



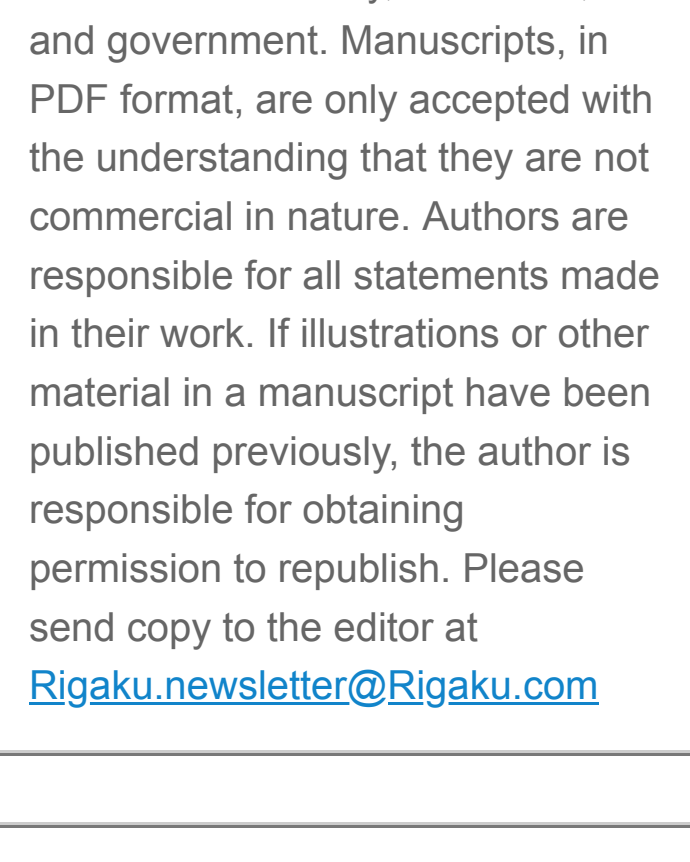
Benchtop chemical crystallography system for 3D small molecule structure determination



XtaLAB mini II

The Rigaku XtaLAB mini II benchtop X-ray crystallography system is a compact single crystal X-ray diffractometer designed to produce publication-quality 3D structures. The perfect addition to any synthetic chemistry laboratory, the XtaLAB mini II will enhance research productivity by offering affordable structure analysis capability without the necessity of relying on a departmental facility. With the XtaLAB mini II, you no longer have to wait in line to determine your structures. Instead your research group can rapidly analyze new compounds as they are synthesized in the lab. **For more >**

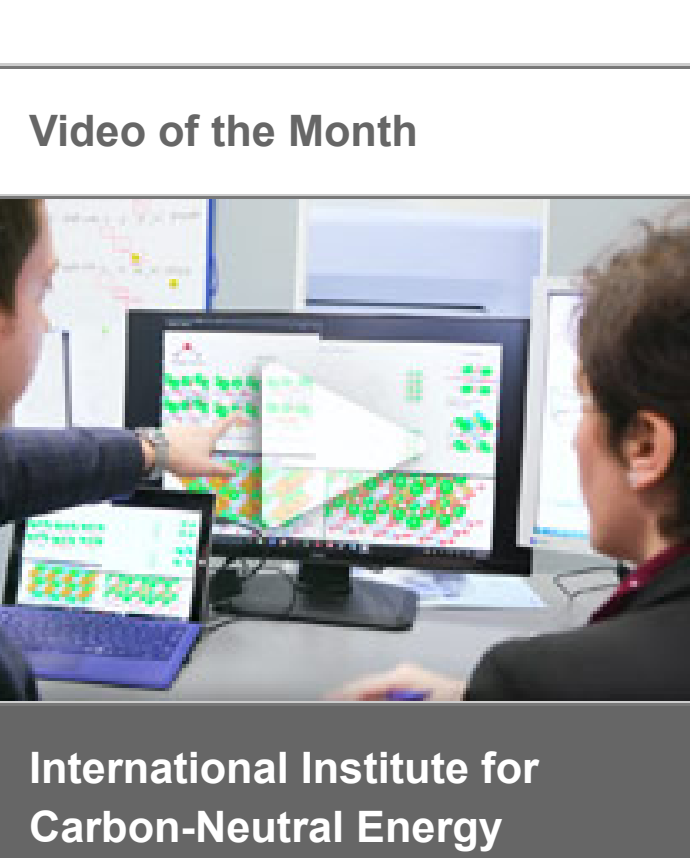
Interested in publishing your work in The Bridge?



