

ENERGY IS OUR MATTER



## „MATERIALS METROLOGY“

Joint HZB-PTB Satellite Workshop to the User Meeting 2019:  
The 1<sup>st</sup> in the BESSY III Foresight Workshop Series

December 3<sup>rd</sup> to 4<sup>th</sup>, 2019, lunch-to-lunch, Berlin-Adlershof (Lecture hall of BESSY II)

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Tuesday, December 3 <sup>rd</sup>			
Registration and Lunch-Snack			12:00-12:45
Welcome	Jan Lüning	Helmholtz-Zentrum Berlin für Materialien und Energie (HZB)	12:45-12:55
Opening	Emil List-Kratochvil	Humboldt-Universität zu Berlin (HUB) and HZB	12:55-13:10
<b>Overview Talks: The need for Materials Metrology</b> (Chair: Emil List-Kratochvil, HUB and HZB)			
Standard operation procedures in heterogeneous catalysis research	Annette Trunschke	Fritz-Haber-Institut der Max-Planck-Gesellschaft	13:10-13:40
Materials Metrology with Synchrotron Radiation	Mathias Richter	Physikalisch-Technische Bundesanstalt (PTB)	13:40-14:10
Political guidance and targets (HGF, BMBF, EU)	Paul Harten	HZB	14:10-14:40
<b>General Discussion</b>			14:40-14:50
Coffee Break			14:50-15:10
<b>Examples of actual activities I</b> (Chair: Michael Krumrey, PTB)			
One step forward, two steps back: About the challenges in hybrid X-ray metrology for nanostructured surfaces	Victor Soltwisch	PTB	15:10-15:35
Materials science for grand challenges: What can synchrotron research do for us?	Franziska Emmerling	Bundesanstalt für Materialforschung und -prüfung	15:35-16:00
Photoemission tomography: a quantitative tool for investigating molecular films	Michael Ramsey	Karl-Franzens-Universität Graz	16:00-16:25
X-ray spectrometry for advanced energy materials	Burkhard Beckhoff	PTB	16:25-16:50
<b>Discussion and Short Coffee Break</b>			16:50-17:10
<b>Overview Talks: Benefit for the Users and Requirements</b> (Chair: Antje Vollmer, HZB)			
Benefit for Users of Large Research Infrastructures	Astrid Schneidewind	Komitee für Forschung mit Neutronen (KFN)	17:10-17:40
Technical Requirements and involvement of AI	Jens Viefhaus	HZB	17:40-18:10
<b>General Discussion</b>			18:10-18:20
<b>Poster Session with Snacks</b>			18:20

Wednesday, December 4 <sup>th</sup>			
<b>Overview Talk: FAIR Data Infrastructure</b> (Chair: Antje Vollmer, HZB)			
FAIRmat – a FAIR data infrastructure for materials science and related research fields	Christoph Koch	HUB	9:00-9:35
<b>Examples of actual activities II</b> (Chair: Frank Scholze, PTB)			
VUV ellipsometry with synchrotron radiation: Instrumentation characteristics, optical component development and applications in material science	Norbert Esser	Leibniz-Institut für Analytische Wissenschaften - ISAS	9:35-10:00
Small-angle X-ray scattering for the characterization of Nanoparticles in medical applications	Zoltan Varga	Research Centre for Natural Sciences Budapest	10:00-10:25
Coffee Break			10:25-10:45
<b>Panel Discussion: Metadata</b> (Chair: Jan Lüning, HZB)			
Helmholtz Metadata Collaboration	Sünje Dallmeier-Tiessen	Helmholtz-Gemeinschaft deutscher Forschungszentren	10:45-12:15
Overview (EU activities)	Mirjam van Daalen	Paul Scherrer Institute (PSI)	
ExPaNDS	Alun Ashton	PSI	
DAPHNE	Astrid Schneidewind	KFN	
Implementation at BESSY II	Heike Görzig	HZB	
<b>Summary and Closing Remarks</b>			12:15-12:30
Lunch			12:30

