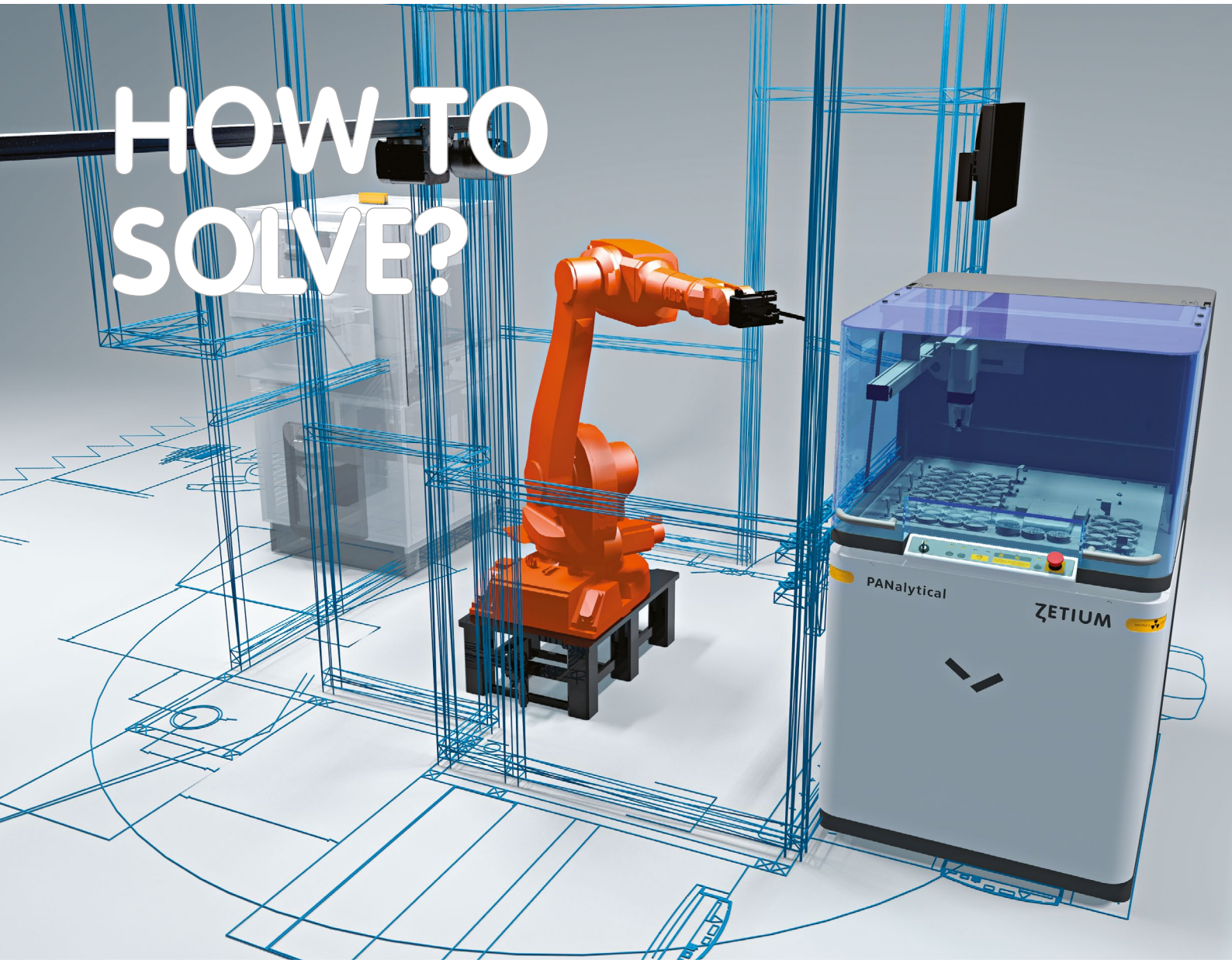
ISSUE 2/2016



# X'PRESS




PANalytical
get insight

# A gallery of **solutions**

Pieter de Groot
*Corporate marketing director*

'How to solve' is the theme of this issue of X'Press and a challenge many of us have to deal with at some time. Whether you are active in any industry or in research & development – you will be confronted with demands for more efficiency, better cost-effectiveness and faster return of better and more precise results, to name just a few of the most urgent requirements.

In our interview, PANalytical's Mark Pals describes his group's strategy when being faced with our industrial customers' requests to solve their analytical problems. They have to deal with the above-mentioned demands on a daily basis. The solution can be small and based on software or a large automated installation (as for Yara, Finland), and of course everything in between these two extremes. Mark and his group have the ambition of never giving up before the perfect tailor-made solution has been found.