Publish Your Work Here

The Bridge now welcomes manuscripts, communications, and papers that describe techniques and applications of all forms of X-ray fluorescence (XRF) and X-ray diffraction (XRD, including SAXS) that are of interest to fellow scientists in industry, academia, and government. Manuscripts, in PDF format, are only accepted with the understanding that they are not commercial in nature. Authors are responsible for all statements made in their work. If illustrations or other material in a manuscript have been published previously, the author is responsible for obtaining permission to republish. Please send copy to the editor at Rigaku.newsletter@Rigaku.com

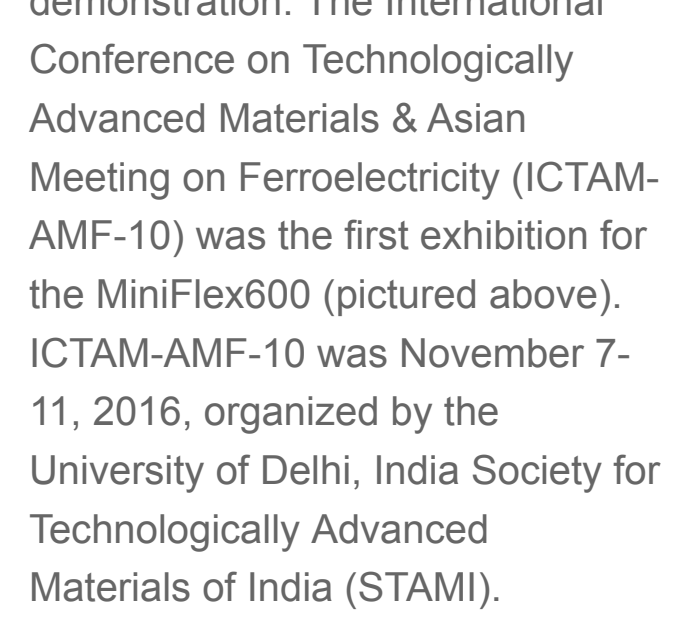
Powder diffraction, thin film diffraction, SAXS, in-plane scattering



SmartLab®

The SmartLab is the most novel high-resolution X-ray diffractometer available today. Perhaps its most novel feature is the SmartLab Guidance software, which provides you with an intelligent interface that guides you through the intricacies of each experiment. It is like having an expert standing by your side. **For more >**

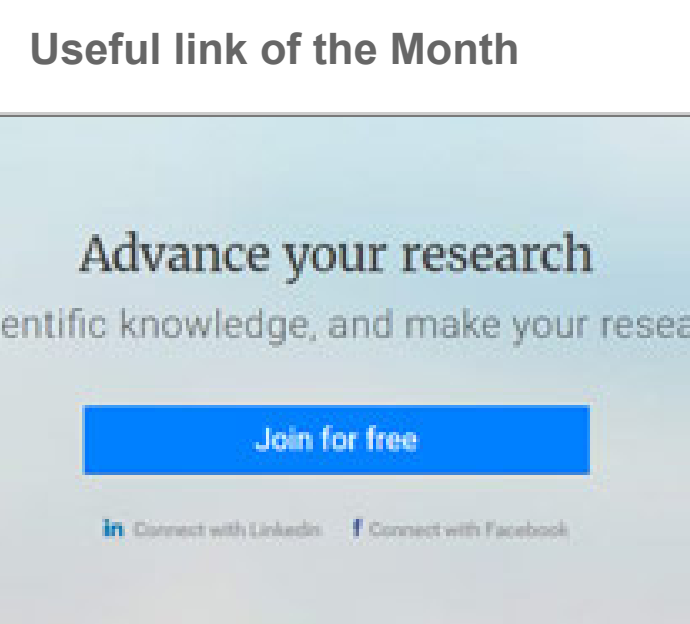
Video of the Month



International Institute for Carbon-Neutral Energy Research (I²CNER), Japan

The research objective at I²CNER is to reduce CO₂ emissions while creating a new generation of carbon-neutral energy solutions. **Watch video >**