## “Materials Metrology”

Joint HZB-PTB Satellite Workshop to the User Meeting 2019:  
 The 1st in the BESSY III Foresight Workshop Series  
 3-4.12.2019 lunch-to-lunch, Lecture hall BESSY II  
 Albert-Einstein-Str. 15, 12489, Berlin

## **Abstracts of “The need for Materials Metrology” session**

Tuesday, December 3<sup>rd</sup>

## **Materials Metrology with Synchrotron Radiation**

Mathias Richter

Physikalisch-Technische Bundesanstalt (PTB), 10587 Berlin, Germany

For more than 35 years, PTB has been using synchrotron radiation for metrology. Currently, the electron storage ring BESSY II in the X-ray range and PTB's own Metrology Light Source (MLS) for lower photon energies are used for this purpose. The work is based on radiometry with storage rings and cryogenic radiometers as primary standards. Detectors, radiation sources and optical components are characterized and calibrated within the scope of services. On this basis, however, the main tasks today lie in two areas of funded research: (a) optical technology for research and industry and (b) quantitative materials research in cooperation with external partners. The requirements for the combination of materials research and metrology are discussed in the present contribution and its possible impact on fundamental science and cutting-edge technologies as well.

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## Political guidance and targets (HGF, BMBF, EU)

Paul Harten<sup>1</sup>, Martin Hoffmann<sup>1</sup>, Nicolas Villacota<sup>2</sup>

1 Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

2 Hermann von Helmholtz-Gemeinschaft Deutscher Forschungszentren e.V., Berlin, Germany

We analyse research programs and strategies starting on the European scale, then looking at the national German federal government level into the realm of the Federal Ministry of Education and Research, and finally visiting the implementation of these programs and strategies within the Helmholtz Association of German Research Centres.

We are looking at recent and future versions of research agendas and strategies with the aim of identifying starting and connecting points as well as boundary conditions for future research in materials metrology.

Strategic Research Agenda for Metrology in Europe, EURAMET, 2016

Measurement research - European Partnership on metrology

(Horizon Europe programme), EC 2019

Research and innovation that benefit the people, The High-Tech Strategy 2025, BMBF 2018

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## **Abstracts of “Examples of actual activities I” session**

Tuesday, December 3<sup>rd</sup>

## One step forward, two steps back: About the challenges in hybrid X-ray metrology for nanostructured surfaces

Victor Soltwisch<sup>1</sup>, Anna Andrlé<sup>1</sup>, Burkhardt Beckhoff<sup>1</sup>, Nando Farchmin<sup>1</sup>, Analía Fernández Herrero<sup>1</sup>, Philipp Hönicke<sup>1</sup>, Yves Kayser<sup>1</sup>, Konstantin Nikolaev<sup>1</sup>, Mika Pflüger<sup>1</sup>, Jürgen Probst<sup>2</sup>, Qais Saadeh<sup>1</sup>, Thomas Siefke<sup>3</sup>, Dieter Skroblin<sup>1</sup>, Frank Scholze<sup>1</sup>

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3 Universität Jena, Jena, Germany

The development of methods for characterizing nanostructures with X-rays has made significant progress in the last decade, but still falls behind the requirements of industry in many aspects. Scattering under grazing incidence angles (GISAXS) allows to extract a very detailed reconstruction of the dimensional shape of the structure. At the same time, the X-ray standing wave fields generated in the grazing incidence geometry can be used to spatially resolve the nanostructures using their fluorescence emission with sensitivity for the elemental composition. A combination (hybridization) of both methods is obvious as they are also theoretically linked to a near and far field simulation of the same model. The metrological challenge lies in the exact theoretical simulation of the entire experimental chain in order to achieve quantitative results.

Uncertainty determination in X-ray experiments can best be validated with modern statistical methods. However, these statistical methods require an enormous numerical effort which can quickly explode with increasing demands on the simulation of the full experiment and increasing complexity of the investigated structures. New ways have to be found to balance the need for accurate (rigorous) simulations and fast reconstructions, through approximation methods.

