; Illinois Institute of Technology, USA

9:10 D-8 What Happens When Nanoparticles are not Spherical?
**A. Corrao*, M. Cosby, P. Khalifah**, Stony Brook University, USA
**V. Petrova, C. Coaty, P. Liu**, University of California San Diego, USA

9:30 D-14 A New Procedure for Decomposing the Powder Diffraction Pattern of a Mixture into Individual Component Patterns Including the Component with No Pattern Model
**H. Toraya**, Rigaku Holding Corporation, Japan

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| 9:50 | | Break |
| 10:10 | D-34 | Microstructural Analysis of ZnO Nanoparticles Using Rietveld Refinement of X-ray Diffraction Data<br>**S. Rath*, G. Gupta**, University of Delhi, India |
| 10:30 | D-57 | Application of Phase Identification and the Rietveld Method on XRPD data of Deposits and Zeolite Catalysts by using ICDD PDF4+ Database and HighScore(Plus) Software – An Important Industrial Challenge<br>**H. Sitepu**, Saudi Aramco, Saudi Arabia<br>**T. Degen**, Malvern Panalytical B. V., The Netherlands |
| 10:50 | D-18 | Structural and Texture Refinement of X-ray Powder Diffraction Data of the Modified Zeolite-Y and Synthesized Catalysts for Crude Oil Direct Hydrocracking by Rietveld Method<br>**H. Sitepu, L. Ding, M.F. Aljishi, S.J. Al-Khaldi, I.M. Zahrani**, Saudi Aramco, Saudi Arabia |
| 11:10 | D-65 | Anomalous X-ray Diffraction of NMC Battery Cathode Materials using a Laboratory Diffractometer<br>**S.A. Speakman**, Malvern Panalytical, USA |
| 11:30 | D-49 | Joint PDF-Rietveld Refinements of $LiMn_2O_4$ from Laboratory Data<br>**M. Evans***, Bruker, Germany<br>**N. Henderson, B. Jones**, Bruker, USA |

## Industrial and General XRF — Glen Echo

Chair: **C.G. Worley**, Los Alamos National Laboratory, USA, cworley@lanl.gov

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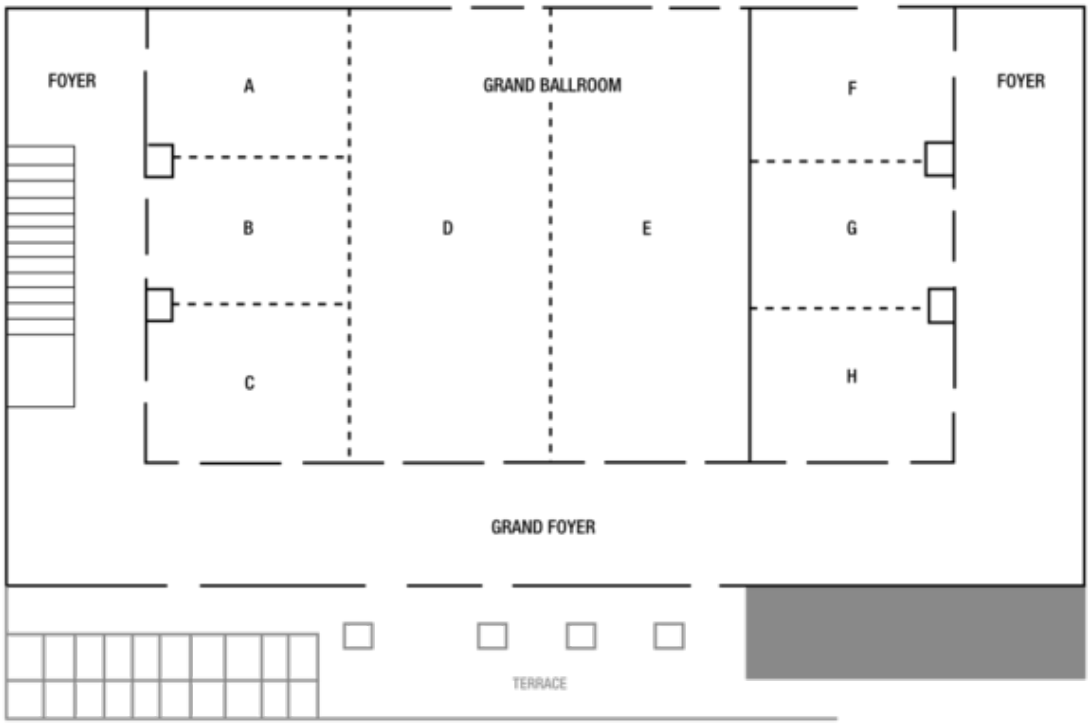
| 8:30 | F-24 | Invited - The Capability of XRF For Solving Analytical Problems in Industry and Forensic Investigations<br>**S. Mamedov**, HORIBA Scientific, USA |
| 9:00 | F-3 | Invited - How XRF Has Become Integrated Into Precious Metal Determinations Over the Past 25 Years<br>**M. Hinds**, MHinds Analytical Consulting Inc, Canada |
| 9:30 | F-16 | Analytical Validation of Elemental Impurities in Pharmaceutical Matrices by Energy Dispersive X-ray Fluorescence Spectroscopy<br>**J. Langford, H. Chen, J. Peters**, Shimadzu Scientific Instruments, USA |
| 9:50 | | Break |
| 10:10 | F-32 | XRF in Feed and Forage Applications<br>**T. Shalapska, J. Sedlmair**, Bruker AXS LLC, USA |
| 10:30 | F-4 | Additively Manufactured Polymer Lattice Experiments and Modeling<br>**B.M. Patterson, J. Brett, A. Chov, S.G. Young, B.K. Hunter, D. Zhang, A. Ionita**, Los Alamos National Laboratory, USA |
| 10:50 | F-2 | Toward a Road Map in Total Reflection X-ray Fluorescence Analysis<br>**D. Eichert**, Elettra - Sincrotrone Trieste, Italy |
| 11:10 | F-43 | Picoliter Derived Artificial Samples and Their Investigation with Gracing Incidence XRF<br>**S. Hampel*, U.E.A. Fittschen**, Clausthal University of Technology, Germany |