This is equally true for scientists in any research lab. Irene Margiolaki and her team at the University of the Patras (Greece) are investigating protein structures and have now been able to solve them from powder X-ray diffraction data. This has become possible by employing modern X-ray detectors and optics with their superb performance. These detectors also enable researchers to study the behavior of their samples *in situ*: variable temperature, humidity and pressure can be applied. Phase transitions, caused by these changing conditions, result in a change of the diffraction patterns and can easily be recorded by the fast new detectors.

It was exactly this kind of experiments Ms. Arianna Lanza from the University of Bern (Switzerland) used for her investigation of a highly flexible metal-organic framework (MOF). A jury of five leading scientists chose her article describing the research and its convincing and original results as the winning entry of the PANalytical Award 2015. Arianna investigated how a metal-organic framework reversibly interacts with guest molecules when variable pressure or temperature are applied to the crystals. You can read more in our article on page 10.

I hope our examples of solutions for various challenges can inspire your work. I wish you a productive and creative summer.

With kind regards,

Pieter de Groot

LATEST NEWS

## LeDoser™ – Scale up your analytical precision

Claisses's new automatic weigher, LeDoser™, is specifically designed to weigh and dispense borate flux with high precision. Three different weighing modes ensure a seamless integration in laboratory standard operation procedures, the instrument is LIMS-ready and data transfer is simple and straightforward. A tank stirrer option makes sure that LeDoser's performance is constant for both high and low throughput.

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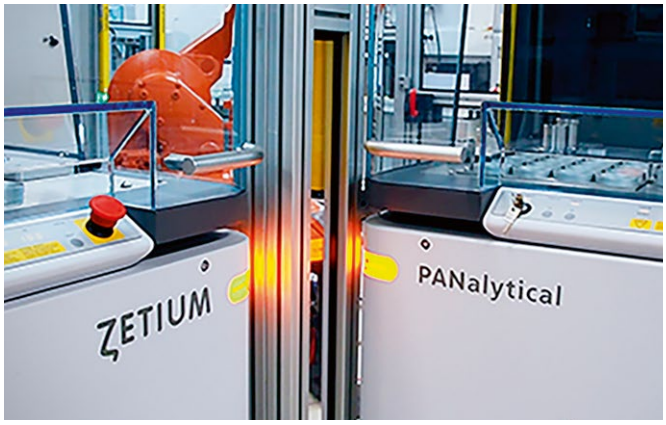
**LeDoser™**
- Quick return on investment
- Low cost of ownership
- Easy to use

www.panalytical.com/news/ledoser

# In this issue




**4** A tailor-made solution for Yara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*Yara's mine in Siilinjärvi (Finland) is the only apatite mine in Western Europe and ca. 3 km long, 1 km wide and with a deepest point of 240 m.*

# A tailor-made solution for Yara

**Yara's Siilinjärvi mine has been in continuous operation since 1979. The carbonatite deposit is mined in two large open pits and is subsequently processed on-site to extract apatite from the host rock with tailings stored in a tailings pond. Yara is continuously investing in guaranteeing that their operations are safe, reliable and profitable at the same time. When they noticed that production recovery and quality of the apatite concentrate were sometimes below their target values, they consulted PANalytical for a possible solution of these problems.**

The desired solution should cover a few aspects at the same time. The mine is not very homogeneous and therefore it is important to receive accurate feedback on the mined material. In this way inefficient mining of less useful rock can be avoided. Additionally Yara wants to precisely control their beneficiation process of apatite to achieve an increased recovery rate and enhance their product quality. This can be realized by frequent analyses of the concentrates and tailings, delivering fast results. The methods of choice are X-ray diffraction (XRD) and X-ray fluorescence (XRF), which can be automated and deliver quantitative elemental and qualitative mineralogical information in a relatively short time.

Together with Yara, PANalytical developed a unique automated installation, which is now taking care of Yara's demands. Incoming samples from 5 control points in the production process are split into several portions for XRD, XRF, LOI (loss on ignition) and combustion analyses. Robots take care of the sample transport between various sample preparation stations (such as a mill, press and bead maker) and the analytical instruments. In this way laboratory technicians can concentrate on other tasks as well.

**"With this customized automation, feedback time is now approximately half of that in the past. This allows us to make informed decisions about our mining and production processes much faster, resulting in a more efficient process control."**

*- Pauli Moilanen, Chemist, Project Manager XR-automation at Yara's Siilinjärvi site*

Samples are mostly delivered in continuous batches and processed automatically 24 hours per day excluding 2-3 hours maintenance break. If necessary, however, high-priority samples can always be inserted manually and are analyzed as soon as a station has been freed. The analysis time is one hour and 15 minutes excluding LOI; with LOI the typical analysis time is one hour and 50 minutes, including the sample taking.