Phys. Rev. B 94, (2016)

J. Appl. Cryst. 50, (2017)

Nanoscale 13, (2018)

Optics Express 27, (2019)

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**Materials science for grand challenges:  
What can synchrotron research do for us?**

Franziska Emmerling, Ana de Oliveira Guilherme Buzanich, Martin Radtke,  
Uwe Reinholz, Adam Michalchuk

Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

The modern world is one of materials. From everyday electronics to pharmaceuticals, energy production, and energy storage, we are in constant contact with materials in one form or another. In order to make use of these materials, and design more advanced materials, a thorough understanding of the design, synthesis, and function are needed. Moreover, an understanding of the material is required over wide ranges of scale, from their structure at the atomistic scale through to the macroscopic structure and properties of buildings.

The need to develop and apply advanced analytical technologies and processing strategies are critical for driving the study and design of new materials. BAM is actively pushing the boundaries of modern materials science across the areas of design, manufacture, and testing. We routinely apply and develop state-of-the-art materials characterization methods at both laboratory and synchrotron sources. This allows extensive investigation of materials across all scales.

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## Photoemission Tomography: a quantitative tool for investigating molecular films

Michael G. Ramsey

Physics Institute, University of Graz, Graz, Austria

The frontier orbitals of molecules are the prime determinants of their chemical, optical, and electronic properties. Arguably, the most direct method of addressing the (filled) frontier orbitals is ultra-violet photoemission spectroscopy (UPS). Although UPS is a mature technique from the early 1970s on, the angular distribution of the photoemitted electrons was thought to be too complex to be analyzed *quantitatively*. Recently angle-resolved UPS work on conjugated molecules, both in ordered thick films and chemisorbed monolayers, has shown that the angular (momentum) distribution of the photocurrent from orbital emissions can be simply understood when a plane wave final state is assumed. This approach, becoming known as orbital or photoemission tomography (PT), relates the emission distribution to the Fourier transform of the ground state orbitals [1]. Examples will be shown for using PT to reconstruct real space orbitals, determine molecular orientation, and quantifying the charge transfer to molecules on surfaces. These will introduce photoemission tomography and demonstrate its potential as a technique to determine both electronic and geometric structures not just complementary but also competitive to methods as diverse as scanning tunneling microscopy and near-edge X-ray absorption spectroscopy.

P. Puschnig and M.G. Ramsey, Encyclopedia of Interfacial Chemistry, 2018, 380

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## Characterization of energy conversion and storage materials by X-ray spectrometry

Burkhard Beckhoff, Philipp Hönicke, Yves Kayser, Florian Peinl, Christian Stadelhoff,  
Cornelia Streeck, Rainer Unterumsberger, André Wählich, Jan Weser, Claudia Zech

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The development of new energy materials and the assessment of nanomaterials require the correlation of the materials' functionality with their chemical and physical properties. To probe these properties, analytical methods that are both sensitive and selective at the nano- and microscales are required. The reliability of most analytical methods is based on the availability of reference materials or calibration samples, the spatial elemental composition of which is as similar as possible to the matrix of the specimens of interest. However, there is a drastic lack of reference materials in particular at the nanoscale. PTB addresses this challenge by means of a bottom-up X-ray analytical method where all instrumental and experimental parameters are determined with known contributions to the uncertainty of the analytical results. This first-principle based approach does not require any reference materials but a complete characterization of the analytical instruments' characteristics and, in addition, of the X-ray fundamental parameters related to the elements composing the sample. X-ray spectrometric methods allow for the variation of the analytical sensitivity, selectivity, and information depth needed to effectively reveal the spatial, elemental, and chemical specimen parameters of interest. Examples of interfacial speciation, elemental depth profiling, as well as layer composition and thickness characterizations in different energy materials will be given. Recent instrumental achievements provide access to the operando speciation of nanoscaled battery materials in order to reveal conversion, transportation and degradation processes.