Conferences and Workshops



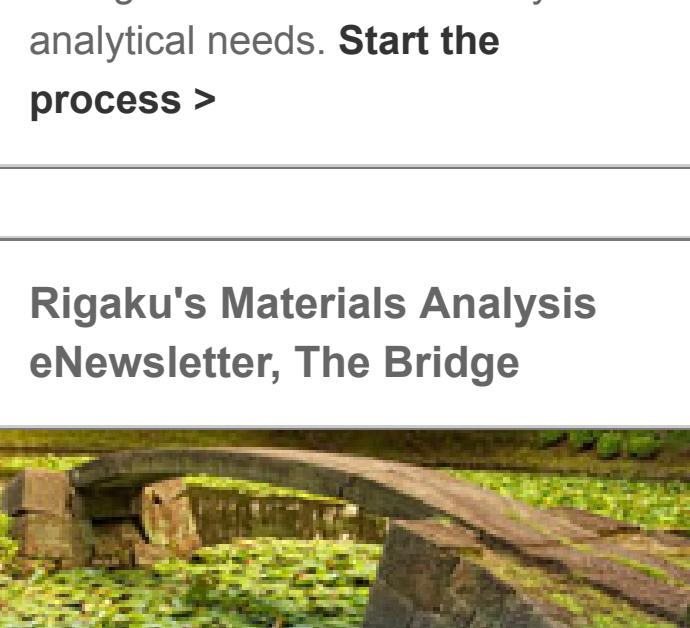
Join Rigaku at future meetings

Indian Rigaku distributor IR Technology Services Pvt. Ltd. now has a Rigaku MiniFlex600 X-ray diffractometer available for demonstration. The International Conference on Technologically Advanced Materials & Asian Meeting on Ferroelectricity (ICTAM-AMF-10) was the first exhibition for the MiniFlex600 (pictured above). ICTAM-AMF-10 was November 7-11, 2016, organized by the University of Delhi, India Society for Technologically Advanced Materials of India (STAMI).
Rigaku will be sponsoring, attending or exhibiting at the following conferences and trade shows:

- PITTCON 2017**
Chicago, Illinois, USA
March 5 – 9, 2017
- AWPA 2017**
Las Vegas, Nevada, USA
April 9 – 11, 2017
- MRO Americas 2017**
Orlando, Florida, USA
April 25 – 27, 2017

See the complete list >

Useful link of the Month



ResearchGate

ResearchGate is a social networking site for scientists and researchers to share papers, find and answer questions, and find collaborators. According to a study by *Nature* and an article in *Times Higher Education*, it is the largest academic social network in terms of active users, although other services have more registered users and more recent data suggests that almost as many academics have Google Scholar profiles.
People that wish to use the site need to have an email address at a recognized institution or to be manually confirmed as a published researcher in order to sign up for an account. Members of the site each have a user profile and can upload research output including papers, data, chapters, negative results, patents, research proposals, methods, presentations, and software source code. Users may also follow the activities of other users and engage in discussions with them. Users are also able to block interactions with other users. **For more >**

Planning to Submit a Grant?



Rigaku is happy to assist

If you are planning on submitting an instrument grant proposal, Rigaku will be happy to assist you. We can help you determine the correct instrument and configuration best suited for your analytical needs. **Start the process >**