# Bethesda North Marriott Hotel & Conference Center
# Rockville, Maryland, USA

MAIN LEVEL

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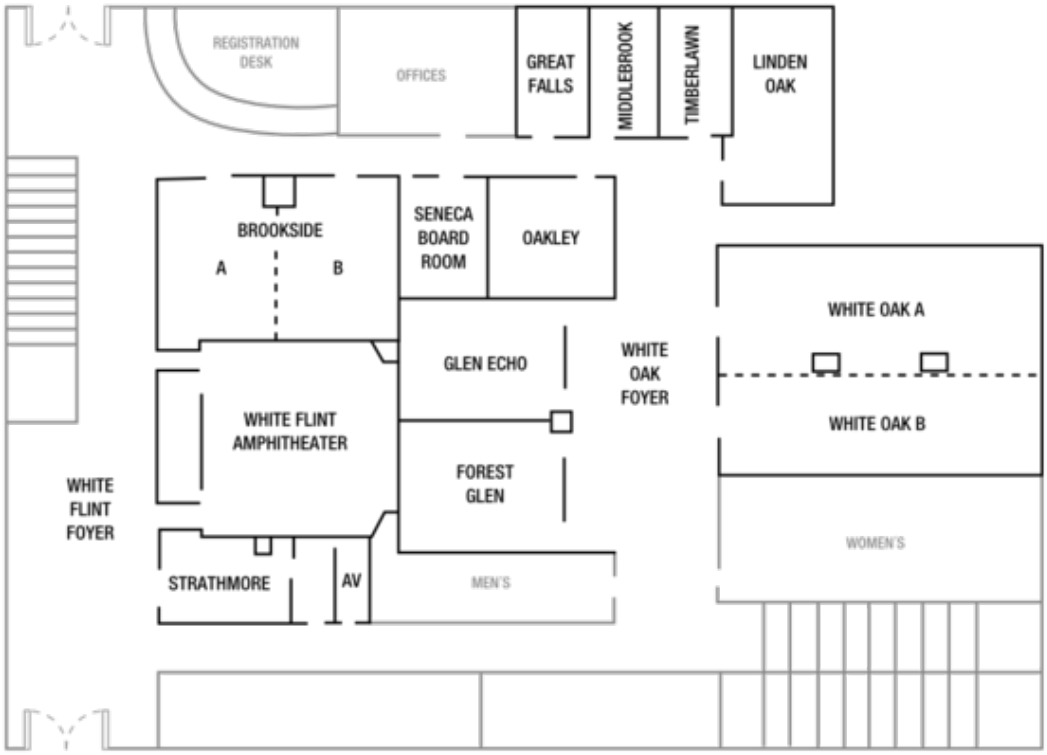