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|--|---|
| [1] Anal. Chem. 79, 7873 (2007)          | [7] Phys. Rev. Lett. 113, 163001 (2014) |
| [2] Anal. Chem. 81, 1770 (2009)          | [8] Spectrochimica Acta B 94-95, 22     |
| [3] Nucl. Instrum. Methods B 268, 370    | (2014)                                  |
| (2010)                                   | [9] Anal. Chem. 87, 2685 (2015)         |
| [4] Anal. Chem. 83, 8623 (2011)          | [10] Anal. Chem. 87, 7705 (2015)        |
| [5] Anal. Chem. 85, 193 (2013)           | [11] Anal. Chem. 87, 10117 (2015)       |
| [6] Appl. Phys. Lett. 103, 113904 (2013) | [12] J. Phys. Chem. C 123, 15802 (2019) |

## **Abstracts of “Benefit for the Users and Requirements” session**

Tuesday, December 3<sup>rd</sup>

## Materials Metrology – Benefit for Users of Large Research Infrastructures

Astrid Schneidewind

Komitee Forschung mit Neutronen  
JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

Scattering experiments have been performed on large scale neutron and photon sources for several decades – to study the properties of a huge variety of materials, from fundamental research to industrial usage. The experimental methods were developed continuously, as well as data collection and processing. Facilities and users are experienced in handling and managing different formats and amounts of data, including large data volumes. But, data management and analysis are changing drastically now, and their use can influence the quality and efficiency of experiments significantly.

Up to now, users perform experiments at facilities, collect data and analyse it mainly at home. Some tools for analysis are widely used, partially maintained by sub-communities or facilities in different ways. Often the data are analysed by young scientists, data and scripts leave with them, as well as information about the samples, their history and details about the experiments. Therefore, the data and their analyses are not sustainable or re-usable, even if the raw data are stored at the facilities.

In our days, several developments provoke us to change procedures: The measurements become (extremely) fast, datasets are much larger in volume and multi-dimensional, analysis tools are more powerful but also challenging in use, development and maintenance. Advanced simulation allows for predicting experimental results, AI to compare the measured data immediately to simulations or to train a network for efficient experimental strategies. The request for data management along the FAIR principles – Findable, Accessible, Inter-operable, Re-usable [1] – changes the facilities' data policies and the ownership of the data, but opens the opportunity to re-think the use of measured data. Being able to store not only the data in catalogues, but also the sample information and history, the experimental metadata, the analysis including used software tools and versions will allow for using them later, deeper and for several demands. Agreed formats allow for combining data from different sources and techniques. Making data available for ML training will finally save experimental time.

The benefit for users is obvious and versatile – we need to invest creativity, communication and effort first.

[1] M. D. Wilkinson et al., The FAIR Guiding Principles for scientific data management and stewardship, *Sci Data* 3, 160018 (2016)  
*Nano Lett* 8, 11 (2008)

## Technical Requirements and Involvement of AI

Jens Viefhaus

Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

In my talk I will make general remarks to "Data Management and Analysis" (DMA) which is being formed as a new programme topic in the research field of matter within the framework of the programme-oriented funding of the Helmholtz-Centres (2021-2027). Specifically, I will address a proposed sub-topic of DMA called "Digital Experiment & Machine". Here it is planned that an AI-based optimization of the experimental infrastructure is combined with near-realtime-analysis of the experiments performed at the corresponding facilities.

Multiple simulation models describing different aspects of the infrastructure and data flow as well as simulations of the experiment will have to be combined. In this context I will describe our recent developments in the field of AI-based synchrotron radiation beamline optimization which may serve as the first step towards the ultimate goal of constructing a digital twin of the whole facility including the experiment.

