



DXC

DENVER X-RAY CONFERENCE

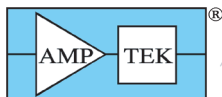
72nd Annual Conference on Applications of X-ray Analysis

7 - 11 August 2023 • Westin Chicago Lombard, Lombard, Illinois, USA

2023 Program



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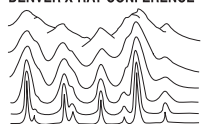


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DENVER X-RAY CONFERENCE®



www.dxcicdd.com



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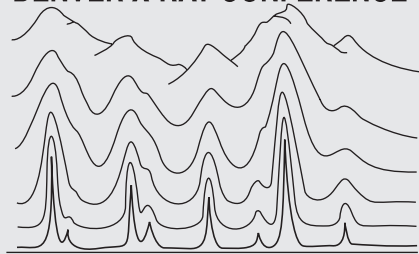
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Paul Predecki, University of Denver, USA

Rene van Grieken, University of Antwerp, Belgium

**Future Conference:
DENVER X-RAY CONFERENCE®**



5 – 9 August 2024

**The Westin Westminster
Westminster, Colorado, USA**

DXC 2023 - HEALTH & SAFETY GUIDELINES

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.

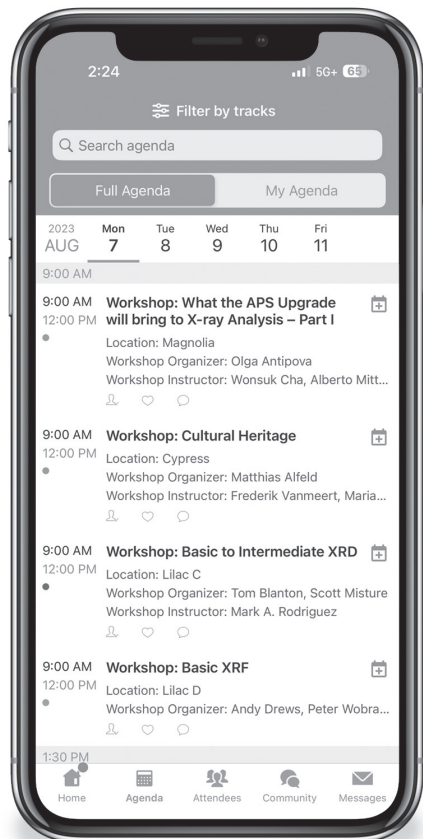
If you become ill onsite, stay in your room and report your illness to Elizabeth Dempsey (dempsey@icdd.com). Seek medical attention to obtain a COVID-19 test, and do not return to the event until you obtain a negative test result.

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.

Health Waiver

In order to attend DXC 2023, all attendees must sign and submit a health waiver acknowledging that there is a risk of contracting COVID-19 by attending the conference. DXC 2023 is not requiring attendees to be fully vaccinated to attend the conference.

LATE ANNOUNCEMENTS – DXC EVENT APP



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

Visit your App Store on your mobile device to download Whova or access using your desktop browser, the event invitation code is: **dxc2023attendee**.

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- Industrial Applications of XRF
- General XRD
- Quantitative Analysis of XRF

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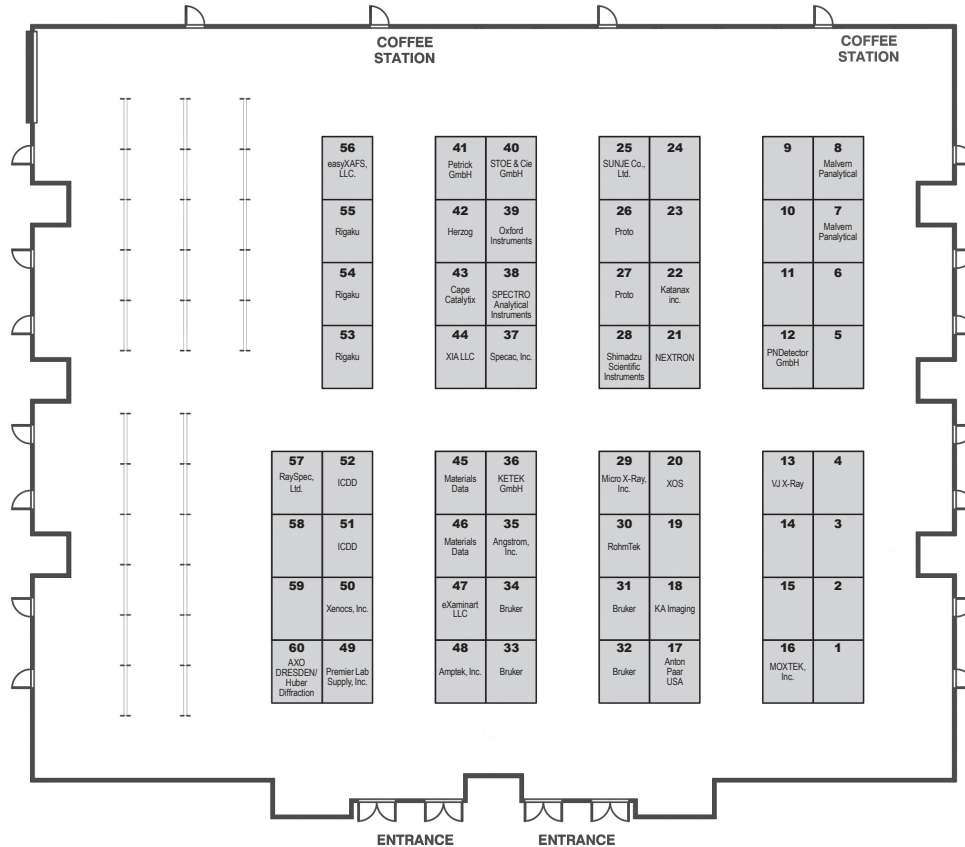
- Energy Storage and Harvesting
- Cultural Heritage
- Applications of Rietveld Analysis
- Micro XRF and Synchrotron Applications

2023 Denver X-ray Conference Exhibitors

Exhibits will be held in the Grand Ballroom.

Exhibit Hours

Monday, 7 August	4:30 pm - 7:00 pm
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Exhibitors

Amptek, Inc.

Booth: 48

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.

Angstrom, Inc.

Booth: 35

Website: www.angstrom-inc.com

Email: sales@angstrom-inc.com

Angstrom is a manufacturer of sample preparation equipment and supplies for XRF analysis. Our product line includes the TE250 Ring & Puck Mill, the 4451AE Pellet Press and the 4452 Programmable Pellet Press. All of our products are rugged and highly regarded in the XRF community - well suited for laboratories that require high sample throughput. A complete line of aluminum sample cups are offered in various depths and diameters.

Anton Paar USA – Ashland, VA

Booth: 17

Website: www.anton-paar.com/us-en

Email: info.us@anton-paar.com

Driven by 60 years of experience in X-ray diffraction (XRD), small-angle X-ray scattering (SAXS) and advanced X-ray optics, Anton Paar provides X-ray analysis solutions for every challenge. Our state-of-the-art X-ray instrumentation is used by customers across a large number of fields in both academia and industry. <https://www.anton-paar.com/us-en/x-ray-analysis/>

AXO DRESDEN / Huber Diffraction Equipment

Booth: 60

Website: www.axo-dresden.de

AXO DRESDEN is a specialist for high precision deposition and multilayer coatings for multilayer X-ray optics, XRD and XRF applications. The Primux 50 micro focus X-ray source system is in our portfolio as well.

HUBER DIFFRACTION is a manufacturer of precise positioning and diffraction equipment for laboratory, synchrotron and neutron applications.

Bruker

Booths: 31, 32, 33, 34

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, micro-XRF, microtomography, EDS, WDS and EBSD systems.

Cape Catalytix

Booth: 43

Website: www.capecatalytix.com

Email: info@capecatalytix.com

Cape Catalytix (Pty) Ltd was established as a spinoff company of the University of Cape Town. Cape Catalytix manufactures patented instrumentation under exclusive license from the University of Cape Town, most notably its IKEY in situ XRD reaction cell and associated controller. The easy-to-use XRD cell is a capillary plug flow reactor suited for controlled-environment studies of engineering materials and heterogeneous catalysis, and can be coupled with laboratory and synchrotron X-ray equipment.

easyXAFS, LLC.

Booth: 56

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.

eXaminart LLC**Booth: 47****Website: www.examinart.com****Email: info@examinart.com**

eXaminart LLC develops innovative analytical systems for space exploration and commercial markets, with a particular interest in cultural heritage. Our commercial line includes:

- Fenix, a general-purpose portable benchtop XRD/XRF for powdered materials (new).
- Duetto-2, a non-invasive portable XRD/XRF specifically developed for cultural heritage (since 2021).
- microScanix, a high-resolution portable mapping microXRF for cultural heritage (since 2022).
- Scanix XRF, a lower-resolution lower-cost counterpart of microScanix (in development).

Herzog Automation Corp.**Booth: 42****Website: www.herzogautomation.com****Email: kburns@herzogautomation.com**

Herzog Automation Corp. is the leading supplier of manual and fully automatic sample preparation systems for spectrographic and X-ray analysis, tube delivery systems for sample transport, and laboratory automation for the cement, mining, steel and aluminum, industries. Please visit our website at www.herzogautomation.com for our full product line.

International Centre for Diffraction Data (ICDD)**Booths: 51, 52****Website: www.icdd.com****Email: info@icdd.com**

We focus on meeting the needs of the scientific community through the publication of the Powder Diffraction File™ (PDF®). We strive to provide quality educational opportunities to exchange new ideas and information. ICDD's carefully curated and edited material identification databases interface with diffractometers and analysis systems of the world's leading X-ray equipment manufacturers and software developers. The Powder Diffraction File is available in a variety of licensing options. Visit our booth for a first look at the new Next-Level Database!

KA Imaging**Booth: 18****Website: www.kaimaging.com****Email: info@kaimaging.com**

KA Imaging produces affordable and easy-to-use 3D phase contrast X-ray microscopes, high-resolution X-ray area detectors and flat panel detectors for medical, scientific, and industrial non-destructive testing (NDT) imaging applications.

Katanax Inc.**Booth: 22****Website: www.katanax.com****Email: info@katanax.com**

Katanax develops automated furnaces for sample preparation by fusion. Katanax® Electric Fluxers prepare fused beads for XRF analysis. They can withstand the worst environment in fusion. Typical samples include cements, ores, slag, sediments, soils, rocks, ceramics, pigments, glasses and even metals. Our fluxers are the ultimate fusion machines and we are proud to support analytical laboratories in their quest for safety, efficiency, and accuracy. Get yourselves "a Katanax" for your lab and prepare to be amazed!

KETEK GmbH**Booth: 36****Website: www.ketek.net****Email: info@ketek.net**

KETEK, the leading manufacturer of Silicon Drift Detectors, presents its next generation electronics. The new generation 3.0 features a low noise analog preamplifier with improved temperature stability and throughput capability as well as a renovated digital signal processing. Moreover, a new version of KETEK's successful VIAMP module product line, featuring a vacuum-compatible flange and compact size, designed for the use in tabletop SEM systems will be introduced.

