Questions that were collected via on-line questionnaire prior Materials Metrology Workshop (December 2019):	
FAIR data	HZB employee

- **How to protect my data from unfair researchers?**
- **How to protect my authorship of data obtained by me from unfair researchers? If someone would perform non-fully correct analysis of my data and provide non-correct explanation how would be possible to complain about this?**

Answer (by Emil List-Kratochvil, Alevtina Smekhova & Antje Vollmer):

The most important questions about a proper use of research data, its authorship and correct citations by others are considered e.g. in "The FAIR Guiding Principles for scientific data management and stewardship“ (https://doi.org/10.1038/-sdata.2016.18). These guiding principles have been mainly set up for the use of data by other individual human scholars as well as for the automatic finding and data recognition by machine algorithms.

Going into detail with respect to the target questions one finds that FAIR use of data does not mean that one gives up control over his/her data; instead, it is just about a clear protocol for accessing the data (specially the meta-data), and this protocol has to be open, free and universally implementable (e.g. from https://www.go-fair.org/fair-principles/a1-2-protocol-allows-authentication-authorisation-required/). In the section "A1.2: The protocol allows for an authentication and authorisation where necessary“ it is explicitly stated that „...often misunderstood ... The ‘A’ in FAIR does not necessarily mean ‘open’ or ‘free’. Rather, it implies that one should provide the exact conditions under which the data are accessible. Hence, even heavily protected and private data can be FAIR. Ideally, accessibility is specified in such a way that a machine can automatically understand the requirements...“. Ideally, “...anyone with a computer and an Internet connection should be able to access at least the metadata. It is important to emphasise that Accessible in FAIR does not mean Open without constraint. Accessibility means that the human or machine is provided - through metadata - with the precise conditions by which the data are accessible and that the mechanisms and technical protocols for data access are implemented such that the data and/or metadata can be accessed and used at scale, by machines, across the web” (https://ec.europa.eu/info/sites/info/files/-turning_fair_into_reality_0.pdf).

That all means that everyone can still control how his/her data is used if he/she provides it in principle to others.

More information could be also found at https://www.go-fair.org/fair-principles/ and https://www.dtls.nl/fair-data/fair-data/.

Imaging, Diffraction	Head of Group
BESSY III - It would be very advantageous if large Institutions (HZB, PTB, BAM, HU, TU, FU) would have several beamlines on their own (multi-purpose) or shared among them (dedicated to specific subjects). Which is the strategy? Are there consultations among such Institutions? Are there any common plans?	
Answer (by Mathias Richter): Already at BESSY I, PTB has operated own beamlines from 1982 to 1999. Currently PTB uses 6 beamlines/stations at BESSY II and 6 at PTB's own Metrology Light Source (MLS, operated by HZB) for various applications in the field of Metrology with Synchrotron Radiation: Radiometry, Reflectometry, Materials Metrology … For hard X-rays, PTB uses also the BAMline. Current discussions between the strategic partners (HZB, PTB, BAM, MPG, Berlin Universities, …) refer to similar structures also for the future (BESSY III & MLS II).	
Optical Constants in the EUV Spectral Range	PTB employee
How to properly determine the uncertainties in the optical constants at the Soft X-ray/ EUV spectral range?	
Answer (by Mathias Richter): The main details could be found in these publications: • Gottwald, K. Wiese, U. Kroth, and M. Richter, Uncertainty analysis for the determination of B4C optical constants by angle-dependent reflectance measurement for 40 nm to 80 nm wavelength, Appl. Opt. 56, 5768 (2017); • A. Gottwald, K. Wiese, T. Siefke, M. Richter, Validation of thin film TiO2 optical constants by reflectometry and ellipsometry in the VUV spectral range, Meas. Sci. Technol. 30, 045201 (2019).	

X-ray spectroscopy	HZB/PTB/academic employee (or any other definition you would prefer)

Which kind of need do you see for absolute measurements to correlate the materials; functionality with the underlying chemical and physical material properties?