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## **Abstract of the “FAIR Data Infrastructure” session**

Wednesday, December 4<sup>th</sup>

## **FAIRmat – a FAIR data infrastructure for materials science and related research fields**

Christoph Koch, Claudia Draxl

Humboldt-Universität zu Berlin, Berlin, Germany

Scientific data are a significant raw material of the 21<sup>st</sup> century. To exploit its value, a proper infrastructure that makes data FAIR – *Findable, Accessible, Interoperable, and Re-purposable* – is a must. For the wider field of the (chemical) physics of condensed matter and materials science, FAIRmat [1], a proposed consortium for the National Research Data Infrastructure (NFDI), sets out to make this happen. Such data infrastructure (DI) enables extensive data sharing and collaborations in data-driven sciences, including artificial intelligence and advances basic science and engineering, reaching out to industry and society. FAIRmat is built on extensive experience with the worldwide biggest database and infrastructure in computational materials science, the Novel Materials Discovery (NOMAD Laboratory [2]), and the association FAIR-DI e.V. [3], and represents numerous researchers from universities and key materials-science institutions in Germany and is also internationally well embedded.

In this talk, the goals of FAIRmat will be presented, which include the establishment of a FAIR digital research data infrastructure for data arising in the areas of synthesis and characterization of materials as well as computational approaches to understand materials properties. In order to create a federated FAIR data infrastructure for materials data it will be important to advance and develop metadata schemas and ontologies, enable efficient exchange of FAIR research data, provide easy accessibility of the data to scientists and engineers across different domains, and reach out to the materials-science and other communities providing advice, training, and user support.

[1] <https://fairdi.eu/fairmat>

[2] <https://nomad-coe.eu>

[3] <https://fairdi.eu/>

## **Abstracts of the “Examples of actual activities II” sessions**

Wednesday, December 4<sup>th</sup>

## VUV-Synchrotron Ellipsometry: Instrumentation and Application to Wide-Bandgap-Semiconductors

Norbert Esser<sup>1</sup>, Maciej Neumann<sup>1,\*</sup>, Rüdiger Goldhahn<sup>2</sup>, Alexander Gottwald<sup>3</sup>,  
Christoph Cobet<sup>4</sup>

- 1 Leibniz-Institut für Analytische Wissenschaften – ISAS e.V., Berlin, Germany
- 2 Institut für Experimentelle Physik, Otto-von-Guericke-Universität Magdeburg, Magdeburg, Germany
- 3 Physikalisch-Technische Bundesanstalt (PTB), Berlin, Germany
- 4 Linz School of Education, Johannes Kepler Universität Linz, Linz, Austria

Spectroscopic Ellipsometry in the VIS-UV spectral range is a standard optical technique to determine the complex refractive index  $n(\omega)$  or the dielectric function  $\epsilon(\omega)$  of materials, thin layers, surfaces or complex layer stacks. A unique ellipsometry setup operating with synchrotron radiation in the visible to vacuum-UV spectral range has been developed by ISAS and is operated in collaboration with the Physikalisch-Technische Bundesanstalt (PTB) at the Metrology Light Source (MLS) in Berlin. The synchrotron ellipsometer is based on a  $\theta / 2 \theta$  goniometer, sample stage (He-cooling, resistive heating) and polarizers, all hosted in UHV and connected to the beamline without any windows. The synchrotron ellipsometer thus allows precise operation in a very broad spectral range between 2eV and 40eV, with very high spectral resolution. The synchrotron ellipsometer setup will be introduced and optical components as well as beamline properties discussed.

In recent years, III-nitride and metal oxide wide band gap semiconductors have been studied in collaboration with external partner groups. Main scientific interest is the fundamental understanding of optical properties, like excitonic absorption at the fundamental band edge, interband transitions at higher energies and shallow core level excitations, respectively. Exemplarily, results of ZnO/MgZnO and GaN/AlGaIn will be presented.

M. D. Neumann, C. Cobet, H. Kaser, M. Kolbe, A. Gottwald, M. Richter, N. Esser,  
Review of Scientific Instruments **85** 5 (2014)

*A synchrotron-radiation-based variable angle ellipsometer for the visible to vacuum ultraviolet spectral range*

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## Small-angle X-ray scattering for the characterization of Nanoparticles in medical applications

Zoltán Varga

Research Centre for Natural Sciences, Budapest, Hungary

The application of nanoparticles (NPs) in medicine opened the continuously growing field of nanomedicine. The first approved nano-drug was Doxil® (Caelyx® in Europe), a PEGylated liposomal formulation of doxorubicin, which was followed by a few other products. Nowadays there are several hundred nanomedicine products that are either approved by the relevant health agencies or are under clinical trials. On the other hand, there is a translational gap between the experimental work devoted to the development of new nano-drug candidates and the clinical realization of their use, which is also reflected in the high number of studies dealing with nanomedicine and the number of approved products on the market. The main reason for this translational gap is that the current characterization techniques possess limitations and there is a need for standardization on this field.