Rigaku's Materials Analysis eNewsletter, The Bridge



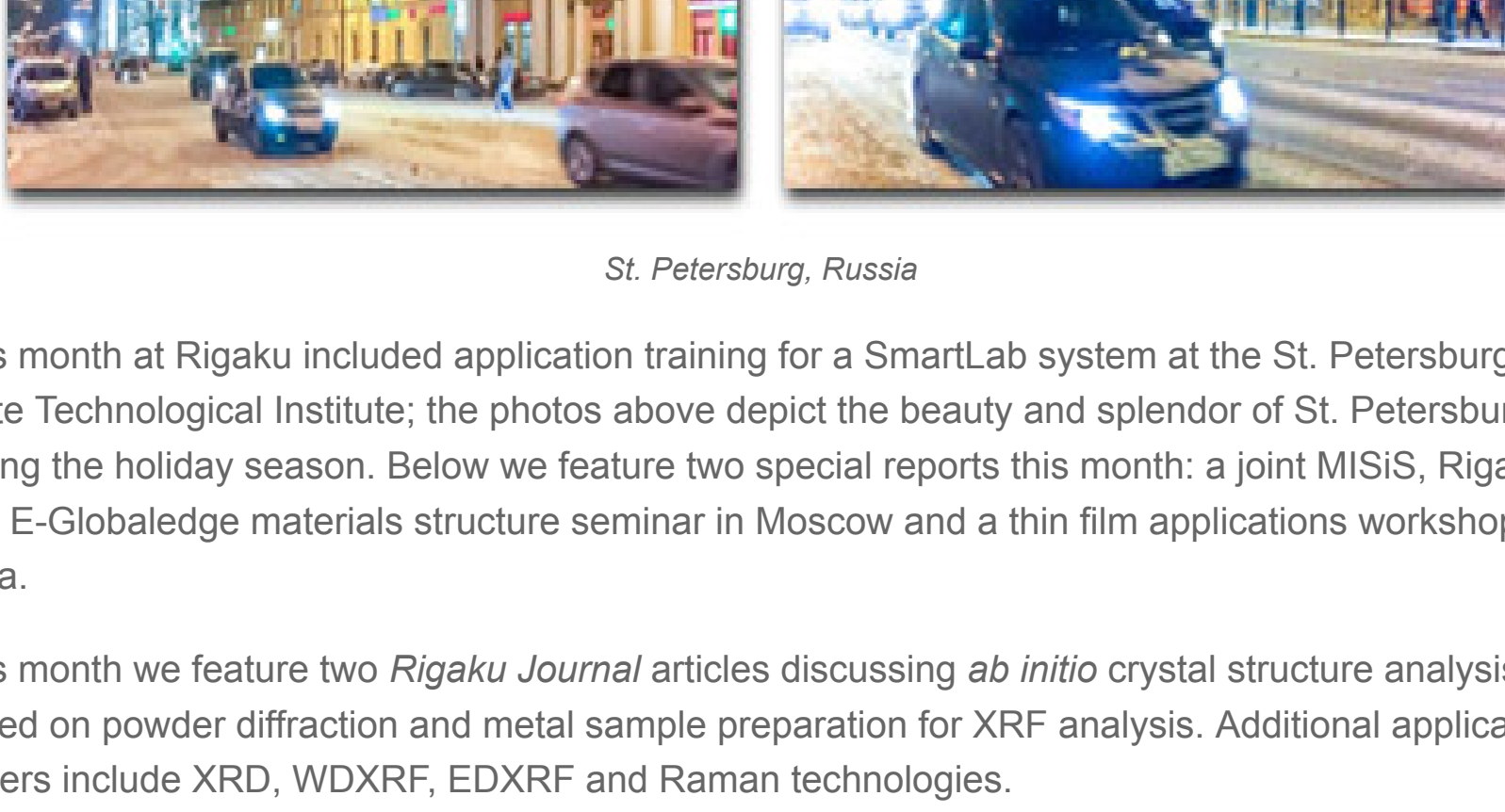
Join us

Each month, Rigaku distributes two eNewsletters: *The Bridge*, which focuses on Materials Analysis, and *Crystallography Times*, which concentrates on life sciences. **Join us >**

Welcome

We want to thank everyone who visited Rigaku at the 14th International Conference of the Asian Crystallographic Association, 4 – 7 December 2016 in Hanoi Vietnam. AI ASCA, the conference banquet was sponsored by Rigaku on Tuesday 6 December and held at one of the most famous restaurants in Hanoi, the Trong Dong Palace. At the banquet, Prof. Gautam Desiraju, Immediate Past President of the International Union of Crystallography (IUCr), gave a special lecture on some general crystallography issues and on the IUCr 2017 Congress in India.

Please come visit Rigaku in the spring at the CCP4 Study Weekend 2017 (Jan 9 – 11, Nottingham, UK), Instrument Society of America 2017 (Feb 22 – 25, Baltimore, MD) and Pitcon 2017 (Mar 5 – 9, Chicago).



St. Petersburg, Russia

This month at Rigaku included application training for a SmartLab system at the St. Petersburg State Technological Institute; the photos above depict the beauty and splendor of St. Petersburg during the holiday season. Below we feature two special reports this month: a joint MISIS, Rigaku, and E-Globalede materials structure seminar in Moscow and a thin film applications workshop in India.

This month we feature two *Rigaku Journal* articles discussing *in situ* crystal structure analysis based on powder diffraction and metal sample preparation for XRF analysis. Additional application papers include XRD, WDXRF, EDXRF and Raman technologies.

The video topic returns to tech in Japan with a spotlight on the International Institute for Carbon-Neutral Energy Research (I²CNER). The book review returns this month for a lighthearted discussion of the music of Bruce Springsteen. Check out the news and papers sections at the bottom of the page for the latest developments in materials science.

Happy New Year and enjoy the newsletter.

R.C. Tisdale, Ph.D. – Editor

Featured XRD Rigaku Journal Article

Ab initio crystal structure analysis based on powder diffraction data using PDXL

Akito Sasaki, Akihiro Himeda, Hisashi Konaka and Norihiro Muroyama, Rigaku Corporation

Physical and chemical properties of a crystalline solid depend strongly on the molecular arrangement, that is, on both the crystal structure and the composition of the molecule comprising the solid. In order to understand the mechanisms and developing properties of a crystalline solid, it is essential to know the crystal structure. Typically, crystal structure analysis has been performed using hundreds or thousands of X-ray intensity data collected from a single crystal. The data is collected with a four-circle diffractometer or a diffractometer equipped with an image plate or other 2D detector. Just 10 years ago, single crystals several hundred microns in diameter were needed. Recent improvements in X-ray sources and detectors enable the collection of intensity data which can be used in the analysis of crystal structures from crystal specimens measuring only a few microns across. **For full article >**