Malvern Panalytical**Booths: 7, 8****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 XRD and XRF systems, and will have application scientists available to answer your questions. Visit us in Booths 7 & 8!

Materials Data

Booths: 45, 46

Website: www.materialsdata.com

Email: mdi@materialsdata.com

Materials Data (MDI), based in California and part of the International Centre for Diffraction Data, creates hardware-independent analysis software for X-ray Powder Diffraction. Our software tools 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 our XRD community. Visit our booth at DXC for a demonstration of JADE™.

Micro X-Ray, Inc.

Booth: 29

Website: www.microxray.com

Email: sales@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.

MOXTEK, Inc.

Booth: 16

Website: www.moxtek.com

Email: info@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.

NEXTRON

Booth: 21

Website: www.microprobesystem.com

Email: sales@nextron.co.kr

Micro Probe System is suitable to analyze the Electrical & Optical properties of the materials. Its advantage is the in-situ measurement of the electrical and optical properties under various environmental conditions with patented smart probes; Vacuum, Temperature, Gas Flow, Humidity, Light Irradiation, and X-ray.

Oxford Instruments

Booth: 39

Website: www.oxinst.com

Oxford Instruments X-Ray Technology is a leading manufacturer of X-ray tubes, power supplies, and integrated X-ray sources.

Our solutions enable breakthrough R&D and high volume OEM's in the global analytical, medical imaging, food quality & packaging inspection, and industrial NDT markets.

Petrick GmbH

Booth: 41

Website: www.petrackgmbh.de

Email: info@petrickgmbh.de

PETRICK GMBH is specialized in the production and development of X-ray tubes and X-ray tube assemblies for medicine and technique since 1991. Apart from our diverse product portfolio, we develop solutions for your specific case of application and also produce small batches and single pieces. We are open to working together with institutes and universities.

PNDetector GmbH

Booth: 12

Website: www.pndetector.de

Email: sales@pndetector.de

PNDetector is developing and manufacturing advanced radiation detectors for material analysis in a wide range of applications such as microanalysis, quality assurance and materials science.

The silicon sensors are fabricated in PNDetector's own cleanroom facilities in Munich. The cleanroom is dedicated to an ultra-pure fabrication with a high level of contamination control, insuring very low dark-current levels. The emphasis in production and development is on Silicon Drift Detectors (SDDs) Backscattered Electron Detectors (BSE) and Charged Coupled Devices (pnCCDs).

Premier Lab Supply, Inc.

Booth: 49

Website: www.premierlabsupply.com

Email: info@premierlabsupply.com

PREMIER manufactures and distributes XRF sample preparation consumables, equipment, and platinum labware items for XRF Analysis. PREMIER's Phoenix and xrFuse fusion equipment brings 25 years of fusion technology and is the leader in platinum labware and borate fusion flux. PREMIER offers manual and automated presses as well as consumables for your press pellet applications: die sets, aluminum cups, and binders. For powder and liquid testing, PREMIER manufactures sample cups and films. For a complete list of products, please visit www.premierlabsupply.com.

Proto Manufacturing

Booths: 26, 27

Website: www.protoxrd.com

Email: info@proxrd.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.

RaySpec, Ltd.

Booth: 57

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: 53, 54, 55

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.

RohmTek
Booth: 30
Website: www.RohmTek.com
Email: info@rohmttek.com

RohmTek is an analytical instrumentation rental and data calibration licensing service provider enabling users with access to instrumentation, analytical labs, expert interpretation, and instrument calibrations to optimize identification and quantification of samples in the laboratory and/or the field. The company provides instrument calibration materials and access to highly utilized laboratory instrumentation rental tools in addition to more traditional laboratory testing and consultancy services.

Shimadzu Scientific Instruments, Inc.
Booth: 28
Website: www.ssi.shimadzu.com
Email: webmaster@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: 37
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? This year, Specac introduces the new APEX 400 press for XRF sample preparation, so be sure to come and visit the team at Booth 37 to learn more! Specac, Inc is based in Fort Washington, PA.

SPECTRO Analytical Instruments
Booth: 38
Website: www.spectro.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 SPECTROCUBE ED-XRF Spectrometers 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. Please visit our resource library at www.spectro.com/resourceLibrary.

STOE & Cie GmbH
Booth: 40
Website: www.stoe.com
Email: info@stoe.com

Originally founded in 1887 with the primary objective of manufacturing equipment for the optical examination of crystals, STOE has been at the forefront of powder and single crystal X-ray diffraction since the 1960s. STOE invented and patented the transmission geometry technique for Powder XRD and additionally, developed the first pixel detector XRD system with an open Eulerian cradle for single crystals. Headquartered in Darmstadt, Germany, STOE keeps the R&D, software programming, electrical and mechanical engineering, and production all in house, allowing to provide customers with standard as well as individual solutions. This integrated approach enables STOE to offer both standard and customized solutions to its customers. STOE is committed to delivering uncompromising quality, distinguishing themselves through their meticulous attention to detail. As a result, they have become THE go-to partner in X-ray Diffraction for crystallographers, chemists, material scientists, and pharmacists worldwide.

SUNJE Co., Ltd.
Booth: 25
Website: www.sunstat.com
Email: jhk1811@sunstat.com

SUNJE is one of the manufacturers who makes the largest number of X-ray tubes in the world. SUNJE can provide optimized X-ray tubes; please do not fit your device for X-ray tubes anymore. Try SUNJE X-ray source, we can deliver faster with a reasonable price.

VJ X-Ray
Booth: 13
Website: www.vjxray.com
Email: info@vjxray.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 & Pharmaceutical, 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: 50
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.

XIA LLC
Booth: 44
Website: www.xia.com
Email: sales@xia.com

XIA LLC is an ISO 9001:2015 certified company that 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 (#44) for more information.

XOS
Booth: 20
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 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

WIN AN AMAZON GIFT CARD!

DXC 2023 EXHIBIT PASSPORT

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	Cape Catalytix
easyXAFS	eXaminart	Herzog Automation	ICDD	KA Imaging	Katanax
KETEK	Malvern Panalytical	Materials Data	Micro X-Ray	MOXTEK	NEXTRON
Oxford Instr.	Petrick	PNDector	PREMIER Lab Supply	PROTO	RaySpec
Rigaku Americas	RohmTek	Shimadzu	Specac	Spectro	
STOE	SUNJE	VJ X-Ray			
Xenocs	XIA	XOS			

VISIT TO WIN!
 Visit: Get:
 10 companies = 1 chance
 20 companies = 2 chances
 All companies = 4 chances

Win one of four \$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.** If you are using this passport card, 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. If you are using the Whova passport card, you will be entered in automatically. **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!**

2023 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

What the APS Upgrade will bring to X-ray Analysis – Part I

Magnolia

Organizer & Instructors:

Olga Antipova, Argonne National Laboratory, USA, oantipova@anl.gov

Wonsuk Cha, Argonne National Laboratory, USA, wcha@anl.gov

Junjing Deng, Argonne National Laboratory, USA, junjingdeng@anl.gov

Katherine Harmon, Argonne National Laboratory, USA, kharmon@anl.gov

Jonathan Lang, Argonne National Laboratory, USA, lang@anl.gov

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The APS Upgrade project (APS-U) will offer an invaluable tool that has the potential to revolutionize the field of hard X-ray research, as it will provide significantly improved coherence and brightness in X-ray beams. With a 500-fold increase in brightness, APS-U will firmly establish itself as a world-leading facility for a wide and rapidly-expanding user community. The upgraded source and novel beamlines will deeply impact many scientific disciplines, including green energy harvesting, energy storage, materials engineering, environmental research, biology, and medicine, among others. X-ray analysis techniques, such as X-ray fluorescence microscopy, micro- and nano-CT, coherent diffraction imaging including ptychography, high-energy imaging, and spectroscopy (XPCS), will be able to push resolution to highest possible, achieve ultra-fast measurements, significantly increase field of view and boost the throughput of the experiments.

Multiple instruments will expand their modalities, allowing for integrated sample measurements even under in-situ or operando conditions, and enable multi-scale imaging of hierarchical systems. The APS-U project will transform existing synchrotron X-ray research and open new frontiers in science and technology on a broad range of scientific disciplines, driving new discoveries and innovations that will benefit society as a whole.

Topics to be covered in Part I: Overview of Microscopy Beamlines Enhancements, Upgrade of Full-field Imaging, and Ptychography after APS-U.

Cultural Heritage

Cypress

Organizer & Instructors:

Matthias Alfeld, TU Delft, Netherlands, m.alfeld@tudelft.nl

Frederik Vanmeert, University of Antwerp (Belgium) & KIK-IRPA (Royal Institute for Cultural Heritage), Belgium, frederik.vanmeert@uantwerpen.be

Maria Kokkori, Northwestern University & Art Institute of Chicago, USA, maria.kokkori1@northwestern.edu

John Okasinski, Argonne National Laboratory, USA, okasinski@anl.gov

Our cultural heritage is more than meets the eye. The material character of heritage artworks provides insight into their creation, their object biography but also their slow decay and degradation. While the first helps us to understand our past, the latter helps us preserve our history for the future. Few analytical techniques are better suited to investigate heritage objects than X-rays as they penetrate through the surface and allow for non-destructive analysis. This workshop will present examples for the most important X-ray techniques used for cultural heritage objects (XRF, XRD and radiography) and discuss their capabilities and limitations. Further, we will show examples of the demands on instruments and scientists during investigations at synchrotron sources, museums, and tombs of ancient pharaohs.

Basic to Intermediate XRD

Lilac C

Organizers & Instructors:

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

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

Mark Rodriguez, Sandia National Laboratories, Albuquerque, USA, marodri@sandia.gov

This workshop will discuss the use of XRD for standard qualitative analysis and will detail progressively more challenging means of XRD characterization including: quantitative analysis, profile fitting, lattice parameter refinement, crystallite size and microstrain determination, texture analysis, and structure refinement (Rietveld). Additionally, some discussion shall be dedicated to characterization of nanomaterials and glasses via pair distribution function analysis, as well as thin film techniques such as grazing incidence XRD and X-ray reflectivity (XRR). The workshop is intended to be a survey for the new user of XRD regarding what experiments can be performed and why one would wish to pursue such measurements.

Basic XRF

Lilac D

Organizers & Instructors:

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

Peter Wobrauschek, Atominstitut – TU Wien, Austria, wobi@ati.ac.at

This workshop provides a basic introduction to the principles of XRF specifically aimed at those new to the field. In the first half, there will be a general overview of the XRF technique, including a discussion of the basic principles of X-ray interactions with matter. The emphasis in the first half will be on understanding the underlying physical phenomena, how the technique is applied, optimization of the signal, and approaches to quantitative analysis. In the second half of the workshop, examples of real-world applications will be presented to illustrate some of the challenges and opportunities that the analyst may face. This half will include a description of a variety of specimen formats and the flexibility of the XRF technique, including a discussion of the capabilities of bench-top EDX instruments, micro analyzers, Total Reflection XRF (TXRF) instruments and handheld analyzers.