## 2022 Denver X-ray Conference ♦ Program-at-a-Glance ♦ Monday – Friday ♦ 1 – 5 August

| | Meeting Rooms | | | |
|---|---|---|---|---|
| | **White Oak A** *(Grand Ballroom / Salon B when noted)* | **White Oak B** *(Grand Ballroom / Salon C when noted)* | **Glen Echo** | **Forest Glen** |
| **Monday Morning Workshops 9:00 am – 12:00 Noon** | | | | |
| Special Topic | Machine Learning Techniques in X-ray Analysis (**Mehta/Cherukara**) | | | |
| XRD | | XRD Sample Preparation (**Fawcett**) | | |
| XRF | | | Sample Preparation of XRF (**Zaitz**) | Layered Structures (**Wobrauschek/Hradil**) |
| **Monday Afternoon Workshops 1:30 pm – 4:30 pm** | | | | |
| Special Topic | | X-ray Absorption Spectroscopy (XAS) (**Seshadri**) | | |
| XRD | 2D Detectors (**He/Blanton**) | | | |
| XRF | | | Basic XRF (**Zaitz**) | Handheld XRF (**Loubser**) |
| **Tuesday Morning Workshops 9:00 am – 12:00 Noon** | | | | |
| Special Topic | X-ray CT in Laboratory Settings (**Cakmak**) | | | |
| XRD | | | Stress Analysis (**Watkins/Murray**) | |
| XRF | | | | Micro XRF (**Tsuji/Zaitz**) |
| **Tuesday Afternoon Workshops 1:30 pm – 4:30 pm** | | | | |
| Special Topic | | | | |
| XRD | Rietveld Analysis for Phase Quantification (**Kaduk/Misture**) | Small-angle X-ray Scattering (SAXS) (**Watkins**) | | |
| XRF | | | Multimodal XRF Microscopy Fitting Tools (**Antipova\Glowacki**) | Trace Analysis (**Wobrauschek**) |
| **Tuesday Evening XRD Poster Session & Reception 5:00 pm – 7:00 pm (Watkins/Cakmak) Grand Ballroom** | | | | |
| **Wednesday Morning Plenary Session – Geology In & Out of This World** Grand Ballroom / Salon B & C, 8:30 am – 11:45 am (**Blanton**) | | | | |
| **Wednesday Afternoon Sessions** | | | | |
| Special Topic | New Developments in XRD & XRF Instrumentation (**Fawcett/Drews**) *(Grand Ballroom / Salon B)* | | X-ray Absorption Spectroscopy (XAS) (**Tian**) | |
| XRD | | General XRD (**Murray**) *(Grand Ballroom / Salon C)* | | |
| XRF | | | | |
| **Wednesday Evening XRF Poster Session & Reception 5:00 pm – 7:00 pm (Schmeling) Grand Ballroom** | | | | |
| **Thursday Morning Sessions** | | | | |
| Special Topic | | Cultural Heritage (**Schmeling**) | | |
| XRD | Industrial Applications of XRD (**Fawcett**) | | | |
| XRF | | | Quantitative Analysis of XRF (**Heirwegh/Ganly**) | |
| **Thursday Afternoon Sessions** | | | | |
| Special Topic | Machine Learning Techniques in X-ray Analysis (**Mehta/Cherukara**) | | | |
| XRD | | Non-ambient Analysis (**Misture**) | Stress Analysis (**Watkins**) | |
| XRF | | | | Trace Analysis (**Eichert**) / Micro XRF using Imaging (**Zaitz/Wobrauschek**) |
| **Friday Morning Sessions** | | | | |
| Special Topic | | | | |
| XRD | Small-angle X-ray Scattering (SAXS) (**Bras/Yang**) | Applications of Rietveld Analysis (**Misture/Kaduk**) | | |
| XRF | | | Industrial & General XRF (**Worley**) | |