Featured XRF Rigaku Journal Article

Sample preparation for X-ray fluorescence analysis VI. Metal samples

Takao Moriyama and Eiichi Furusawa, Rigaku Corporation

Sample preparation methods for X-ray fluorescence analysis (XRF) featuring powder samples were discussed in the previous issues. Preparation of metal samples is introduced in this issue. XRF is superior to ICP and optical emission spectroscopy in reproducibility. However most of analysis errors in XRF can be caused by nature of sample itself and sample preparation, as in the case of powder samples discussed before. Analysis errors of metal samples come from (1) internal segregation, (2) defective surface, (3) surface roughness and uneven surface, (4) surface transformation, (5) metallurgical history, etc. Consideration of these points will provide more accurate analysis results. **For full article >**

Joint MISIS, Rigaku, and E-Globalede Seminar in Moscow

Report on "Modern method of material structure analysis and its application for Materials Science" seminar in Moscow

Reported by S. Sakamoto, E-Globalede Corporation

A joint seminar called "Modern method of material structure analysis and its application for Materials Science", organized by the Institute of Steel and Alloy (MISIS), Rigaku, and E-Globalede, was held on November 28 and 29, 2016. The event took place at MISIS in Moscow. **For full report >**

Rigaku – Thin Film Application Workshop in India

Report on Thin Film Workshops

Reported by Tomikatsu KUBO, International Sales Department at Rigaku Corporation

In November 2016, two workshops were held in India. The first was held at the Indian Institute of Science (IISc) in Bangalore and the Jamia Millia Islamia (JMI) in Delhi. Approximately 200 people interested in Thin Film applications by SmartLab attended the workshop. **For full report >**

XRD Application Note

Qualitative Analysis of an Ancient Glass Bead

Rigaku Corporation

The Oldo tunnel tombs in Wakuyacho, Miyagi (Japan) are tumuli that have been constructed between the late 7th century and the early 8th century. During scientific investigations between 1962 and 1964, a glass bead with a spotted pattern (concentric circles) rare to Japan was excavated, which is believed to be originated in South Asia or Southeast Asia. By evaluating the colored portion of the glass bead using the SmartLab Automated Multipurpose X-ray Diffractometer, it was possible to determine its chemical composition and provide a scientific basis for assumptions on the fabrication technique and a reevaluation of its origin. The research was conducted by the Nara National Research Institute for Cultural Properties in 2013, and presented at the 31st Congress of the Japan Society for Scientific Studies on Cultural Properties in 2014. **For more >**

WDXRF Application Note

Beryllium Analysis in Beryllium Copper Alloy

Rigaku Corporation

Beryllium copper alloy has almost as high strength as steel, and is the strongest among copper alloys. In addition, it has various features such as non-magnetic and non-sparking characteristics, having high electrical conductivity and ductility. Owing to these features, beryllium copper has many uses, springs, electric connectors, tools in environments with explosive vapors and gases, and musical instruments. Since characteristics and uses of beryllium copper alloys depend on beryllium concentration, it is important to analyze beryllium in beryllium copper. **For more >**

EDXRF Application Note

Chemical Bath for Copper Foil Surface Treatment

Applied Rigaku Technologies

Surface treating is an important part in the manufacture of copper foil for the electronics industry. Surface treatments are used to clean the copper foil, to create roughing and heat resistance treatments, and to make single or multiple layer thin film coatings to prevent oxidation or enhance the electro-chemical properties of the copper foil. The chemical baths must be constantly monitored to ensure the highest quality surface treatments. **For more >**

Featured Raman Article

Comparison of rapid detecting optical techniques for the identification of New Psychoactive Substances in Legal High preparations

The number of newly reported synthetic psychoactive "Legal High" preparations has grown and poses a significant danger to the public. Rapid identification of unknown substances in the field can be a challenge. Funded in part by the European Commission's "SPICE II" project, a collaborative study performed by researchers at the Westfälische Wilhelms Universität und Bundeskriminalamt (BKA) compared handheld technologies for identifying unknown substances in the field. Analysis results using Rigaku's Progeny 1064 nm handheld Raman demonstrated advantages in spectral specificity for more accurate identification, when compared to a 785 nm and another 1064 nm based handheld Raman system. **For more >**

Scientific Book Review

Born to Run

In 1979 I first heard the WMMS broadcast of Springsteen's 1978 concert at the Cleveland Agora. I knew that my life would never be the same. **Full review >**

Material Analysis in the News

News for December 2016

December 1, 2016. Prof. Keon Jae Lee's research group at the Center for Multidimensional Carbon Materials within the Institute for Basic Science (IBS) and Prof. Choi Sung-Yool's team at KAIST discovered a **graphene synthesis mechanism using laser-induced solid-state phase separation** of single-crystal silicon carbide (SiC).