Small-angle X-ray scattering (SAXS) is based on the elastic scattering of X-ray photons by the sample's electrons at low angles and it is a method of choice for the characterization of materials in the 1 nm to 300 nm size range. SAXS is capable of traceable size determination for sufficiently monodisperse NPs. This presentation will summarize the use of SAXS for various NPs used in medicine ranging from silica particles to drug delivery liposomes. Biological NPs such as extracellular vesicles (EVs) attracted significant attention in the recent years due to their roles in intercellular communication. However, the heterogeneous distribution of EVs makes it difficult to use SAXS for their characterization, this method can play an important role in the standardization of size and concentration measurement of EVs, which will be highlighted in the last part of my talk.

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## **Abstracts of “Metadata” Panel Discussion session**

Wednesday, December 4<sup>th</sup>

## Helmholtz Metadata Collaboration

Sünje Dallmeier-Tiessen<sup>1</sup>, Sören Lorenz<sup>2</sup>

1 Helmholtz Association, Berlin, Germany

2 GEOMAR Helmholtz Centre for Ocean Research, Kiel, Germany

Data are produced in huge quantities in the Helmholtz Association. This frequently involves unique data sets that take considerable time and effort to prepare. It is therefore very important that these data are processed in such a way that they can be used by researchers and all interested parties now and in the future. This involves carefully documenting research data and making them available, particularly through metadata.

In this context, metadata are essential standardized information about research data, which allow the latter to be found and interpreted, networked, and reused.

This is the Helmholtz Metadata Collaboration's (HMC) task: to promote the qualitative enrichment of research data by means of metadata – and implement this approach across the whole organization.

The platform pools the scientific expertise on metadata from the domains in special metadata hubs for the research fields. Association-wide services offer advice and provide infrastructure services for storing, reusing, and exchanging metadata. The work is always embedded in the national and international context.

HMC aims to keep the research data “alive”. The platform is intended to make it possible to access specific data even after many years, and to make the data available and usable to interested parties in various disciplines. By combining research data and metadata from different sources, researchers can work on new interdisciplinary research topics or validate models, for example. Research in the field of artificial intelligence is also reliant on excellent reference data sets.

Support in the implementation of scientific standards ensures that data providers attain greater visibility for the collection of data. On the one hand, services for the citation and re-use of data increase trust and international visibility; on the other hand, the high quality of research data (through their description via metadata) improves scientific reputation.

In order to establish discipline-specific and Association-wide services in a way that is both broad and at the same time tailor-made, the platform will comprise hubs in each research field as well as centralized services. The research fields introduce expertise, ideas, and demands from their own subject areas through the metadata hubs. Generically applicable processes, technical solutions, and training and consultancy services are centrally organized. These are made available Association-wide to all hubs and can be customized and utilized according to the specific subject.

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## **ExPaNDS and other European PaN activities leading towards FAIR data and the eventual benefits for data producers**

Alun W. Ashton

Paul Scherrer Institut (PSI), Switzerland

The ambition of the new European HORIZON2020 project ExPaNDS (EOSC Photon and Neutron Data Services) and similar initiatives, is to enrich the European Open Science Cloud (EOSC) with data management services and to coordinate activities to enable national Photon and Neutron (PaN) Research Infrastructure (RIs) to make the majority of their data 'open' following FAIR principles (Findable, Accessible, Interoperable, Reusable) and to harmonise their efforts to make their data catalogues and data analysis services accessible through the EOSC, thereby enabling them to be shared in a uniform way.