Monday Afternoon Workshops 1:30 pm – 4:30 pm

What the APS Upgrade will bring to X-ray Analysis – Part II

Magnolia

Organizer & Instructors:

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Tongchao Liu, Argonne National Laboratory, USA, liut@anl.gov

Alberto Mittone, Argonne National Laboratory, USA, amittone@anl.gov

Sarah Wieghold, Argonne National Laboratory, USA, swieghold@anl.gov

The APS Upgrade project (APS-U) will offer an invaluable tool that has the potential to revolutionize the field of hard X-ray research, as it will provide significantly improved coherence and brightness in X-ray beams. With a 500-fold increase in brightness, APS-U will firmly establish itself as a world-leading facility for a wide and rapidly-expanding user community. The upgraded source and novel beamlines will deeply impact many scientific disciplines, including green energy harvesting, energy storage, materials engineering, environmental research, biology, and medicine, among others. X-ray analysis techniques, such as X-ray fluorescence microscopy, micro- and nano-CT, coherent diffraction imaging including ptychography, high-energy imaging, and spectroscopy (XPCS), will be able to push resolution to highest possible, achieve ultra-fast measurements, significantly increase field of view and boost the throughput of the experiments.

Multiple instruments will expand their modalities, allowing for integrated sample measurements even under in-situ or operando conditions, and enable multi-scale imaging of hierarchical systems. The APS-U project will transform existing synchrotron X-ray research and open new frontiers in science and technology on a broad range of scientific disciplines, driving new discoveries and innovations that will benefit society as a whole.

Topics to be covered in Part II - Diffraction Imaging Advancements for Material Science, Clean and Resilient Energy Storage, and Photovoltaics Research at New APS.

In situ Battery Measurements

Cypress

Organizer & Instructors:

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

John Okasinski, Argonne National Laboratory, USA, okasinski@aps.anl.gov

Carlo Segre, Illinois Institute of Technology, USA, segre@iit.edu

This workshop will provide an introduction to laboratory- and synchrotron-based approaches to in-situ and in-operando examination of batteries. The workshop will be divided into three sections to cover laboratory XRD methods, high-energy synchrotron XRD and synchrotron-based X-ray absorption spectroscopic (XAS) methods.

In the first section, topics will include a brief overview of batteries, methods and equipment appropriate to laboratory XRD instrumentation, common issues with testing fixtures, data analysis methods and examples of results.

In the second section, high-energy XRD methods (>50 keV) will be covered. High energy X-rays have the ability to penetrate through significant amounts of material and enable observation of chemical and structural changes of materials within their processing and/or operating environments and deep inside of battery cells, including large format commercially produced cells. Several high-energy XRD techniques that measure spatio-temporal changes inside of batteries will be discussed.

In the third section, X-ray absorption spectroscopy methods will be discussed. XAS methods are powerful tools to study the electronic and local geometric structure in battery materials, that can occur during cycling. In situ and operando XAS studies are limited by the need to work at energies near the absorption edge of the target elements which has important implications to the measurement methods. Options for sample environments and data collection modalities will be discussed.

Quantitative XRF

Lilac C

Organizers & Instructors:

Kosuke Kawakyu, Rigaku Corporation, Japan, kawakyu@rigaku.co.jp

Maggi Loubser, University of Pretoria, South Africa, maggi.loubser@gmail.com

This workshop will cover an introduction to fundamental parameters for quantitative XRF analysis by Maggi Loubser and examples using fundamental parameters for semi-quantitative analysis by Kosuke Kawakyu.

Sample Preparation for XRF

Lilac D

Organizer & Instructor:

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

Yusniel Cruz Hernandez, Rigaku, USA, yusniel.cruzhernandez@rigaku.com

Ivan Rodriguez Duran, Malvern Panalytical, Canada, ivan.rodriguez.duran@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.

Tuesday Morning Workshops 9:00 am – 12:00 noon

Intro to GSAS-II

Magnolia

Organizers & Instructors:

Brian Toby, Argonne National Laboratory, USA, brian.toby@anl.gov

Robert Von Dreele, Argonne National Laboratory, USA, vondreele@anl.gov

Two workshops will be presented on GSAS-II. The first, Introduction to GSAS-II, will be oriented for novice Rietveld refinement practitioners. It will assume that attendees have a reasonable understanding of diffraction and crystallography. This introductory workshop will provide an overview of the capabilities offered by GSAS-II; how the graphical user interface is organized; key concepts used in the software; basics on the GSAS-II profile model; how to get information in and out of the program and will introduce the concept behind sequential refinements in GSAS-II that allows hundreds or thousands of datasets to be analyzed. Attendees will then use their own laptops to perform one of several provided tutorial exercises.

GSAS-II is a comprehensive package for the analysis of all types of X-ray and neutron diffraction data, including single-crystal and powder diffraction, constant-wavelength, pink-beam and time-of-flight data types from lab, synchrotron, spallation and reactor sources. It offers data reduction and instrument calibration facilities. It integrates state-of-the-art visualization with a complete GUI implementation and an applications interface (API) for scripted use. In addition to traditional crystallographic capabilities and Rietveld analysis, it includes support for 3+1 superspace structures and commensurate magnetism. It offers small-angle scattering and reflectometry analysis, structure solution capabilities and interfaces to several other types of analysis tools, such as for pair distribution functions, faulted materials, maximum entropy Fourier maps and symmetry analysis. GSAS-II is distributed open-source at no cost and runs on Windows, MacOS, Linux and Raspberry Pi computers. It currently receives ~500 citations/year.

Texture

Cypress

Organizer & Instructors:

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

Sean Agnew, University of Virginia, USA, sra4p@virginia.edu

Adam Creuziger, NIST, USA, adam.creuziger@nist.gov

Nathan Peterson, Colorado School of Mines, USA, nepeterson@mines.edu

Dan Savage, Los Alamos National Laboratory, USA, dansavage@lanl.gov

Texture is concerned with the statistical and spatial distribution of crystallographic orientations within multiphase and polycrystalline specimens. It is a constitutive material characteristic and determines in first order approximation its behavior except for grain boundary effects. The workshop will address diffraction experiments (X-ray, synchrotron, neutron, electron back-scatter) providing either integral pole intensity data or individual orientation data, including ODF-adaptive texture goniometry, mathematical models, numerical methods and software to analyze and interpret the orientation data, in particular to determine the orientation density function (ODF), its Fourier coefficients and other characteristic entities, associated mis-orientation distributions, examples of applications, e.g. determination of anisotropic tensorial material properties.

It is emphasized that spatially resolving EBSD orientation data takes texture analysis far beyond its classical tasks towards a comprehensive fabric analysis as envisioned by Sander including reconstruction of crystallites and their boundaries, misorientation analysis, classification of grain boundaries, grain size distribution, grain shape analysis and other features.

Micro XRF

Lilac C

Organizer & Instructors:

Kouichi Tsuji, Osaka Metropolitan University, Japan, k-tsuji@omu.ac.jp

Hitomi Nakano, Horiba Techno Service Co., Ltd., Japan, hitomi.nakano@horiba.com

Brian Patterson, Los Alamos National Laboratory, bpatterson@lanl.gov

The workshop will cover the basic principles of Energy Dispersive X-ray Fluorescence (EDXRF) analysis including theory, instrumentation, software, spectral processing, and qualitative & quantitative analysis. Advances in EDXRF instrumentation have made the technique one of the most versatile spectrometers available for elemental analysis. EDXRF instruments have been applied for manufacturing process control, environmental field analysis, planetary exploration, and so on. Micro-XRF utilizes any one of a subset of optics to reduce the analysis area and is used to provide spatial 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. This technique is used to investigate contaminated particles in the laboratory and elemental mapping of various samples. We will discuss the state-of-the-art instruments (X-ray source, X-ray optics for micro beam, and detectors), confocal micro-XRF for 3 dimensional analysis, and applications including elemental mapping. Recent applications of micro XRF analyzers in various fields such as industry, environmental science and artwork will also be discussed.

XRF of Layered Structures

Lilac D

Organizer & Instructors:

Peter Wobrauschek, Atominstitut – TU Wien, Austria, wobi@ati.ac.at

Klaudia Hradil, TU Wien X-ray Center, Austria, klaudia.hradil@tuwien.ac.at

Dieter Ingerle, Atominstitut – TU Wien, Austria, dieter.ingerle@tuwien.ac.at

Christina Strelj, Atominstitut – TU Wien, Austria, strelj@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 Strelj. 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.

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

Advanced Topics in GSAS-II

Magnolia

Organizers & Instructors:

Brian Toby, Argonne National Laboratory, USA, brian.toby@anl.gov

Robert Von Dreele, Argonne National Laboratory, USA, vondreele@anl.gov

Two workshops will be presented on GSAS-II. The second workshop, Advanced Topics in GSAS-II, is intended for experienced Rietveld refinement practitioners to cover aspects of the software that are not usually presented in workshops. Input from attendees on their interests will be taken into account (if received at least six weeks prior to the workshop) but potential topics include: details on performing sequential fits; an introduction to scripting GSAS-II; advanced visualization capabilities; using rigid bodies to simplify fits for MOFs and organic species; preferred orientation analysis; advanced background fitting capabilities; PDF-fitting interfaces.

XRD Methods for Complex Multi-Phase Identification

Cypress

Organizer & Instructors:

Tim Fawcett, ICDD, Emeritus, USA, dxcfawcett@outlook.com

Stephen Hillier, James Hutton Institute, Scotland, stephen.hillier@hutton.ac.uk

With advances in laboratory instrumentation, databases, and software one can analyze more materials at lower concentrations than ever before. It is not uncommon to have 8 or more phases in several types of common samples. This would include cements, soils, core drillings, industrial slags, formulated paints and pharmaceutical tablets. In the cases of advanced building materials and formulated pigments and drugs, small amounts of key ingredients are added to impart desirable physical properties, whilst in soils minor amounts of some minerals may be key to understanding their functional properties; so, there is a common desire to identify and quantify these materials.

When analyzing these samples, one frequently encounters severe peak overlap, with and without the complication of non-crystalline or nanomaterials. This causes the typically high accuracy d-spacings, required for identification, to be merged, shifted or even hidden. Decomposing peak profiles and intensities needed for quantitative analysis will have similar difficulty. This workshop will provide an overview of methods used to tackle such difficult problems. This will include using customized subfiles for identification, control files for quantitation, full pattern matching methods, baseline determination, cluster analyses, multi-specimen and graphics techniques.

Organizer & Instructors:

Maggi Loubser, University of Pretoria, South Africa, maggi.loubser@gmail.com

Alexander Seyfarth, SGS Minerals, Canada, alexander.seyfarth@sgs.com

Handheld XRF spectrometers have increased market share 100-fold in the past ten years. Because 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, because, 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 artefact 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.

The presenters will share some specific case studies from their fields, a set of geological “exploration” based studies will illustrate how to get fit-for-purpose data in various scenarios. Taking hhXRF applications a step further is the approach of quantitative analysis of plant material to manure. Lastly, art conservation case studies, illustrating the application of a non-destructive, in-situ technique to the actual art object has changed how scientists and conservators approach their work, but again, not without potential pitfalls.