December 2, 2016. Experiments using laser light and pieces of gray material the size of fingernail clippings may offer clues to a fundamental scientific riddle: **What is the relationship between the everyday world of classical physics and the hidden quantum realm that obeys entirely different rules?**

December 5, 2016. A collaborative effort between research groups at the Technical University of Freiberg and the University of Siegen in Germany demonstrates that the **physical properties of SrTiO₃ or strontium titanate, a mineral often studied for its superconducting properties, can be changed in its single crystal form by a relatively simple electrical treatment.** The treatment creates the effect known as piezoelectricity, where electricity results from mechanical stress in the material which did not originally see piezoelectric effects.

December 8, 2016. **3D computed tomography (CT) images of six mummies** from between 900 B.C. and A.D. 140 to 180 from ancient Egypt, which have been held at the British Museum but never physically unwrapped, give an insight into what it was like to live along the Nile river thousands of years ago.

December 10, 2016. The campus of the **Japan Advanced Institute of Science and Technology** is about as cosmopolitan as it gets in Japan. More than half of the students at this graduate school hall from elsewhere, making it something of a shining light among the country's universities.

December 11, 2016. Perovskite solar cells, invented in Japan, combined with conventional easy-to-produce silicon type, could open doors to wider applications. Hong Kong Polytechnic University professor Charles Chee Surya demonstrates a **prototype of the new perovskite-silicon tandem solar cell.**

December 13, 2016. the National Institutes for Quantum and Radiological Science and Technology (QST), Sumitomo Heavy Industries, Ltd., Toshiba Corporation, Hitachi, Ltd., and Mitsubishi Electric Corporation signed an **"Agreement on Comprehensive Cooperation on Fifth-Generation Quantum Beam Cancer Treatment Facility"**. QST successfully developed the world's first heavy ion beam treatment facility for treating cancer in 1994.

December 15, 2016. Some of the most prized diamonds on Earth are unusually clear, exceedingly rare, and often extraordinarily large. Researchers have long wondered how such gems formed. A new **analysis of imperfections trapped within the diamonds provides the first direct evidence** that they were forged within blobs of liquid metal hundreds of kilometers below Earth's surface.

December 16, 2016. Singapore's two main research universities, Nanyang Technological University (NTU) and National University of Singapore (NUS), are pushing back the frontiers of materials science. NTU is pouring US\$20 million (\$28.5 million) into the effort over the next few years and will be one of the first places in the world with a new US\$160,000 machine that can create and test new nanomaterials many times faster than existing methods. NUS Centre for Advanced 2D Materials is utilised by about 50 professors and 200 scientists from different disciplines.

December 20, 2016. Researchers have discovered the partial tail of a **feathered dinosaur** that was preserved in amber some 99 million years ago. Lida Xing from the China University of Geosciences, happened upon the feathered dinosaur fossil at an amber market in Myanmar last year.

December 22, 2016. A **four-day workshop on Innovative Approach to Materials Research** (AMR 2016) was inaugurated at the PEC University of Technology, Chandigarh. Dr Renu Vigi inaugurated the workshop and emphasised the significance of material research in various disciplines of engineering.

Recent Scientific Papers of Interest

Papers for December 2016

Recent Scientific Papers of Interest is a monthly compilation of material analysis papers appearing in recently released journals and publications. **See below**

X-ray plane-wave diffraction effects in a crystal with third-order nonlinearity. Balyan, M. *Crystallography Reports*. Dec2016, Vol. 61 Issue 7, p1039-1046. 8p. DOI: [10.1134/S106377451600704X](https://doi.org/10.1134/S106377451600704X).

Investigation of recrystallization of amorphous hydroxyapatite through hot-humidity stage X-ray powder diffraction. Jógari-Laczakovich, Orsolya; Katona, Gábor; Algher, Zoltán; Szabó-Révész, Piroska. *European Journal of Pharmaceutical Sciences*. Dec2016, Vol. 95, p145-151. 7p. DOI: [10.1016/j.ejps.2016.08.003](https://doi.org/10.1016/j.ejps.2016.08.003).

Experimental verification of the hydrogen concentration around a crack tip using spot X-ray diffraction. Takakuwa, S. V.; Fujisawa, T.; Soyama, H. *International Journal of Hydrogen Energy*. Dec2016, Vol. 41 Issue 48, p23188-23195. 8p. DOI: [10.1016/j.ijhydene.2016.10.083](https://doi.org/10.1016/j.ijhydene.2016.10.083).