In this completely automated solution the analyses are performed by PANalytical's HighScore (XRD) and SuperQ (XRF) software packages; SamTracs takes care of the automated process and seamlessly communicates all results to Yara's LIMS (laboratory information management system).

**Knowledge grows**

Yara is the world's largest producer of ammonia, nitrates and fertilizers with 12,000 employees working in 51 countries worldwide. Their fertilizers, crop nutrition programs and technologies increase yields, improve product quality and reduce the environmental impact of agricultural practices.

The Siilinjärvi site in Finland employs 400 people and produces mainly fertilizers and phosphoric acid, but also other industrial chemicals. It consists of a mine, two sulfuric acid plants, one phosphoric acid plant, one nitric acid plant and one NPK-fertilizer plant. The mine is the only apatite mine in Western Europe, and it's main product is apatite concentrate.

**Fertilizers** are natural or synthetic materials applied to plants in order to enhance their growth. They contain precisely formulated targeted nutrition to suit each specific situation. Besides a number of micronutrients such as copper, iron or manganese they typically contain the three macronutrients nitrogen, phosphorus and potassium in varying proportions (NPK-fertilizers).

85% of the world phosphate utilization goes into the production of fertilizers. With the continuous growth of the world population the demand for nutrients and subsequently for phosphates is still increasing. The main source for phosphates is apatite, a group of phosphate minerals.

# Together towards the optimal solution

**This new issue of X'Press deals with the question 'How to solve'. Solving means 'effectively dealing with a problem' and dealing with very complex problems is one of the major tasks of PANalytical's Priority Lane department. X'Press asked Mark Pals, manager of this versatile project automation group, to describe his strategies for solving the very diverse customers' requests.**

***Mark, the Priority Lane department is dealing with many different requests. What are the extremes you handled in the past?***
We have been asked to do very small automations, like for instance special software that facilitates announcing samples to a spectrometer. Also we frequently deliver software pieces called 'protocol converters' that let the PANalytical spectrometer software talk a different protocol to the outside world. This comes in handy when you want to replace an existing non-PANalytical spectrometer in an existing automation with a PANalytical one, without disturbing the automation itself. For example after the installation of your new Zetium instrument, your automation will continue to work like before without any changes to your automated installation.

On the other end of the scale, we have had request for, and later executed, big automation projects for steel factories, where we not only provided the complete automated laboratory, but also the complete 300 m² laboratory building, the amenities and the air tube lines to the factory. We always jokingly say that the project in question was so complete, it even included the necessary coffee machine.

**"We try to be a real sparring partner for the customer, to get the most out of a project."**

*- Mark A. Pals, manager Priority Lane group at PANalytical*

***Can you give a few examples?***
There are so many to choose from. We have done projects for all important metals companies, like ThyssenKrupp, ArcelorMittal, TATA Steel, Salzgitter, Aperam, Otto Fuchs, LDM and so on, and we are also known in the mining world. We have recently delivered a very extensive laboratory for Yara mining in Finland, which is described in this X'Press on pages 4 and 5.

People have come to know that we have the ability to build just the laboratory that the customer needs, and that we never walk away from a problem. One of the most important values that we live by is 'Do as you promise', which in case of automation is very important. These automations tend to get complex when they are bigger than a single line, and then attention to details, and completing the tasks at hand is key.

***Your examples are all located in Europe. Is there no demand for automation in other regions?***
Of course the ever increasing demand for automation is not only to be found around Europe. As we started our automation activities in the European regions more than twenty years ago, it is natural that our presence in Europe is the biggest chunk of our installed base, but we also have a good number of installations in the USA.

Asia was always a bit too far for us, but as our competences have grown significantly over the last years, we are active now in expanding into the Asian Pacific region. We are actively supporting the worldwide sales teams with information that they need to start discussions with possible automation customers. When they find these prospective customers, the consultative work begins.

We are not very well known for automation in Asia yet, but we expect that this will soon change. People already know PANalytical is a dependable partner for spectrometry, and they will find out that we are quite good at building customized automated solutions as well.

***What is the approach you usually take when your group receives a new inquiry?***
We follow a consultative concept. This means that when we get an inquiry, usually via our sales organization, we try to visit the prospective customer to find out their needs. Some customers have a very clear view of their requirements, but others need some more help.