XRF Trace Analysis

Organizer & Instructors:

Peter Wobrauschek, Atominstitut – TU Wien, Austria, wobi@ati.ac.at

Gakuto Takahashi, Rigaku Corporation, Japan, g-takaha@rigaku.co.jp

Christina Strelj, Atominstitut – TU Wien, Austria, streli@ati.ac.at

Kouichi 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, should 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 – Monday Evening

Grand Ballroom

**Signifies presenting author, when noted*

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

Chairs:

Ercan Cakmak, Oak Ridge National Laboratory, USA, cakmake@ornl.gov

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

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- D-2 Use of Rietveld Refinement Method for Describing Structural, Texture and Phase Analysis of X-ray Diffraction Data of a Siliciclastic Succession
Mohamed Soua*, **H. Sitepu**, Saudi Aramco, Saudi Arabia
- D-6 Fast Non-destructive Characterization of Si/SiGe Superlattice for Sequential CFET Layer Transfer Using X-ray Scattering Metrology
Lixia Rong*, **W. Hong**, **L. Thomas**, **H. Zhou**, **Q. Fu**, **M. Phillips**, **B. Liu**, **H. Jiang**, **N. Yoshida**, **M. Naik**, Applied Materials Inc, USA
- D-7 Glancing Angle Deposition and Structural Characterization of Al/Si Thin Films
Qiyin Lin*, Irvine Materials Research Institute, UC Irvine, USA
- D-9 Crystal Structures of Large-Volume Commercial Pharmaceuticals
James Kaduk*, **T. Ens**, **N. Boaz**, North Central College, USA
T. Blanton, **A. Dosen**, ICDD, USA
- D-12 Quantification of Calcite and Dolomite in Polymer Blends - A Simplified XRD QC Approach Combining the Accuracy of Rietveld Analysis and the Simplicity of an Intensity Ratio Approach
Pierre Ricou*, Arkema Inc., USA
- D-14 Accurate Quantification of Cement by Combining Amorphous Phases in Rietveld Method
Ekaterina Vinogradova*, **M. Sharma**, **K. Saito**, **A. Tripathi**, Rigaku Americas Corporation, USA
- D-15 New Challenges in Non-Ambient XRD – New Solutions from Anton Paar
Petra Kotnik*, **B. Pühr**, **B. Schrode**, **M. Kremer**, **A.O.F. Jones**, Anton Paar GmbH, Austria
- D-22 Combined Powder X-ray Diffraction and Raman Spectroscopy Studies of Ti-doped LiMnO₂ Compounds
Yong Il Kim*, **H.S. Kwon**, **K.B. Kim**, KRISS, South Korea
D.K. Choi, **D.W. Han**, Hallym University, South Korea
- D-24 Influence of the Experimental Setup for In-situ and Operando X-ray Diffraction of Batteries
Benedikt Schrode*, **A.O.F. Jones**, **M. Kremer**, **B. Pühr**, **P. Vir**, Anton Paar GmbH, Austria
- D-27 Optimized XRD Measurement Configurations for Porous Materials with XRDynamic 500
Semih Gulec*, **B. Schrode**, **A.O.F. Jones**, **M. Kremer**, **P. Vir**, Anton Paar USA, USA
- D-28 Strain Profiles and Dislocations Density of GaN Layers Grown On Silicon Deduced From X-ray Diffraction Scans
Patrice Gergaud*, **V. Yon**, **M. Latusas**, **S. Torrenço**, **F. Nolot**, **M. Charles**, University Grenoble Alpes, France
- D-31 Investigation on X-ray Photoelectron Spectroscopy, Structural, Electronic, and Luminescent Properties of Copper Doped ZnO Nanostructures
Abdel Khaleq Alsmadi*, **B. Salameh**, Kuwait University, Kuwait
- D-36 Development of a High Brilliance Laboratory SAXS/WAXS Beamline with Optimized User Interface for High Throughput Structural Characterization
Phillip Kohl*, **Y. Li**, **M. Zepeda-Rosales**, **C. Barcelon**, **R. Willat**, **A. Pan**, BioPACIFIC MIP, California NanoSystems Institute, University of California, USA
- D-38 Crystal Structure Solution and Thermal Expansions of CaZr₄(PO₄)₆ and SrZr₄(PO₄)₆
Benjamin S. Hulbert*, **J.E. Brodecki**, **W.M. Kriven**, University of Illinois at Urbana-Champaign, USA

- D-39 Exploring the Structural Evolution in Li-Rich Layered Materials via Operando XRD
Hao Lin*, **C. Segre**, Illinois Institute of Technology, USA
- D-40 Development of 3D-XRD with X-ray Optical Elements
Shotaro Fukumoto*, Nippon Electric Glass Co., Ltd. and Osaka Metropolitan University, Japan
M. Okuda, **T. Matsuyama**, **K. Tsuji**, Osaka Metropolitan University, Japan
- D-42 Powder Pattern Denoising Using Haar Wavelets and a Thresholding Rule Designed For Poisson Noise
Richard McClurg*, Curia Indiana, USA
- D-45 Structural Analysis of 2D Noble Metal Telluride Exploiting X-ray Diffraction
Chang-Soo Kim*, **M.H. Choi**, **M.K. Jo**, **J.T. Min**, **S.W. Song**, Korea Research Institute of Standards and Science, Republic of Korea
- D-46 High Entropy Oxide Tungsten Bronzes as Anodes for Lithium Ion Batteries
Dana Alramahi*, **O. Marques**, **C. Segre**, Illinois Institute of Technology, USA
- D-48 The High Intensity Diffractometer for Residual stress Analysis (HIDRA), a 3rd Generation Residual Stress Mapping Neutron Diffractometer at the High Flux Isotope Reactor
Jeff Bunn*, **C. Fancher**, **E.A. Payzant**, **W.B. Bailey**, **R. Gregory**, Oak Ridge National Laboratory, USA
- D-60 Texture and Residual Stress Analysis on a D6 PHASER Benchtop Diffractometer
Jonathan M. Gentile*, **B. Krueger**, **S. Rodesney**, **N. Henderson**, **J. Giencke**, **B. Jones**, Bruker AXS, USA
- D-61 D6 PHASER: Thin Film Analysis on a Benchtop
Benjamin Krueger*, **N. Rodesney**, **J. Gentile**, **N. Henderson**, **B. Jones**, Bruker AXS, USA
- D-62 High-End Powder Diffraction Data on the D6 PHASER Benchtop
Steven N. Rodesney*, **N. Henderson**, **B. Krueger**, **J. Gentile**, **B. Jones**, Bruker AXS, USA
- D-66 Determining the Best Internal Standard for Use in Iron Slags, Steel Slags, and Other Complex Materials
Lucas Sy*, Edward C. Levy, Co. and Purdue University West Lafayette, USA
J. Lyza, **S. Page**, Edward C. Levy, Co., USA
T. Fawcett, International Centre for Diffraction Data, USA
- D-67 Control Files as a Model for Dealing with the QPA of Complex Materials within an Industrial Setting
Jessica Lyza, **S. Page**, Edward C. Levy, Co., USA
T. Fawcett, International Centre for Diffraction Data, USA
- D-68 A Lab Based Simultaneous and Co-Registered X-ray Diffraction Computed Tomography and Color Transmission Computed Tomography System
Ashkan Ajeer*, **R Moss**, University College London, United Kingdom
- D-69 Direct Conversion 7.8-Micron Pitch Hybrid CMOS X-ray Detector for New Applications in Material
Chris Scott*, **K.S. Karim**, KA Imaging, Canada

WITHDRAWN

XRF Poster Session – Tuesday Evening Grand Ballroom

**Signifies presenting author, when noted*

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

Sponsored Awards:

Amptek Award for Best Student XRF Poster - Best Student Poster during the XRF Poster Session and awarding the winner with an Apple iPad. *This award is separate from the DXC Best Student Poster Award.*

XOS Innovation Award™ - recognizes the Best Poster Presentation at the Denver X-ray Conference characterized by the spirit of innovation, excellence in research, and scientific and/ or community impact. Selection Criteria can be found within the WhoVA event app, under the XRF Poster Session. The awardee(s) receive a \$750 prize from X-ray Optical Systems, Inc. A second award in the amount of \$250 may be given to the runner-up(s).

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

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| F-1 | Determination of Gold, Silver and Rhodium in Liquid Samples via WD- XRF Instrument
Mohammed Abdelbarie* , GOEIC, Egypt |
| F-4 | Development of New Substrate Pretreatment Method Using Ammonia-Hydrogen Peroxide Mixture for Total Reflection X-ray Fluorescence Analysis
Tsugufumi Matsuyama* , Y. Tanaka , N. Taniguchi , K. Tsuji , Osaka Metropolitan University, Japan
Y. Mori , Doshisha University, Japan |
| F-5 | Elemental Characterization of 3D-printed Polymers Using Micro X-ray Fluorescence Spectrometry for Forensic Applications
Ruthmara Corzo* , NIST, USA
J. Stallworth , T. Gluodenis , Lincoln University, USA |
| F-6 | ICH-Q3D Elemental Impurity Analysis of Oral Drugs and Active Pharmaceutical Ingredients by EDXRF
Haihan Chen* , Shimadzu Scientific Instruments, USA
T. Nakao* , E. Terashita , K. Suzuki , H. Furukawa , Shimadzu Corporation, Japan
T. Sakamoto , T. Shoda , National Institute of Health Sciences, Japan |
| F-8 | Challenges in Performing Chromium Speciation Analysis using Synchrotron X-ray Absorption Spectroscopy for the Development of Reference Materials
Hana Cho* , Y. Lim , K.S. Lee , Korea Research Institute of Standards and Science, Republic of Korea
K.B. Dasari , Gyeongsang National University, Republic of Korea
S.H. Choi , Pohang Accelerator Laboratory, Republic of Korea |
| F-10 | Multifaceted Evaluation of Gemstones using UV-Vis-NIRs and EDXRF — Tanzanite and Zoisite
Hirokazu Moriya* , A. Urushizaki* , X. Yan , A. Goto , R. Ogawa , Shimadzu Corporation, Japan |
| F-12 | Quantitative Analysis of Black Mass from Spent Lithium-Ion Batteries Using EDXRF
Aya Urushizaki* , Shimadzu Corporation, Japan |
| F-14 | Analysis for the Focal Spot Size According to the Focusing Structure of the Transmission X-ray Tube
Jeongdong Kim* , D. Lee , SUNJE, Korea |
| F-17 | Performance of KETEK's New Generation 3.0 SDD Electronics
Thomas Ganka* , F. Krieglner , C. Zacher , N. Willems , C. Berger , C. Luckey , R. Fojt , J. Knobloch , KETEK GmbH, Germany |
| F-28 | Successful Picoliter Printing of 65 Elements for TXRF Analysis and Related Methods
Sven Hampel* , F. Sand , U.E.A. Fittschen , Clausthal University of Technology, Germany
G. Pepponi , Fondazione Bruno Kessler, Italy |
| F-29 | ENFORCE TXRF: A European Network for Chemical Elemental Analysis by Total Reflection X-ray Fluorescence
Diane Eichert* , ELETTRA - Sincrotrone Trieste, Italy
L. Borgese , University of Brescia, Italy |