The burden of making data FAIR inevitably falls on data producers, but a close collaboration between science communities and facilities greatly reduces the workload and raises the potential benefits for every stage of the experiment and data lifecycle.

ExPaNDS: [www.expands.eu](http://www.expands.eu),

European Open Science Cloud Photon and Neutron Data Services

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## Research data management and metadata at HZB

Heike Görzig, Rolf Krahl

Helmholtz-Zentrum Berlin für Materialien und Energie, Berlin, Germany

In recent years efforts have been undertaken to facilitate sharing and reuse of research data. The HZB has been and is still involved in various projects concerning research data management in Photon and Neutron sciences as [1][2] and has organized two workshops [3][4].

In 2016 the HZB has agreed on a data policy [5] requiring open access to research data with an embargo time of five years. Since August 2018 the HZB has a data repository using the ICAT [6] as a data catalog for searching the data.

Currently there are three experimental stations connected to the ICAT and datasets can be found and retrieved via the portal offered by the ICAT. The files should be archived in the NeXus format [7] which is based on HDF5 [8]. The NeXus format is a standard which defines the file structure and the vocabulary for metadata in a file. In order to accomplish reusability of the created and archived datasets, its comprehensibility and traceability also after the projects runtime has to be achieved. Therefore, data and metadata from various sources have to be integrated into the NeXus file for archival.

Next steps are to continuously connect experimental stations to the ICAT. This involves converting the created research data to the standardized NeXus format, preparing search parameter for finding the datasets in the data catalog and transferring datasets to the ICAT.

Usability and integration into existing workflows are very important criteria when connecting an experimental station to the ICAT. Therefore, this process is carried out with a strong input and cooperation from the instrument scientist, but also input from users is very welcome. We are very interested that the different scientific communities define their standard in order to make their research data interoperable.

[1] <http://pan-data.eu/>; [2] <https://expands.eu/>; [3] [https://www.helmholtz-berlin.de/events/scientific-data-management/program\\_en.html](https://www.helmholtz-berlin.de/events/scientific-data-management/program_en.html);

[4] [https://www.helmholtz-berlin.de/events/datenmanagement/index\\_en.html](https://www.helmholtz-berlin.de/events/datenmanagement/index_en.html)

[5] <https://www.hz-b.de/datapolicy>; [6] <https://icatproject.org/>

[7] <https://www.nexusformat.org/>; [8] <https://www.hdfgroup.org/>

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## Participants of the Workshop

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① Dorint hotel

② Airporthotel

③ Wista centre

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This Lunch-to-Lunch Workshop is organized in cooperation with the Physikalisch-Technische Bundesanstalt (PTB), Germany's National Metrology Institute, and is a part of Foresight Workshops Series dedicated to the BESSY III project.



## HZB 2030: DER WEG ZU BESSY III

BESSY III is expected to be a globally competitive synchrotron radiation source in the field of XUV, soft and tender X-rays for research and industry and will be optimally tailored to the needs of HZB and strategic partners like PTB, MPG, BAM, Berlin Universities, guest researchers and external Users. In the BESSY III Foresight Workshops Series, HZB is establishing a discussion forum of future projects and research activities in strong interaction with current and new User groups.

The main goal of the 1<sup>st</sup> workshop in this series is to underline the significance of Materials Metrology nowadays, to point attention to a special importance of standardized, validated, and authenticated measurements, to show the necessity of quality management and developing standardized procedures of SI-units traceable measurements, data acquisition, storage and archiving, including their effective implementation in research of new functional materials. Further aspects are related to Fair Data and Open Science that will become relevant or even mandatory in the near and long-term future as well as to the question of Metadata, widely discussed in scientific community and politics.

HZB and PTB cordially welcome you to this workshop and invite you to start or intensify the discussion about all these points as well as your expectations and requirements for future scientific research and successful experiments at our facilities.

When are you coming to visit?  
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## “MATERIALS METROLOGY” - SATELLITE WORKSHOP TO THE HZB USER MEETING 2019

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### FURTHER INFORMATION

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