In any case we try to do something that we call the 'Ping-Pong-game' internally: When defining the scope and the specifications for a project, PANalytical and the customer need to get into a discussion that goes back and forth, revision by revision, in which we define the specifications and designs together. This back-and-forth is necessary because normally, even when the customer has a very clear view of the requirements, our expertise can add to or change the items in scope to improve the overall setup of the automation.

It is a joint search for the optimal, cost-effective way to automate a laboratory. For the smaller projects this normally takes between three and five iterations, but we have been known to get up to fifteen iterations for the really big and complex laboratories. In short, we try to be a real sparring partner for the customer, to get the most out of a project.

***How would you describe your strategy and what is special about it?***
Our strategy for all we do revolves around modularity. We strive to make our software, instruments and auxiliaries to be as modular as possible. This makes it easy to extend existing automations over time, which makes the investment into the laboratory automation more worthwhile and future-proof than with closed non-modular systems.

When designing a new laboratory with the client, we always ask: "what is the next step after this one?" and then we try to fit that into our design, for example by leaving some space for future instruments.

In software, modularity is also key: changes, swaps and additions to the system should always be possible, also in the far future. We have been known to do eleven subsequent upgrades in ten years for a certain customer, growing from a moderate to a very big automation over time. This is very good for keeping the value of the customers' assets high.

**Mark A. Pals** was born in Enschede and educated at the University of Twente and the Saxion Hogeschool in Mechanical Engineering, with a specialism in machine automation engineering.

His career started as sales support engineer for machine motion products and he subsequently became project leader for metal surface damage measurement systems for steel plants. After working as process improvement engineer at a cable factory, he became project leader for automation projects at PANalytical and has subsequently been leading this automation group since 2007.

This automation group with the not-so-ordinary name 'Priority Lane' is specialized in designing and building fully automated laboratories for production control in metals, mining and other production environments.

**Get an impression of our automated solutions in the new movie on www.panalytical.com/automation**

*Members of the Laboratory of Structural Biology at UPAT (left to right): Stefanos Saslis (BSc), Magda Christopoulou (MSc), Souzana Logotheti (BSc), Stavroula Fili (MSc), Fotini Karavassili (PhD), Irene Margiolaki (group leader), Eleftheria Rosmaraki (lecturer, Department of Biology, UPAT), Alexandros Valmas (PhD), Maria Spiliopoulou (BSc), Paraskevi Kontou (BSc), Nikos Nikolopoulos (BSc), Katerina Pappa (BSc)*

# Smaller crystals, faster experiments, brighter beams

## Drug screening & innovation via XRPD

**Knowledge of the 3D structures of proteins is a key element for understanding functions and mechanisms necessary for the conception of drugs. Drugs can be proteins, as insulin, or small molecules that interact with biological targets. To date, more than 100 proteins are approved for clinical use in the European Union and the USA. The need for a large number of experimental structural data is common in all drug-related projects and demands continuous improvement of methods for determination of protein structures.**

Until now, the majority of protein structures are determined by X-ray diffraction on single crystals with typical sizes > 5-10 μm at micro-focus synchrotron beam lines. Despite significant progress there are still limitations of the research on single crystals. Difficulties in protein crystallization are the major bottleneck for single crystal diffraction. Polymorph screening – critical for drug innovation – is not possible and last but not least single crystal diffraction is not ideal for time-resolved studies (dynamics).

Already in 1999 the power of X-ray powder diffraction (XRPD) for revealing protein structures was demonstrated for hen egg white lysozyme by Bob Von Dreele. Since 2003, Irene Margiolaki and her colleagues at the ESRF and later at UPAT, have proved that protein structures can also be obtained from sub-micron crystals with typical sizes > 0.1 μm via X-ray powder diffraction using synchrotron and laboratory sources [i,ii]. This approach provides medium-resolution structural models (3-10 Å) and allows for the study of low-quality crystals; polymorph screening is a routine practice and time-resolved studies are also possible[iii,iv].

In addition, powder data reveal characteristics of the microcrystalline samples such as purity, sample homogeneity, highly accurate cell dimensions and lattice strains induced by sample preparation; critical parameters for the development of therapeutic formulations.