- F-31 Process and Quality Control of Phosphate Rock as Inorganic Resource of Phosphate Fertilizer by WD-XRF Analysis
Tetiana Shalapska*, J. Sedlmair, Bruker AXS, USA
- F-34 Synthesis and Characterization of MoP Nanoparticles Used as a Catalyst in CO₂ Reduction Reaction
Karen A. Castañeda*, I. Senevirathna, C. Segre, M. Asadi, Illinois Institute of Technology, USA
- F-35 Improving the Performance of Silicon Drift Detectors
Andrew Jarrett*, M. Zhang, E. Tikhomirov, Y. Tomimatsu, Hitachi High-Tech America, Inc., USA
- F-36 In Situ EXAFS Study on Pd @ Ni(OH)₂ during Electrocatalytic CO₂ Reduction Reaction
Ishani S. Senevirathna*, K.A. Castañeda, N. Su, C. Segre, Illinois Institute of Technology, USA
- F-37 XAS Study Local Atomic Environment Mn-Edge in MnO_xGO Nanocomposites as Air-Cathode for Metal-Air Battery Application
Benard L. Patawah*, Illinois Institute of Technology, USA
E. Timofeeva, G.S. Pourb, Inluit Energy, LLC, USA
C. Segre, Illinois Institute of Technology and Inluit Energy, LLC, USA
- F-38 Nondestructive Micro X-ray Fluorescence Analysis of Cultural Samples
Kazuaki Mori*, T. Matsuyama, K. Tsuji, Osaka Metropolitan University, Japan
T. Hourai, Fuji Computer Co., Japan
S. Zhuo, Shanghai Institute of Ceramics, China
- F-40 Benchtop ED-XRF Analysis for Improved Quantification of Total Rare Earth Content
Julia Sedlmair*, Bruker AXS, USA
- F-50 Environmental Sampling of Chicago Industrial Corridors
Alyssa Tovar*, M. Schmeling, Loyola University Chicago, USA
- F-54 Characterization of MoS₂ Films via Simultaneous Grazing Incidence X-ray Diffraction and Grazing Incidence X-ray Fluorescence (GIXRD/GIXRF)
Mark A. Rodriguez*, T.F. Babuska, J. Curry, J.J.M. Griego, M.T. Dugger, Sandia National Laboratories, USA
- F-56 Statistical and Systematic Errors in Laboratory-Based X-ray Absorption Spectroscopy
Ursula E.A. Fittschen*, J. Hiller, J. Kolny-Olesiak, Clausthal University of Technology, Germany
- F-57 GIMOXs - A New Spectrometer for GIXRF for the Nondestructive Characterization of Light Element Containing Nanomaterials in the Laboratory
Dieter Ingerle*, P. Wobrauschek, C. Strelj, Atominstitut – TU Wien, Austria
F. Meirer, K. Siebers, Utrecht University, Netherlands
- F-58 Mini Beam – A Compact X-ray Microbeam Generator for Micro X-ray Analysis
Brendan Waffle*, Ning Gao*, XOS, USA
- F-60 The Evidence of Cu²⁺ and Zn²⁺ Modulation of Key HSA, HCC, and Aβ Proteins Activity in Neurodegenerative Processes
Wojciech M. Kwiatek*, Institute of Nuclear Physics PAN, Poland
M. Nowakowski, Paderborn University, Germany
J. Wolak, K. Rucinska, J. Maksim, M. Taube, D. Wojciechowska, E. Banachowicz, Adam Mickiewicz University in Poznan, Poland
M. Kozak, Adam Mickiewicz University in Poznan and Jagiellonian University, Poland
- F-61 Phase Study within the Fe-Si System
Thomas Watkins*, G. Muralidharan, Oak Ridge National Laboratory, USA
R. Kamath, D. Singh, Argonne National Laboratory, USA

Plenary Session – Wednesday Morning, 9 August, 8:30 am – 11:45 am Lilac C & D

**Signifies presenting author, when noted*

Energy Storage

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

-
- 8:30 Welcoming Remarks and Awards
Scott Misture, Chairman of the Denver X-ray Conference, NYS College of Ceramics at Alfred University, USA
- 2023 Barrett Award presented to **Ashfia Huq**, Sandia National Laboratories, USA. Presented by the Chair of the Barrett Award Selection Committee, **Conal Murray**, IBM T.J. Watson Research Center, USA.
- 2023 Jenkins Award presented to **Tim Elam**, University of Washington, USA. Presented by the Chair of the Jenkins Award Selection Committee, **Tim Fawcett**, Emeritus ICDD, USA.
- 2022 Hanawalt Award presented to **Karena Chapman**, Stony Brook University, USA. Presented by **Tom Blanton**, Executive Director, ICDD, USA.
- 2023 Robert L. Snyder Student Awards to be announced by **Tom Blanton**, Executive Director, ICDD, USA.
- Remarks by the Plenary Session Chair, **Scott Misture**.
- 9:00 P-3 Designing Better Materials for Future Batteries
Y. Shirley Meng*, Laboratory for Energy Storage & Conversion, The University of Chicago & Argonne Collaborative Center for Energy Storage Science (ACCESS), USA
- 9:45 P-2 X-ray Visions: Operando Insights into Functional Energy Materials
Karena W. Chapman*, Stony Brook University, USA
- 10:30 Break
- 11:00 P-1 Dynamic Electrochemical Phenomena at the Mesoscale
William Chueh*, Stanford University, USA

Oral Sessions – Wednesday Afternoon, 9 August

**Signifies presenting author, when noted*

New Developments in XRD & XRF Instrumentation

Magnolia

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

-
- 1:00 S-21 Battery Cell and Other In-Operando Investigations in Transmission Geometry
Thomas Hartmann*, Stoe & Cie GmbH, Germany
- 1:15 S-2 X-ray Detector Technology at Amptek
Robert Redus*, **A. Huber**, **P. Bennett**, **T. Lantela**, Amptek, USA
- 1:30 S-30 Utilising X-ray Scattering for High Accuracy Early Diagnostics of Breast Cancer
Barbara Gerbelli*, **C. Greenwood**, Keele University, United Kingdom
K. Rogers, Cranfield University, United Kingdom
- 1:45 S-3 Characterization of Strong Metal-Support Interaction (SMSI) Using X-ray Standing Wave Analysis
Igor A. Makhotkin*, **A. Tiwari**, **K. Matveevskii**, **M.D. Ackermann**, University of Twente, Netherlands
L. Mandemaker, **M. Monai**, **F. Meirer**, Utrecht University, Netherlands
S.N. Yakunin, NRC KI, Russia
- 2:00 S-18 Improvements in PNDetector's Versatile Compact Systems with Silicon Drift Detectors
Moritz Kopetzki*, **D. Schlosser**, **M. Bornschlegl**, **A. Bechteler**, **K. von Mirbach**, **S. Aschauer**, **A. Niculae**, **H. Soltau**, PNDetector GmbH, Germany
- 2:15 S-19 PDF-5+: A Comprehensive Powder Diffraction File™ For Materials Characterization
Suri Kabekkodu*, **J. Blanton**, **T. Blanton**, International Centre for Diffraction Data, USA

- 2:30 S-40 Easy PDF Analysis From Start To Finish – Highscore(Plus) V.5.2
Thomas Degen*, **M. Sadki**, **M. Gateshki**, **E. Bron**, Malvern Panalytical, Netherlands
- 2:45 S-7 Latest Generation of Silicon Drift Detectors and Readout Electronics
Andreas Pahlke*, **M. Fraczek**, **L. Höllt**, **M. Hofmann**, **J. Knobloch**, **J. Stoib**, KETEK GmbH, Germany
- 3:00 Break
- 3:30 S-37 D6 PHASER: The Powerful, Versatile, and Accessible Benchtop XRD Platform
Jon Giencke*, **B. Jones**, Bruker AXS, USA
- 3:45 S-31 MetalJet X-ray sources for Experiments at Non-ambient Pressures and Temperatures
Geethanjali Gopakumar*, **J. Hållstedt**, Excillum, Sweden
R. Drake, Proto Manufacturing, USA
- 4:00 S-16 Energy-Position Dispersive X-ray Fluorescence
Jack Webster*, CSIRO, Australia
R. Ninan, University of New South Wales, Australia
B. Ganly, CSIRO, Australia
- 4:15 S-13 Latest Advancements in Laboratory Powder XRD Instrumentation from Anton Paar
Benedikt Schrode*, **A.O.F. Jones**, **M. Kremer**, **B. Puhr**, **P. Vir**, Anton Paar GmbH, Austria
- 4:30 S-33 Free-Form Approach for the Analysis of XRR Data for Thin Films
Igor A. Makhotkin*, **J.F. Woitok**, **H.W. Lokhorst**, **K. Matveevskii**, **A. Tiwari**, **M.D. Ackermann**, University of Twente, Netherlands
S.N. Yakunin, RNC KI, Russia
G. Tye, Malvern Panalytical, Netherlands
- 4:45 S-10 XSPA-400 ER: High-Energy Resolution Seamless 2-D Detector
Ekaterina Vinogradova*, **E. Kagami**, **K. Saito**, Rigaku Americas Corporation, USA
- 5:00 S-43 FORJ: The Newest Malvern Panalytical Fusion Solution for XRF Brings Sample Preparation to a Higher Level
Iván Rodríguez Durán*, **C. Audet**, Malvern Panalytical, Canada
- 5:15 S-45 Novel Operando X-ray Reaction Cell from Cape Catalytix
Michael Claeys*, Cape Catalytix, South Africa

Imaging

Cypress

Chair: Peter Wobrauschek, Atominstitut – TU Wien, Austria, wobi@ati.ac.at

- 1:30 S-28 Invited – First Results with the X-ray Color Camera Microscope
Arno Frank*, **D. Ingerle**, **K. Hradil**, **C. Strelt**, TU Wien, Austria
P. Cook, **H. Lichtenegger**, **M. Kerber**, IPM, BOKU Wien, Austria
R. Hartmann, PNSensors GmbH, Germany
- 2:00 S-8 X-ray Computed Tomography as a Metrology Technique for the Analysis of Additively Manufactured Materials
Bryan K. Hunter*, **E. Jacobson**, **I.T. Cummings**, **A. Wachtor**, **B.M. Patterson**, Los Alamos National Laboratory, USA
- 2:20 S-29 Invited – X-ray Microfluorescence Imaging of Asteroid Samples
Laszlo Vincze*, Ghent University, Belgium
- 2:50 S-4 X-ray Absorption, Raman, and Fluorescence Imaging and Spectroscopy at Beamline 25-ID of the Advanced Photon Source
George E. Sterbinsky*, **J. Huang**, **M.A. Solovyev**, **M. Wolfman**, **C. Sun**, **S.D. Kelly**, Argonne National Laboratory, USA
G.T. Seidler, University of Washington, USA
Y. Chen, **D.M. Meira**, Canadian Light Source Inc., Canada