Answer (by Mathias Richter):

In order to correlate the functionality of a device with its materials properties, the latter must be determined in terms of absolute analytical measurements, traceable to SI-units with a reliable uncertainty budget. For this purpose, the requirements are:

(i) stable storage ring operation with respect to beam current and position (lifetime);

(ii) optimized and well-characterized beamlines (stable flux monitor, high spectral purity, stable and calibrated photon flux detector, diagnostics for beam position and size);

(iii) quality management system with respect to beamline and analysis setup documentation, characterization, and operation; measurement procedures and data acquisition, documentation and storage; the calculation of uncertainty budgets.

Open data	HZB employee

Would it be possible to increase an embargo period for data before make them open from 5 to 15 years in the fields NOT related to e.g. medical studies? It would protect the young researches from unfair competition. To whom such questions could be addressed?

Answer (by Jens Viefhaus): This question has to be discussed with the funding bodies, if possible. These constraints are defined by them as they are the ones pushing primarily for “open data”.

Answer (by Heike Görzig): The embargo period of five years is defined in the HZB Data Policy. This Data Policy has been set into force as a decision of the HZB management after discussion in several panels and committees at HZB, involving among others: the "BER Runde", the "BESSY Runde", the User's committee, the Scientific-Technical Council (WTR), and the Scientific Advisory Council (SAC). If one wants to change this regulation, one needs to start a new decision process that will likely involve again all these panels.

I shall note that I believe that it is simply unrealistic that a proposal to extend the embargo period in the policy to 15 years would have a chance to be adopted. Such a long embargo would mean the de facto abandon of open access to research data. There are very clear guidelines from funders and policy makers, such as European Commission, the Alliance of German Science Organisations, and Deutsche Forschungsgemeinschaft, just to name a few, all demanding open access to research data. There is also a decision of the Assembly of Members of the Helmholtz Association that requires all Helmholtz institutes to implement an open access policy for research data.

Metadata	HZB employee
Are there some time-milestones for a unification of definition of "Metadata"? Would it be acceptable that different facilities will determine their own definitions for it?	
Answer (by Heike Görzig): There are no time-milestones. It would be a progress if facilities define their metadata and not every measuring instrument. The MX community found it useful to have standard and generated lots of synergies. If there are other communities willing to have a standard we start with them. **Answer (by Jens Viefhaus):** Along the line of the NFDI-Initiative, it is expected that the research domains rather than the facilities will make the definitions. Facilities will then have to implement the definitions. There is still the challenge to coordinate this on an international level.	
AI for Big Data	HZB employee
Currently there are a lot of activities related to Big Data in a business domain. Is smth. planned for the research-domain within BESSY III upgrade (not-related to MX crystallography)?	
Answer (by Jens Viefhaus): Regarding Beamlines and Spectrometers, the answer is yes, already now. Ideally the compete research facility will be globally optimized with AI-methods and the whole research data flow will be designed by taking "big data"-algorithms and practices into account. Realizing the latter will require substantial resources that will be increasingly in high demand.	
ExPaNDS	academic employee
In which way the communication of people from ExPaNDS project with Users of large-scale facilities is managed? How the real needs of Users will be taken into account? What will be done if new standards will not be convenient enough?	
Answer (by Heike Görzig): ExPaNDS does not interfere with users. At HZB the needs of users will be taken into account when beamlines are connected to the ICAT. The standard is mainly the format for the repository. If required we keep writing the format that is produced at the experimental stations now. There is no standard approach pros and cons have to be discussed with beamline scientist. We also try to take needs of users or usages into account that are not previewed in the moment of data production. Lots of information is missing or not clear in the self-tailored not standardised files. That is one reason why standards have to be applied. **Answer (by Jens Viefhaus):** Provide a one-stop-shop for the data (analysis) needs of scientific facility users. Organise workshops/tutorials, provide e-learning platforms in cooperation with EOSC.	