**"Our X'Pert PRO equipped with the fast PIXcel detector delivers extremely useful powder diffraction data from proteins which are employed not only for indexing but also structure refinements".**

*- Dr. Irene Margiolaki, head of the Structural Biology Laboratory, University of Patras (UPAT)*

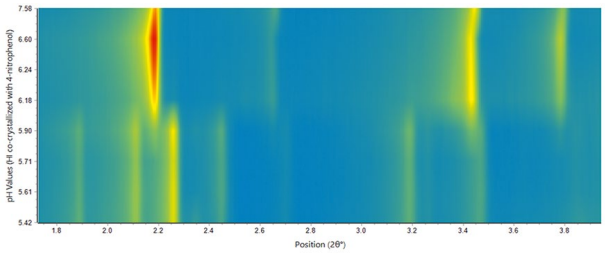
In 2013, the UPAT team installed a PANalytical X'Pert PRO diffractometer, which is routinely employed for structural studies of proteins. Data collection in the lab prior to synchrotron measurements is a major advance. The X'Pert PRO also allows for high-throughput crystal screening and optimization, polymorph identification and delivers high statistics due to the much slower radiation damage of the biological samples in the lab.

Currently, researchers at the structural biology lab at UPAT study human insulin (HI) complexes with phenol-based ligands at different crystallization conditions. They could for example show that phenol-based molecules bind on HI and affect both HI conformation and the crystal forms adopted; they revealed very high polymorphism upon variation of crystallization pH and type of ligand and disclosed 4 novel polymorphs with enhanced characteristics as potential drug targets[v,vi,vii].

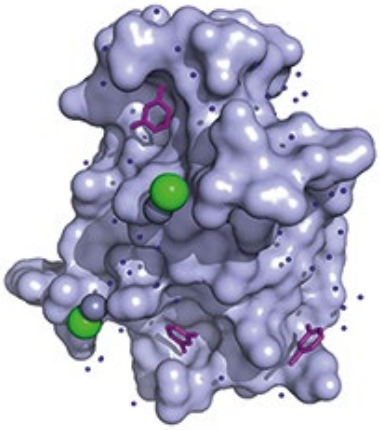
In collaboration with the R&D scientists at PANalytical, preliminary variable temperature and relative humidity studies indicated rapid phase transitions and previously unidentified polymorphs associated with distinct biological activity. Finally, combined data collected using laboratory and synchrotron instruments, allowed for the detailed structural characterization of several HI-ligand polymorphs determining not only the protein structure but also the ligand binding sites necessary for rational drug design[viii].

These studies manifest that powder diffraction is moving 'beyond demonstration experiments' and is ready to become a strategic technique for routine characterization of micro-crystalline proteins.

Laboratory data of human insulin 4-nitrophenol complex crystallized at different pHs. The data reveal a first-order phase transition at pH ~ 6 from monoclinic to hexagonal phase[vi].




Surface of an insulin dimer obtained from combined laboratory and synchrotron powder diffraction, illustrating how phenol-based ligand molecules (magenta) fit within deep cavities (binding sites). Grey and green show zinc and chloride anions involved in crystallization, while blue dots represent oxygen atoms belonging to water molecules[viii].



*References:*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[iii] *Margiolaki, I. et al. (2005). Acta Cryst., D61, 423-432*

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[v] *Karavassili, F. et al. (2012). Acta Cryst., D68, 1632–1641*

[vi] *Valmas, A. et al. (2015). Acta Cryst., D71, 819-828*

[vii] *Fili, S. et al. (2015). IUCrJ., 2, 534-544 (open access)*

[viii] *ESRFnews, Cover & article p. 18; Karavassili et al,* March 2015


**University of Patras (UPAT)**

Founded in 1964 UPAT includes 22 departments, which operate 112 labs and 14 clinics for about 25,000 students. The UPAT has a reputation for quality and innovative research and a number of its departments, laboratories and clinics have been designated as Centers of Excellence on the basis of international assessment.

ΠΑΝΕΠΙΣΤΗΜΙΟ ΠΑΤΡΩΝ
UNIVERSITY OF PATRAS

The Department of Biology at UPAT was established in 1967 and was the first biology department in the Greek university system. It includes the Laboratory of Structural Biology, headed by Irene Margiolaki and is well equipped with advanced instrumentation for protein expression, purification, crystallization and X-ray diffraction studies.

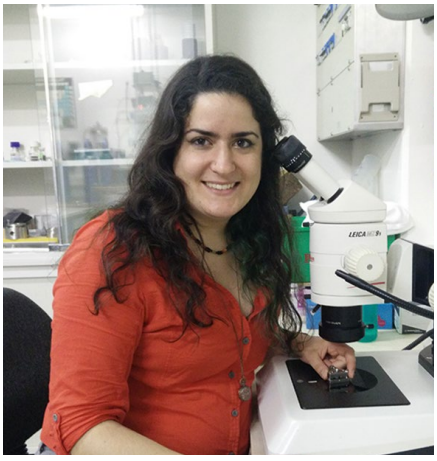
# **Arianna Lanza**, winner of the 4th PANalytical Award