X-ray diffraction (XRD)-studies on the temperature dependent interface reactions on hafnium, zirconium, and nickel coated monocrystalline diamonds used in grinding segments for stone and concrete machining. Tillmann, W.; Tolan, M.; Pinho Ferreira, M.; Paulus, M.; Becke, M.; Stangier, D. *Materialwissenschaft und Werkstofftechnik*. Dec2016, Vol. 47 Issue 12, p1193-1201. 9p. DOI: [10.1002/mawe.201600713](https://doi.org/10.1002/mawe.201600713).

Time-resolved *in situ* powder X-ray diffraction reveals the mechanisms of molten salt synthesis. Moorhouse, Saul J.; Wu, Yue; Buckley, Hannah C.; O'Hare, Dermot. *Chemical Communications*. 12/14/2016, Vol. 52 Issue 96, p13865-13868. 4p. DOI: [10.1039/C6CC08133A](https://doi.org/10.1039/C6CC08133A).

A multi-scale simulation algorithm for grazing-incidence small-angle X-ray scattering. Venkatakrisnan, S. V.; Donatelli, Jeffrey; Kumar, Dinesh; Sarje, Abhinav; Sinha, Sunil K.; Li, Xiaoye S.; Hexemer, Alexander. *Journal of Applied Crystallography*. Dec2016, Vol. 49 Issue 6, p1876-1884. 8p. DOI: [10.1107/S1600576716013273](https://doi.org/10.1107/S1600576716013273).

Dispersed SiC nanoparticles in Ni observed by ultra-small-angle X-ray scattering. Xie, R.; Ilavsky, J.; Huang, H. F.; Zhou, X. L.; Yang, C.; Wang, Y. Z.; Xu, H. J. *Journal of Applied Crystallography*. Dec2016, Vol. 49 Issue 6, p2155-2160. 5p. DOI: [10.1107/S1600576716015090](https://doi.org/10.1107/S1600576716015090).

Composition and microstructural changes in an aged cement pastes upon two heating-cooling regimes, as studied by thermal analysis and X-ray diffraction. Sabeur, Hassen; Platret, Gérard; Julien, Julien. *Journal of Thermal Analysis & Calorimetry*. Dec2016, Vol. 126 Issue 3, p1023-1043. 21p. DOI: [10.1007/s10973-016-5639-8](https://doi.org/10.1007/s10973-016-5639-8).

Curvature determination of embedded silicon chips by *in situ* rocking curve X-ray diffraction measurements at elevated temperatures. Angerer, Paul; Schöngrundner, Ronald; Macurova, Katerina; Wiessner, Manfred; Keckes, Jozef. *Powder Diffraction*. Dec2016, Vol. 31 Issue 4, p267-273. 7p. DOI: [10.1017/S0885715616000488](https://doi.org/10.1017/S0885715616000488).

Neutron and high-pressure X-ray diffraction study of hydrogen-bonded ferroelectric rubidium hydrogen sulfate. Binns, Jack; McIntyre, Garry J.; Parsons, Simon. *Acta Crystallographica: Section B: Structural Science, Crystal Engineering & Materials*. Dec2016, Vol. 72 Issue 6, p855-863. 9p. DOI: [10.1107/S2052520616013494](https://doi.org/10.1107/S2052520616013494).

Uncertainty in flow stress measurements using X-ray diffraction for sheet metals subjected to large plastic deformations. Jeong, Y.; Gräuper-Herold, T.; Iadicola, M.; Creuziger, A. *Journal of Applied Crystallography*. Dec2016, Vol. 49 Issue 6, p1991-2004. 13p. DOI: [10.1107/S1600576716013662](https://doi.org/10.1107/S1600576716013662).

Versatile electrochemical cell for Li/Na-ion batteries and high-throughput setup for combined operando X-ray diffraction and absorption spectroscopy. Soltmann, Jonas; Homs-Regajo, Roberto; Wragg, David S.; Fjellvåg, Helmer; Margadona, Serena; Eckerl, Hermann. *Journal of Applied Crystallography*. Dec2016, Vol. 49 Issue 6, p1972-1981. 9p. DOI: [10.1107/S160057671601428X](https://doi.org/10.1107/S160057671601428X).

X-ray diffraction from magnetically oriented microcrystal suspensions detected by a shutterless continuous rotation method. Tsuboi, Nobuhiko; Shi, Kimura; Fumiko; Kimura, Tsunehisa; Hasegawa, Kazuya; Baba, Seiichi; Mizuno, Nobuhiko. *Journal of Applied Crystallography*. Dec2016, Vol. 49 Issue 6, p2100-2105. 5p. DOI: [10.1107/S160057671601534X](https://doi.org/10.1107/S160057671601534X).