Stress and Texture Analysis

Lilac C

Chair: Tom Watkins, Oak Ridge National Laboratory, USA, watkinstr@ornl.gov

- 1:00 D-55 Invited – Texture and Stress-state Evolution during Dynamic Compression in Titanium Characterized with the XFEL at LCLS-2
Daniel Savage*, **S. Vogel**, **C. Bolme**, **D. Brown**, Los Alamos National Laboratory, USA
L. Lutterotti, Universita di Trento, Italy
- 1:30 D-52 Invited – On the Estimation of Elastic Constants in Low Symmetry Materials with In-situ Neutron Diffraction Measurements
Nathan Peterson*, Colorado School of Mines, USA
S. Agnew, University of Virginia, USA
D. Brown, **B. Clausen**, **D. Savage**, Los Alamos National Laboratory, USA
A. Stebner, Georgia Institute of Technology, USA
- 2:00 D-26 Bulk Elastic Constants and Their Role in Diffractive Stress Analysis
Thomas Gnaupel-Herold*, NIST Center for Neutron Research, USA
- 2:20 D-54 Impact of Bragg Edges on Residual Stress as Measured by Neutron Diffraction
E. Andrew Payzant*, **J.R. Bunn**, Oak Ridge National Laboratory, USA
- 2:40 D-23 Energy Dispersive Diffraction Tomography of Shark Vertebrae
Stuart Stock*, Northwestern University, USA
J. Park, Argonne National Laboratory, USA
R. Horn, Purdue University, USA
H. Chen, Stonybrook University, USA
M. Passerotti, **K. James**, **L. Natanson**, NOAA, USA
- 3:00 Break
- 3:30 D-20 Invited – Stress Measurements across Length Scales
Adam Creuziger*, **M. Iadicola**, **J. Robinson**, **E. Rust**, **M. Cox**, **C. Calhoun**, **T. Gnaupel-Herold**, NIST, USA
A. Bucsek, **C. Perez**, University of Michigan, USA
M. Cox, **K. Findley**, Colorado School of Mines, USA
- 4:00 D-33 Characterizing Nanoscale Thin-Film Residual Stresses for Stress Mitigation and Engineering in Next Generation X-ray Optics
Taylor Wood*, **D. Pagan**, **R. McEntaffer**, The Pennsylvania State University, USA
H. Seren, ASML Holding, N.V., USA
A. Woll, **L. Smieska**, **K. Page**, Cornell High Energy Synchrotron Source, USA
- 4:20 D-59 Texture and Residual Stress Analysis using the D6 PHASER Benchtop XRD
Brian Jones*, **N. Rodesney**, **J. Gentile**, Bruker AXS, USA
- 4:40 D-44 Recent Progress in Stress Analysis with 2D Detectors
Bob He*, Bruker AXS, USA
- 5:00 D-58 Different Crystallization Behavior of Polypropylene and Polyethylene within Existing Oriented Crystal Network from MDO Process
Minqiao Ren*, **X. Yao**, **X. Liu**, **H. Shi**, **L. Zhang**, SINOPEC (Beijing) Research Institute of Chemical Industry Co. Ltd., People's Republic of China

Trace Analysis

Lilac D

Chair: Diane Eichert, Elettra Sincrotrone Trieste, Italy, diane.eichert@elettra.eu

- 2:00 F-18 Invited – Using X-rays to Study the Fate of Nanoparticles in Fuel Conversion Processes and Environmental Samples
Laura Torrent*, **H. Xiang**, **D. Baudouin**, **F. Vogel**, **C. Ludwig**, **K. Kilchhofer**, **K.Y. Cheung**, **P.A. Alpert**, **M. Ammann**, Paul Scherrer Institute, Switzerland
M. Iglesias, **E. Marguí**, **M. Hidalgo**, University of Girona (UdG), Spain
C. Ludwig, École Polytechnique Fédérale de Lausanne, Switzerland
- 2:30 F-39 Heavy Metal Pollution within the Calumet Industrial Corridor
Martina Schmeling*, **M. Gende**, Loyola University Chicago, USA

- 2:50 F-30 A Round Robin Test for Total Reflection X-ray Fluorescence Analysis Using Preselected and Well Characterized Samples
Buckhard Beckhoff*, **R. Unterumsberger**, Physikalische-Technische Bundesanstalt, Germany
A. Gross, H. Stosnach, Bruker Nano GmbH, Germany
S. Nowak, Y.P. Stenzel, MEET - Battery Research Center, Germany
M. Kraemer, AXO DRESDEN GmbH, Germany
A. von Bohlen, Leibniz-Institut für Analytische Wissenschaften – ISAS – e.V., Germany
- 3:10 F-44 Evaluating Multi-Elemental Reference Materials for EDXRF Measurements of Atmospheric Aerosols
Nicole Hyslop*, **S. Yatkin, K. Trzepla, J. Giacomo, Y. Liu**, University of California Davis, USA
- 3:30 Break
- 4:00 F-15 Invited – Elemental Analysis and Mapping of Biological Tissues
Po-Wah So*, King's College London, United Kingdom
- 4:30 F-59 Tackling Low Z Element Quantification with TXRF
Philipp Ziegler*, **M. Weinberger, D. Krstajic, P. Wobrauschek, C. Strel, D. Ingerle**, Atominstytut – TU Wien, Austria
- 4:50 F-51 Analysis of Heavy Metals and Pesticides in Balsamic Vinegar
Monika Rasic*, **C. Halcin, M. Schmeling**, Loyola University Chicago, USA

Oral Sessions – Thursday Morning, 10 August

**Signifies presenting author, when noted*

Machine Learning Techniques in X-ray Analysis – Part I

Magnolia

Chairs: **Mathew Cherukara**, Argonne National Laboratory, USA, mcherukara@anl.gov

Apurva Mehta, Stanford University / SLAC National Accelerator Laboratory, USA, mehta@slac.stanford.edu

- 9:00 S-36 Invited – High-Throughput Crystal Structure Solution Using Diffraction and DFT
Chris Wolverton*, **S. Griesemer**, Northwestern University, USA
L. Ward, Argonne National Laboratory, USA
- 9:30 S-1 Deploying Machine Learning Based Segmentation for X-ray Diffraction Images at Synchrotron Facilities
Howard Yanxon*, **H. Parraga, J. Weng, W. Xu, U. Ruett, N. Schwarz**, Argonne National Laboratory, USA
E. Roberts, P. Zwart, Lawrence Berkeley National Laboratory, USA
- 9:50 S-6 X-ray Powder Diffraction Patterns as Features to Represent Atomic Distributions for Learning through Artificial Intelligence
Xim Bokhimi*, Instituto de Fisica, Universidad Nacional Autónoma de México, Mexico
J.I. Gómez-Peralta, CINVESTAV-IPN, Mexico
- 10:10 S-17 Deep Neural Network Application for Phase Identification in Powder X-ray Diffraction
Akihiro Himeda*, **T. Shibasaki, T. Ohta**, Rigaku Corporation, Japan
- 10:30 Break
- 11:00 S-22 Rapid Screening for Novel Crystal Structures in High Uncertainty, Low Quality Synchrotron XRD Data
Nathan Johnson*, **D. Van Campen, O. Hoidn, A. Mehta**, SLAC National Accelerator Facility, USA
J. Chen, A.A. Yakovenko, U. Ruett, Argonne National Laboratory, USA
H.P. Patel, J. Sha, K.M. Schaab, A.H. Bond, DeNovX, USA
- 11:20 S-35 Invited – AI-Guided Analysis for Coherent Scattering Time Series
Andi Barbour*, **T. Konstantinova, L. Wiegart, N. Nellikunmel, H. Chen, M. Rakitin, J. Lynch, A. DeGennaro**, Brookhaven National Laboratory, USA

Synchrotron Applications in XRD

Cypress

Chairs: **Jon Almer**, Argonne National Laboratory, USA, almer@anl.gov

Matt Miller, Cornell University, USA, mpm4@cornell.edu

- 9:00 D-49 Invited – Multi-Modal Materials Characterization at the P21.2 High-Energy Beamline at PETRA III (DESY)
Ulrich Lienert*, **S. Gutschmidt, Z. Hegedüs, M. Blankenburg**, Deutsches Elektronen-Synchrotron DESY, Germany

- 9:30 D-4 Atomic-scale Dynamics of Metallic Glasses under Elastic Stresses Probed via Coherent XRD
Amlan Das*, Cornell High Energy Synchrotron Source, USA
P.M. Derlet, Paul Scherrer Institute, Switzerland
E.M. Dufresne, Argonne National Laboratory, USA
R. Maass, Federal Institute of Materials Research and Testing (BAM), Germany
- 9:50 D-10 *In-situ* 3D High-energy X-ray Diffraction Study on Deformation Behavior of Neutron-Irradiated Fe-9%Cr
Dominic Piedmont*, **J. Stubbins**, University of Illinois Urbana Champaign, USA
X. Zhang, **M. Li**, **J. Almer**, Argonne National Laboratory, USA
- 10:10 Break
- 10:40 D-51 Invited – X-ray Diffraction-Based Tools for Structural Materials Characterization at CHESS
Kate Shanks*, **A. Das**, **K. Nygren**, **J. Ko**, CHESS, USA
- 11:10 D-30 Microstructure Quantification of Shark Vertebral Mineralized Cartilage
Stuart Stock*, Northwestern University, USA
K. James, **M. Passerotti**, **L Natanson**, NOAA, USA
P. Shevchenko, Argonne National Laboratory, USA
- 11:30 D-50 Invited – Microstructure Imaging for Engineering Materials Using High-Energy X-rays after the Advanced Photon Source - Upgrade (APS-U)
Jun-Sang Park*, **J. Almer**, **P. Kenesei**, **C.A. Chuang**, **L. Gallington**, **J. Okasinski**, **H. Sharma**, **S. Shastri**, Argonne National Laboratory, USA

Industrial Applications of XRD

Lilac C

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

- 9:00 D-8 Invited – Powder Crystallography: Providing Basic Scientific Infrastructure for Industry
James Kaduk*, **C. Scherry**, North Central College, USA
W. Wong-Ng, NIST, USA
- 9:30 D-13 Quantitative Phase Analysis of Cement Using the New Compact X-ray Diffractometer, MiniFlex XpC
Ekaterina Vinogradova*, **M. Sharma**, **K. Saito**, **A. Tripathi**, Rigaku Americas Corporation, USA
- 9:50 D-35 High Throughput Mechanocrystallization and Synchrotron X-ray Powder Diffraction: Actionable Information from Imperfect Pharmaceutical Specimens
Andrew H. Bond*, **H.P. Patel**, **J. Sha**, **Y. Ma**, **K.M. Schaab**, DeNovX, USA
J. Chen, **A.A. Yakovenko**, **S. Lapidus**, **U. Ruett**, Argonne National Laboratory, USA
N.S. Johnson, **D. Van Campen**, **A. Mehta**, SLAC National Accelerator Laboratory, USA
- 10:10 Break
- 10:40 D-18 Invited – Obtaining Accurate QPA on Highly Complex Materials like Iron Slag, Steel Slag, and Cement
Jessica Lyza*, **S. Page**, Edward C. Levy, Co., USA
T. Fawcett, International Centre for Diffraction Data, USA
- 11:10 D-5 ICDD® Polymer Diffraction Data Project – Raw Data Entries for Materials Characterization
Tom Blanton*, **M. Rost**, **D. Bohnenberger**, ICDD, USA
- 11:30 D-63 Structural Analysis of Small Molecule Pharmaceuticals with the D6 PHASER Benchtop XRPD
Nathan Henderson*, **N. Rodesney**, **B. Jones**, Bruker AXS, USA
- 11:50 D-56 A Study on the Diffraction Intensity of Isotactic-Polypropylene
Xuanbo Liu*, **M. Ren**, SINOPEC (Beijing) Research Institute of Chemical Industry Co., Ltd., China