**The PANalytical Award, founded in 2012, aims at supporting excellent young scientists at the beginning of their career. They are invited to submit a scientific paper describing outstanding work that used laboratory-scale X-ray equipment as the primary analytical technique. Ms. Arianna Lanza has recently been selected as winner of the 4th PANalytical Award. She is currently working on her PhD at the University of Bern, Switzerland.**

Ms. Lanza's article: 'Solid-state Reversible Nucleophilic Addition in a Highly Flexible MOF' (published in the Journal of the American Chemical Society in September 2015) was highly rated by all of the six members of the jury. They were impressed by the convincing and original results, which open the way to even more exciting possibilities in designing metal-organic frameworks. Ms. Lanza's high competence and confidence in X-ray analysis were explicitly mentioned by the jurors, all leading experts in their research fields.

For this 2015 edition of the PANalytical Award a record number of 95 articles was received. Many of these were of superior quality, which made the jury's task especially difficult. In the end the winner's proven scientific leadership was the crucial factor: Arianna Lanza has designed, initiated and carried out the project, as a part of her ongoing PhD work and is as such a worthy first author and winner of the award. X-ray diffraction experiments were performed at the Department of Chemistry and Biochemistry of the University of Bern (Switzerland) and at the Materials Science beam line of the Swiss Light Source at the Paul Scherrer Institute in Villigen, Switzerland.

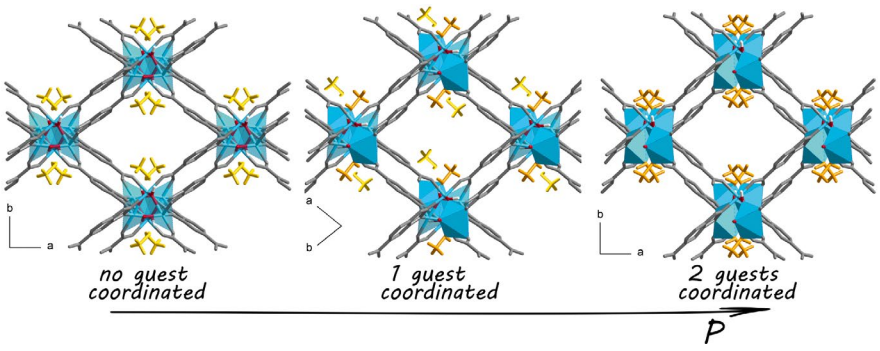
The award will be handed over to Arianna at this year's Meeting of the European Crystallographic Association (ECM 30) in Basel at the end of August where she will present her work to the scientific community.



In her **winning article** Arianna Lanza describes in detail a flexible and porous metal-organic framework, based on $Co^{II}$ connectors with benzotriazolide-5-carboxylato linkers and its selective reaction with guest molecules.

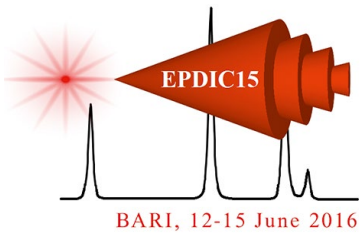
X-ray diffraction at various pressures and temperatures clearly revealed changes in the framework and in the host-guest interactions.

The investigated system is an extraordinary example of temperature- or pressure-induced chemisorption with enormous implications for catalysis, storage or selective sieving.




*The coordination number of $Co^{II}$ (blue polyhedra) increases after pressure-induced coordination of additional ligands (in yellow).*

# Winner of **the EPDIC Award** for Young Scientists




**Dr. Kirsten Marie Ørnsbjerg Jensen from University of Copenhagen (Denmark) is the winner of this year's EPDIC Award for Young Scientists. This award is assigned at each European Powder Diffraction Conference and honors outstanding scientific achievements by young scientists in the field of powder diffraction. The award has a value of € 1000 and is sponsored by PANalytical. It was presented to Dr. Jensen at the opening ceremony of EPDIC in Bari (Italy) on 12 June 2016.**

Kirsten obtained her PhD from Aarhus University (Denmark) where she worked in Prof. Bo B. Iversen's group in the Center for Materials Crystallography on understanding the mechanisms that take place when inorganic materials form in solution. She did postdoctoral work at Columbia University (USA), working with new methods in nanostructure characterization using X-ray total scattering.

Kirsten Jensen is currently an assistant professor in the Department of Chemistry at University of Copenhagen (Denmark) where she does research in materials chemistry, using X-ray and neutron scattering to study the structures of nanoscale materials.