Determination of the analytical performance of EDXRF and FAAS techniques in the determination of metal species concentrations using protocol 3050B (USEPA). da Silva, Paulo Roberto Barros; Makara, Cleyton Nascimento; Munaro, Ana Paula; Schivater, Danielle Caroline; Wastowski, Airci Dirceu; Poleto, Cristiano. *International Journal of River Basin Management*. Dec2016, Vol. 14 Issue 4, p401-406. 6p. DOI: [10.1080/15715124.2016.1203792](https://doi.org/10.1080/15715124.2016.1203792).

Study of the elemental composition of saliva of smokers and nonsmokers by X-ray fluorescence. Jr Poles, Antonio A.; Baldo, Victor M.; Chaud, Marco V.; Vila, Maria M.D.C.; Aranha, Norberto; Yoshida, Valquíria M.H.; Jr Oliveira, José M. *Applied Radiation & Isotopes*. Dec2016, Vol. 118, p221-227. 7p. DOI: [10.1016/j.apradiso.2016.09.007](https://doi.org/10.1016/j.apradiso.2016.09.007).

X-ray diffraction (XRD)-studies on the temperature dependent interface reactions on hafnium, zirconium, and nickel coated monocrystalline diamonds used in grinding segments for stone and concrete machining. Tillmann, W.; Tolan, M.; Pinho Ferreira, M.; Paulus, M.; Becke, M.; Stangier, D. *Materialwissenschaft und Werkstofftechnik*. Dec2016, Vol. 47 Issue 12, p1193-1201. 9p. DOI: [10.1002/mawe.201600713](https://doi.org/10.1002/mawe.201600713).

Raman, FT-IR and XRD investigation of natural opals. Sodo, A.; Casanova Munichiana, A.; Barucca, S.; Bellatreccia, F.; Della Ventura, G.; Ricci, M. A. A.; Butini, F. *Journal of Raman Spectroscopy*. Dec2016, Vol. 47 Issue 12, p1444-1451. 8p. DOI: [10.1002/jrs.4972](https://doi.org/10.1002/jrs.4972).

Relative adsorption excess of ions in binary solvents determined by grazing-incidence X-ray fluorescence. Witala, Monika; Kononov, Oleg; Nygård, Kim. *Journal of Colloid & Interface Science*. Dec2016, Vol. 484, p249-253. 5p. DOI: [10.1016/j.jcis.2016.09.005](https://doi.org/10.1016/j.jcis.2016.09.005).

Analytical capabilities of total reflection X-ray adsorption studies. Torrent, Laura; Iglesias, Mónica; Hidalgo, Manuela; Margul, Eva. *Spectrochimica Acta Part B*. Dec2016, Vol. 126, p71-78. 8p. DOI: [10.1016/j.sab.2016.10.019](https://doi.org/10.1016/j.sab.2016.10.019).

Identification of secondary salts and their sources in deteriorated stone monuments using micro-Raman spectroscopy, SEM-EDS and XRD. Marszałek, Mariola. *Journal of Raman Spectroscopy*. Dec2016, Vol. 47 Issue 12, p1473-1485. 13p. DOI: [10.1002/jrs.4972](https://doi.org/10.1002/jrs.4972).

The effect of damp heat-illumination exposure on CIGS solar cells: A combined XRD and electrical characterization study. Theelen, Mirjam; Hendriks, Ruud; Barreau, Nicolas; Steijvers, Henk; Böttger, Antramite. *Solar Energy Materials & Solar Cells*. Dec2016, Vol. 157, p943-952. 10p. DOI: [10.1016/j.solmat.2016.07.051](https://doi.org/10.1016/j.solmat.2016.07.051).

Hydration products in sulfoloaminate cements: Evaluation of amorphous phases by XRD/solid-state NMR. Gastaldi, D.; Paul, G.; Marchese, L.; Irico, S.; Boccolari, E.; Mukte, S.; Buzzi, L.; Canonico, F. *Cement & Concrete Research*. Dec2016, Vol. 90, p162-173. 12p. DOI: [10.1016/j.cemconres.2016.05.014](https://doi.org/10.1016/j.cemconres.2016.05.014).

Headspace thin-film microextraction onto graphene membranes for specific detection of methyl(cyclopentadienyl)-tricarbonyl manganese in water samples by total reflection X-ray fluorescence. Romero, V.; Costas-Mora, I.; Lavilla, I.; Bendicho, C. *Spectrochimica Acta Part B*. Dec2016, Vol. 126, p65-70. 6p. DOI: [10.1016/j.sab.2016.10.011](https://doi.org/10.1016/j.sab.2016.10.011).