General XRF

Lilac D

Chair: **Ursula E.A. Fittschen**, Clausthal University of Technology, Germany, ursula.fittschen@tu-clausthal.de

- 9:00 F-47 Invited – The Role of MA-XRF in the Concert of Methods for the Investigation of Cultural Heritage Artefacts
Matthias Alfeld*, TU Delft, Netherlands
- 9:30 F-26 A Historical Review of Miniaturized X-ray Sources Over the Last Twenty Years
Sterling Cornaby*, **K. Kozaczek**, Moxtek, USA

- 9:50 F-49 XRF under Grazing Incidence Investigations of Potential Calibration Samples for the Quantification of Heavy Elements in Particulate Matter
Diane Eichert*, ELETTRA - Sincrotrone Trieste, Italy
L. Borgese, P. Cirelli, University of Brescia, Italy
T. Hase, University of Warwick, United Kingdom
- 10:10 Break
- 10:40 F-43 Invited – Illuminating BOF-Slags By μ -XRF – Vanadium Distribution and Its Structural Influences
Sophie Wunderlich*, **S. Hampel, K. Sanyal, U.E.A. Fittschen, T. Schirmer**, Clausthal University of Technology, Germany
D.F. Sanchez, Paul Scherrer Institute, Switzerland
- 11:10 F-27 Determination of Diffusion Coefficients of Vanadium Inside Polymer Electrolyte Membranes
Sven Hampel*, **F. Mähler, C. Lutz, U.E.A. Fittschen, N. Merkert**, Clausthal University of Technology, Germany
G. Falkenberg, Deutsches Elektronen-Synchrotron DESY, Germany
- 11:30 F-7 Portable X-ray Fluorescence in the Assessment of Mineral Provision from Okra and Spices in East Africa
David Fleming*, Mount Allison University, Canada
H. Hailu, D. Woldetsadik, Wollo University, Ethiopia

Oral Sessions – Thursday Afternoon, 10 August

**Signifies presenting author, when noted*

Machine Learning Techniques in X-ray Analysis – Part II

Magnolia

Chairs: **Mathew Cherukara**, Argonne National Laboratory, USA, mcherukara@anl.gov

Apurva Mehta, Stanford University / SLAC National Accelerator Laboratory, USA, mehta@slac.stanford.edu

- 1:30 S-32 Unsupervised Deep Learning for Lensless Imaging
Oliver Hoidn*, **A. Mishra, M. Seaberg, A. Mehta**, SLAC National Accelerator Laboratory, USA
- 1:50 S-27 A Stochastic Minibatch Approach to the Ptychographic Iterative Engine
Ashish Tripathi*, **Z. Di**, Argonne National Laboratory, USA
S. Wild, Lawrence Berkeley National Laboratory, USA
- 2:10 S-41 Invited – Experience with Integrated Systems for Online Physics Modeling, Adaptive ML Modeling, and Model- Based Control for Particle Accelerators
Auralee Edelen*, SLAC National Accelerator Laboratory, USA
- 2:40 S-26 Prediction of X-ray Fluorescence Intensity Based on Bayesian Estimation
Tsugufumi Matsuyama*, **M. Nakae, S. Yasuda, K. Tsuji**, Osaka Metropolitan University, Japan
M. Machida, Japan Atomic Energy Agency, Japan
K. Hayashi, Kyoto University, Japan
- 3:00 Break
- 3:30 S-23 Data Analysis Algorithms for the Energy Dispersive X-rays Detectors
Sarmad Adeel*, **M. Tolkiehn**, FS-PETRA-D Deutsches Elektronen-Synchrotron DESY, Germany
- 3:50 S-12 Subpixel Resolution for Pixelated Semiconductor Tracking Detectors Based on Neural Networks
Björn Eckert*, PNDetector GmbH and University of Siegen, Germany
S. Aschauer, M. Huth, P. Majewski, H. Soltau, PNDetector GmbH, Germany
L. Strüder, PNSensor GmbH and University of Siegen, Germany

Industrial Applications of XRF

Cypress

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

- 1:30 F-11 Invited – Trace Heavy Metal Analysis in Food Products by X-ray Fluorescence Spectroscopy, the Disruptive Nature of Introducing X-ray Fluorescence into the World of Atomic Spectroscopy
Joel Langford*, **H. Chen**, Shimadzu Scientific Instruments, USA

- 2:00 F-2 Invited – Unraveling the Power of X-ray Fluorescence for Accurate Inorganic Quantitative Analysis in Industrial Applications
Poulami Dutta*, Dow Inc., USA
- 2:30 F-16 Application of Micro-XRF in the Pharmaceutical Industry
Sergey Mamedov*, HORIBA Scientific, USA
- 2:50 Break
- 3:40 F-42 Invited – XRF Assays for Critical Minerals in Mining and Processing: Comparison of WDXRF, EDXRF and PXRF Capabilities for Cobalt in Ore, Tails and Concentrates
Alexander Seyfarth*, SGS Natural Resources, USA
- 4:10 F-48 XRF Simultaneous Measurements of Density and Thickness of Thin Films
Tianqing He*, Bowman Analytic, Inc., USA
- 4:30 F-3 Optimizing Sample Preparation for Ferrochrome Analysis with Latest Developments in Fusion Instrument
Iván Rodríguez Durán*, **C. Audet**, **J. Asselin**, Malvern Panalytical, Canada

+ The previously advertised talk, *X-ray Fluorescence Analysis of Portland Cement and Clinker for Major and Trace Elements Using XRF Technique*, Mohammed Abdelbarie*, GOEIC, Egypt, was withdrawn from the Program.

General XRD

Lilac C

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

- 1:40 D-32 A Comparative X-ray Diffraction Analysis of Calcifications in Normal and Diseased Prostates
Sarah Gosling*, **C. Greenwood**, **M. Kitchen**, Keele University, United Kingdom
E. Arnold, **K. Rogers**, **I. Lyburn**, Cranfield University, United Kingdom
P. Cool, The Robert Jones and Agnes Hunt Orthopaedic School, United Kingdom
K. Geraki, **T. Snow**, Diamond Light Source, United Kingdom
N. Stone, Exeter University, United Kingdom
- 2:00 D-21 Austenite Calculator – Phase Fraction Quantification with Expanded Uncertainty Estimates
Adam Creuziger*, **D. Newton**, **T. Gnaupel-Herold**, NIST, USA
M. Garman, **C. Schenck**, Colorado School of Mines, USA
- 2:20 D-57 Determination of Two Structures of the Solvent 3-Hydroxypropionitrile Crystallized at Low Temperature
Scott Misture*, Alfred University, USA
P. Whitfield, Excelsus Structural Solutions, Switzerland
- 2:40 D-64 Crystallite Size Distribution Evaluation of PuO₂ as a Function of Calcination Temperature Using Whole Powder Pattern Modeling and Transmission Electron Microscopy Imaging
Lucas E. Sweet*, **E.C. Buck**, **J.F. Corbey**, **A.J. Casella**, **D.E. Meier**, **F.D. Heller**, **A.D. Nicholas**, **D.D. Reilly**, **R.A. Clark**, **S.H. Swenson**, Pacific Northwest National Laboratory, USA
M. Leoni, University of Trento, via Mesiano, Italy
- 3:00 Break
- 3:30 D-37 Specimen Displacement Correction for Powder X-ray Diffraction in Debye-Scherrer Geometry with a Flat Area Detector
Benjamin S. Hulbert*, **W.M. Kriven**, University of Illinois at Urbana Champaign, USA
- 3:50 D-34 Thin Film Thickness Measurement by X-ray Diffraction Peak Intensities of Film or Substrate Using Symmetric or Asymmetric Scans
William Boyer*, Proto Manufacturing, Inc., USA
- 4:10 D-43 Powder Pattern Spectral Deconvolution
Richard McClurg*, Curia Indiana, USA
- 4:30 D-1 Differentiation of Depositional Environments Using X-ray Diffraction Relative Intensities in Siliciclastic Succession
Mohamed Soua*, Saudi Aramco, Saudi Arabia

Quantitative Analysis of XRF

Lilac D

Chair: Maggi Loubser, University of Pretoria, South Africa, maggi.loubser@gmail.com

- 1:30 F-13 Invited – Thickness Measurement and Shape Correction of Resin Thin Films Using Theoretical Intensity of Scattered X-rays
Rie Ogawa*, Shimadzu Corporation, Japan
H. Ochi, Shimadzu General Services, Inc., Japan
- 2:00 F-9 Fitting Compton Scattering Profiles in X-ray Fluorescence Spectroscopy
Bryan Pi Ern Tee*, **B. Ganly**, **M. Kirkpatrick**, CSIRO Mineral Resources, Australia
- 2:20 F-33 Total Reflection X-ray Fluorescence: Not Just About the Physics!
Diane Eichert*, ELETTRA - Sincrotrone Trieste, Italy
- 2:40 F-46 Total-reflection X-ray Fluorescence Analysis of Coffee Samples
Peter Wobrauschek*, **M. Weinberger**, **P. Kregsamer**, **C. Strelj**, Atominstytut – TU Wien, Austria
E. Margui, University of Girona, Spain
J. Jablan, University of Zagreb, Croatia
- 3:00 Break
- 3:30 F-20 Invited – Quantitative Analysis of Materials at the Nanoscale by X-ray Spectrometry
Burkhard Beckhoff*, Physikalisch-Technische Bundesanstalt, Germany
- 4:00 F-23 New Spectroscopic Research Efforts to Refine the Calibration of the Planetary Instrument for X-ray Lithochemistry
Christopher Heirwegh*, **A. Das**, **Y. Liu**, **L. Wade**, Jet Propulsion Laboratory, California Institute of Technology, USA
B. Ganly, CSIRO, Australia
T. Elam, University of Washington, USA
N. Gao, XOS, USA
- 4:20 F-55 Using Synchrotron XFM to Calibrate and Correct for Matrix Effects in LA-ICP-TOF-MS
Andrew Crawford*, **S. Ahn**, **K. Macrenaris**, **T. O'Halloran**, Michigan State University, USA
Q. Jin, **D. Zee**, **Y. Chen**, Northwestern University, USA
C. Jacobsen, Argonne National Laboratory, USA

Oral Sessions – Friday Morning, 11 August

**Signifies presenting author, when noted*

Energy Storage and Harvesting

Magnolia

Chair: Ursula E.A. Fittschen, Clausthal University of Technology, Germany, ursula.fittschen@tu-clausthal.de

- 9:00 S-34 Invited – Multi-Modal Scanning X-ray Microscopy: From Material Properties to Nanoscopic Solar-Cell Performance
Michael Stuckelberger*, DESY, Germany
- 9:30 S-38 Invited – Imaging Chemistry in Space and Time using Synchrotron Light
Dario Ferreira Sanchez*, **M. Grazyna Makowska**, **C. Goncalves Anchieta**, **D. Grolimund**, Paul Scherrer Institut, Switzerland
- 10:00 S-20 Synthesis and Analysis of Synthetic Slags and References Prepared By Sol-Gel-Combustion
Alena Schnickmann*, **T. Schirmer**, TUC Institute of Disposal Research, Germany
S. Hampel, **K. Sanyal**, **Y. Pu**, **U.E.A. Fittschen**, Clausthal University of Technology, Germany
S. Britto, Diamond Light Source, United Kingdom
- 10:20 Break
- 10:40 S-15 Invited – Acceleration of Li-ion Battery Cathode Development with Laboratory X-ray Absorption Spectroscopy
Zachary Lebens-Higgins*, **W. Holden**, **D. Mortensen**, easyXAFS, LLC, USA