**The PANalytical Award 2016**

This year the PANalytical Award celebrates its 5th anniversary. Young scientists who have never held a professorship are invited to submit their scientific articles about groundbreaking research that required the use of a laboratory X-ray diffraction, X-ray fluorescence or X-ray scattering instrument as the primary analytical technique. There are no restrictions on the manufacturer of the equipment used for the published research. The award consists of a € 5,000 cash price and trophy and a certificate.

The deadline for submissions via www.panalytical.com/award is 1 December 2016.

# Determination of **postmortem interval** on human cortical bone

**One of the more difficult aspects of forensic anthropology is to medically and legally estimate a postmortem interval (PMI) of human skeletal remains (i.e. a determination of how long an individual has been deceased). PMI estimation becomes increasingly difficult as time of death becomes more remote, and it is therefore of immediate importance to determine whether remains are forensically significant or of non-significant origin (i.e. historical, archeological). ASD's Goetz Instrument Support Program participant John Servello of the University of North Texas (US) has investigated whether near-infrared (NIR) spectroscopy could be useful for reliable PMI estimation.**

Long-term decomposition-related changes in bone ranging over decades to millennia (due to erosion, infiltration of soil matrix and water, the addition of soil fungi and bacteria, etc.) ultimately lead to the breakdown of collagen and the replacement of normal bone content with new mineral.

It is predicted that the loss of bone organic phase over the extended PMI will manifest spectrally. John Servello, of the University of North Texas, used an ASD LabSpec® 4 benchtop analyzer to determine if NIR spectroscopy could be used to assess and assign a PMI range for human skeletal remains.

The technique of NIR analysis is appealing for examining cortical bone because the shorter wavelength light can penetrate the sample to greater depths than other vibrational techniques, allowing for interaction with the sample constituents. Additionally, NIR analysis requires minimal to no sample preparation, allows for rapid data collection, and is simple to use with minimal prior training whereas the present qualitative and quantitative tests for a determination of the PMI are time-consuming, the methods are destructive, and they require expensive, highly specialized equipment.

Using the 1350-2100 nm band for NIR analysis of femoral bone samples, John's research showed that historic and archaeological materials formed a well-defined and separated cluster, while forensically significant samples formed a broad and overlapping cluster with some suggested gradation with respect to time.

Ultimately, the goal of this research is the development of a robust, quantitative technique that can be used to assess and assign a PMI range for human skeletal remains.

*Setup for data collection using the ASD LabSpec® 4 benchtop analyzer with a bifurcated fiber optic reflectance probe*

Experimental details are described in the complete article on http://discover.asdi.com/Postmortem-Interval

*Collecting spectra directly from a sectioned femoral diaphysis. Diffusion of light through the cortex is clearly visible. The PMI for this sample was short (<6 months).*

# A **jubilant year** for XRD


**As already mentioned in our previous edition of X'Press, 2016 is a special year for X-ray diffraction (XRD): it was 100 years ago that Peter Debye introduced powder diffraction and it was 50 years ago that Hugo Rietveld introduced his method to refine crystal structures from these powder diffraction patterns. In order to honor these achievements of two pioneering Dutch scientists, the Dutch Crystallographic Society together with the University of Delft (the Netherlands) will organize an international scientific symposium.**

The symposium titled '2016: Debye & Rietveld – A 100 & 50 year celebration' will take place on Thursday 22 September at the Shell Technology Centre Amsterdam. Guest of Honor at the symposium will be Hugo Rietveld. A variety of European speakers will address the history of X-ray diffraction methods, the state-of-the-art in powder diffraction and the latest developments in the field. Scientists and students can present their work during poster sessions.

The Debye-Rietveld Scientific Symposium aims to be a worthy celebration of the anniversaries of two major events that have made X-ray diffraction a standard technique for scientists around the world.
More information about the program and registration can be found on https://debye-rietveld.nl

# **Get familiar** with X-ray diffraction solutions

**On 4 October 2016 the University of Twente (Enschede, the Netherlands) will host this year's PANalytical XRD User Day, a special event for our European users.**

Participants and PANalytical specialists will share the latest applications and advancements in X-ray diffraction, from powder and thin film analysis to small-angle X-ray scattering (SAXS). In the afternoon the PANalytical headquarters open their doors for a guided tour – see for yourself how our instruments are built, tested and serviced for you!
www.panalytical.com/xrd-user-day

**If you want to know even more about XRD solutions you are welcome to continue your stay at the University of Twente and follow an X-ray Metrology Workshop (XRM) on 5 and 6 October.**

The program will concentrate on the application of X-ray scattering techniques for research on soft condensed matter. Powder diffraction and pair distribution function analyses will be discussed in detail as well as thin film analysis by means of X-rays.

Five invited scientific lectures will be accompanied by oral and poster contributions from the participants. The workshop will be concluded by interactive sessions where participants can present and discuss their own analytical problems.
www.panalytical.com/xrm-workshop

# Get ready for **unrivalled analytical performance** with our new option for TheOx® fusion instrument

**Do you want to increase the durability of your fusion instrument? Claisses's TheOx can now be configured with a carriage made from very high-quality ceramic, ensuring the sturdiness of the parts even at high temperatures.**

These total ceramics cantilevers can easily be installed as an update kit directly on TheOx instrument – the perfect solution to extend the instrument's life at a lower cost. For TheOx Advanced users, the option can be built in at the time of purchase.

The resistant ceramic material allows fusion at higher temperatures without prematurely damaging the parts involved, thus leading to a greater return on investment. The option is also perfect if you need to analyze samples containing very low metal concentrations (<0.5%).

At Claisse, our priority is to remain at the forefront of spectrometry analysis and we aim at developing the most efficient sample preparation options for you. Please do not hesitate to contact the product manager Chantal Audet, or your local sales representative for more information.

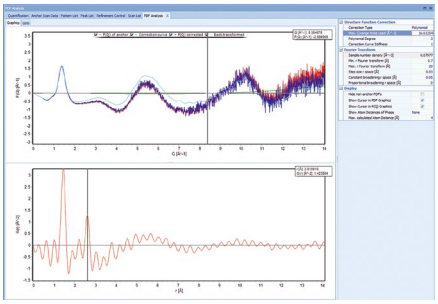

# Solve your **powder diffraction challenges** with HighScore version 4.5

**The HighScore suite is PANalytical's comprehensive powder diffraction software for phase identification, Rietveld, crystallographic and cluster analysis. Version 4.5 of this proven software package has been launched earlier this year. HighScore customers with internet connection have automatically been informed of this update, which runs under all 4.x licenses.**

The new version does not only contain a number of bug fixes but also offers several new features.

Not only has user-friendliness been improved together with the graphical representation but large data sets are now fitted much faster. A unique way of instant search-match suggests candidates just by pointing at any data point.

HighScore now offers ExtSym, the best space group determination algorithm on the market. And last but not least users can now get insight into disorder and local structure by pair distribution function (PDF) calculations from observed XRD scans.



*New: PDF calculations from capillary data in HighScore v. 4.5*

**Check out HSvu, the world's first X-ray powder diffraction app, now supporting the latest document format of HighScore version 4.5.**

**HSvu**

- displays all kinds of X-ray diffraction scans in various formats.
- shows and reports details from an XRD analysis by HighScore.
- opens scans or diffraction analyses from your e-mail account.
- lets you share powder diffraction data with friends by dropbox, facebook or e-mail.

HSvu
PANalytical
Download on the App Store

# Events calendar 2016

**The list shows a selection of events during the next few months where you will find us. Please come by and visit us when you attend any of these events.**

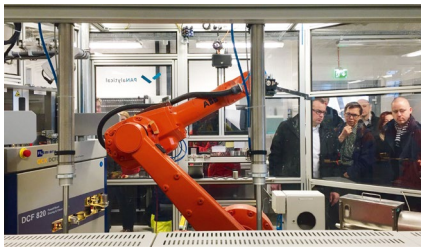
| | | |
|---|---|---|
| 1 – 5 August | Denver X-ray Conference and Exhibit | Rosemont, IL, USA |
| 14 – 19 August | IMRC2016 | Cancun, Mexico |
| 27 August – 4 September | 35th International Geological Congress | Capetown, South Africa |
| 28 August – 1 September | ECM-30 | Basel, Switzerland |
| 21 – 22 September | Food Technology Summit 2016 | Mexico City, Mexico |
| 26 – 28 September | MINExpo | Las Vegas, NV, USA |
| 2 – 7 October | International Workshop on Nitride Semiconductors 2016 | Orlando, FL, USA |
| 3 – 6 October | ICSOBA 2016 | Quebec, Canada |

www.panalytical.com/events

# Automation days hosted by Yara, Finland

**In April this year Yara's Siilinjärvi phosphate mine and processing plant in the middle of Finland (see page 4) hosted the Automation Days. The two-day seminar mainly addressed decision makers from the metals and mining industry and presented PANalytical's automation solutions for those two industry segments.**

During several side meetings some of the participants' analytical challenges could be discussed. One of the highlights of the event was the visit to Yara's new PANalytical X-ray automation. Participants could see the automated laboratory in action and were impressed by the complexity and the possibilities of this installation, which supplies Yara with fast feedback from the mining and production processes.




## Colophon

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