- 11:10 S-25 Polysulfide Driven Degradation in Lithium-Sulfur Batteries during Cycling – A Quantitative and High Time-Resolution Operando X-ray Absorption Study for Dissolved Polysulfides Probed at Both Electrode Sides
Burkhard Beckhoff*, **C. Zech**, **P. Hoenicke**, **Y. Kayser**, Physikalisch-Technische Bundesanstalt, Germany
S. Risse, Helmholtz-Zentrum Berlin, Germany
O. Graetz, **M. Stamm**, Leibniz-Institut fuer Polymerforschung Dresden, Germany
- 11:30 S-24 Investigation of the Genesis of Spinel Solid Solutions in Recycling Slags
Sven Hampel*, **K. Sanyal**, **U.E.A. Fittschen**, **A. Schnickmann**, **T. Schirmer**, Clausthal University of Technology, Germany
S. Britto, Diamond Light Source, United Kingdom

Cultural Heritage

Cypress

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

**Signifies presenting author, when noted*

- 9:00 S-14 Invited – Look But Don't Touch: Non-Invasive Analysis Strategies for Archaeological Glass
Monica Ganio*, Getty Conservation Institute, USA
- 9:30 S-5 Minerals Used for Painting in the Olmec "Red Palace" of San Lorenzo Tenochtitlan
Xim Bokhimi*, **A. Cyphers**, Universidad Nacional Autónoma de México, México
- 9:50 S-39 Compiling a Database of the Chemical Composition of Anton van Wouw's Sculptures and Linking it to the Foundries that Cast Them
Maggi Loubser*, **P. Forbes**, University of Pretoria, South Africa
- 10:10 Break
- 10:30 S-11 X-ray Diffraction and Small Angle Scattering Analyses of Diagenesis of Archeological Human Second Metacarpal Bones
Stuart Stock*, Northwestern University, USA
J.-S. Park, **J. Almer**, Argonne National Laboratory, USA
S. Mays, Historic England, United Kingdom
- 10:50 S-9 Micro-XRF Analysis on an "OUGI-E" Painting for the Production Date Estimation
Chiya Nishimura*, **T. Aoyama**, HORIBA, Ltd., Japan

Applications of Rietveld Analysis

Lilac C

Chair: **Saul Lapidus**, Argonne National Laboratory, USA, slapidus@aps.anl.gov

- 8:30 D-47 Invited – Understanding the Structure and Properties of the Elusive Non-Stoichiometry Lead Dioxide
Tiffany Kinnibrugh*, **T. Fister**, **X. Wang**, **D. Bazak**, **A. Karakoti**, Argonne National Laboratory, USA
V. Murugesan, Pacific Northwest National Laboratory, USA
- 9:00 D-3 Temperature-Induced Static and Dynamic Displacements of Atoms from Diffraction Analysis of Nanocrystalline Powders
Hande Öztürk*, **M. Batyrow**, **H. Hekmatjou**, Özyegin University, Turkey
- 9:20 D-16 Distorted Holandite, Structural, Morphological, Optical and Transport Properties
A.M. Moustafa*, **S.A. Gad**, National Research Centre, Egypt
I.A. Abdel-Latif, **K.M. Roumah**, Egyptian Atomic Energy Authority, Egypt
- 9:40 D-17 Biogenic and Synthetic Hydroxyapatite under Thermal Treatment
Emily L. Arnold*, **S.K. Davies**, **K.D. Rogers**, Cranfield University, United Kingdom
S.B. Gosling, **H.L. Cross**, **C.E. Greenwood**, Keele University, United Kingdom
D.L. Keeble, Diamond Light Source, United Kingdom
J.P.O. Evans, Nottingham Trent University, United Kingdom
- 10:00 Break
- 10:20 D-53 Invited – Mechanistic Understanding of High-Rate Battery Cycling using Operando Synchrotron X-ray Diffraction
Molleigh Preefer*, **V. Thampy**, **K. Stone**, **J. Nelson Weker**, SLAC National Accelerator Laboratory, USA
Y. Luo, **B. Dunn**, UCLA, USA

- 10:50 D-25 Cation Adaptive Networks Understood via Powder Diffraction
Peter Stephens*, Stony Brook University, USA
J. Miller, University of Utah, USA
- 11:10 D-29 Verification of the Method for Determining the Degree of Crystallinity Using Experimental and Simulated Powder Diffraction Patterns
Hideo Toraya*, Rigaku Holdings Corporation, Japan
- 11:30 D-11 GSAS-II in 2023
Brian H. Toby*, **R.B. Von Dreele**, Argonne National Laboratory, USA

Micro XRF and Synchrotron Applications

Lilac D

Chair: **Peter Wobrauschek**, Atominstytut – TU Wien, Austria, wobi@ati.ac.at

- 8:30 F-45 Invited – voxTrace: A Voxel-Based Monte-Carlo Raytracing Code for the Simulation of Confocal Micro-X-ray Fluorescence Measurements
Michael Iro*, **P. Kregsamer**, **C. Strelt**, Atominstytut, TU Wien, Austria
D. Ingerle, X-ray Center, TU Wien, Austria
S. Hampel, **U.E.A. Fittschen**, Clausthal University of Technology, Germany
- 9:00 F-19 A Large Solid Angle X-ray Spectrometer for High Count-Rate XFM Experiments
Giacomo Ticchi*, **B. Pedretti**, **D. Di Vita**, **G. Borghi**, **M. Carminati**, **C. Fiorini**, Politecnico di Milano, Italy
G. Falkenberg, DESY, Deutsches Elektronen-Synchrotron DESY, Germany
- 9:20 F-21 Towards a New Generation of Multichannel X-ray Fluorescence Spectrometers
Beatrice Pedretti*, **G. Ticchi**, **D. Di Vita**, **G. Borghi**, **M. Carminati**, **C. Fiorini**, Politecnico di Milano, Italy
- 9:40 F-22 Micro-X-ray Fluorescence Combined with Optical Microscopy as a Potential Alternative to Scanning Electron Microscopy for Nuclear Materials Applications
Christopher Worley*, **O. Duarte**, Los Alamos National Laboratory, USA
- 10:00 F-24 Full-field Spectroscopic X-ray Microscopy Using the pnCCD Color X-ray Camera
Martin Huth*, **H. Soltau**, PNDetector GmbH, Germany
J. Soltau, **P. Meyer**, **T. Salditt**, University of Göttingen, Germany
R. Hartmann, PNSensor GmbH, Germany
L. Strüder, University of Siegen, Germany
- 10:20 Break
- 10:40 F-53 Invited – Scanning X-ray Microscopy at the Hard X-ray Micro/Nano-Probe Beamline P06 (DESY) for Bio and Bio-Medical Applications
Gerald Falkenberg*, **D. Brückner**, **K.V. Falch**, **J. Garrevoet**, Deutsches Elektronen-Synchrotron DESY, Germany
- 11:10 F-25 A Compact High Solid Angle Four Segmented Annular Silicon Drift Detector System for Synchrotron and Ion Beam Applications for Ambient Conditions
Dieter M. Schlosser*, **A. Bechteler**, **M. Bornschlegl**, **T. Eckstein**, **U. Weber**, **R. Lackner**, **D. Steighöhöfer**, **S. Aschauer**, **A. Niculae**, **H. Soltau**, PNDetector GmbH, Germany
- 11:30 F-32 Manganese Enrichments in Jezero Crater Analyzed by the Planetary Instrument for X-ray Lithochemistry
Kimberly Sinclair*, University of Washington, USA
B. Clark, Space Science Institute, USA
- 11:50 F-52 Correcting for Ice Block Attenuation of X-ray Fluorescence for Fully Hydrated Flash Frozen Cells
Andrew Crawford*, **K. Ok**, **T. O'Halloran**, Michigan State University, USA

Westin Chicago Lombard Hotel Layout



2023 Denver X-ray Conference ♦ Program-at-a-Glance ♦ Monday – Friday ♦ 7 – 11 August

Monday Morning Workshops 9:00 am – 12:00 Noon				
	Meeting Rooms			
	Magnolia	Cypress	Lilac C	Lilac D
Special Topic	What the APS Upgrade will bring to X-ray Analysis – Part I (Antipova)	Cultural Heritage (Alfeld)		
XRD			Basic to Intermediate XRD (Blanton/Misture)	
XRF				Basic XRF (Drews/Wobruschek)
Monday Afternoon Workshops 1:30 pm – 4:30 pm				
Special Topic	What the APS Upgrade will bring to X-ray Analysis – Part II (Antipova)	In situ Battery Measurements (Drews)		
XRD				
XRF			Quantitative XRF (Kawakyu/Loubser)	Sample Preparation for XRF (Cruz Hernandez/Rodriguez Duran)
Monday Evening XRD Poster Session & Reception 5:00 pm – 7:00 pm (Watkins/Cakmak) Grand Ballroom				
Tuesday Morning Workshops 9:00 am – 12:00 Noon				
Special Topic				
XRD	Intro to GSAS-II (Von Dreele/Toby)	Texture (Watkins)		
XRF			Micro XRF (Tsuji)	XRF of Layered Structures (Wobruschek)
Tuesday Afternoon Workshops 1:30 pm – 4:30 pm				
Special Topic				
XRD	Advanced Topics in GSAS-II (Von Dreele/Toby)	XRD Methods for Complex Multi-Phase Identification (Fawcett)		
XRF			How to Get the Best from Your Handheld XRF Spectrometer (Loubser)	XRF Trace Analysis (Wobruschek)
Tuesday Evening XRF Poster Session & Reception 5:00 pm – 7:00 pm (Schmeling) Grand Ballroom				
Wednesday Morning Plenary Session – Energy Storage Lilac C & D, 8:30 am – 11:45 am (Misture)				
Wednesday Afternoon Sessions				
Special Topic	New Developments in XRD & XRF Instrumentation (Fawcett/Drews)	Imaging (Wobruschek)		
XRD			Stress and Texture Analysis (Watkins)	
XRF				Trace Analysis (Eichert)
Thursday Morning Sessions				
Special Topic	Machine Learning Techniques in X-ray Analysis – Part I (Mehta/Cherukara)			
XRD		Synchrotron Applications in XRD (Almer/Miller)	Industrial Applications of XRD (Fawcett)	
XRF				General XRF (Fittschen)
Thursday Afternoon Sessions				
Special Topic	Machine Learning Techniques in X-ray Analysis – Part II (Mehta/Cherukara)			
XRD			General XRD (Murray)	
XRF		Industrial Applications of XRF (Worley)		Quantitative Analysis of XRF (Loubser)
Friday Morning Sessions				
Special Topic	Energy Storage and Harvesting (Fittschen)	Cultural Heritage (Schmeling)		
XRD			Applications of Rietveld Analysis (Lapidus)	
XRF				Micro XRF and Synchrotron Applications (Wobruschek)