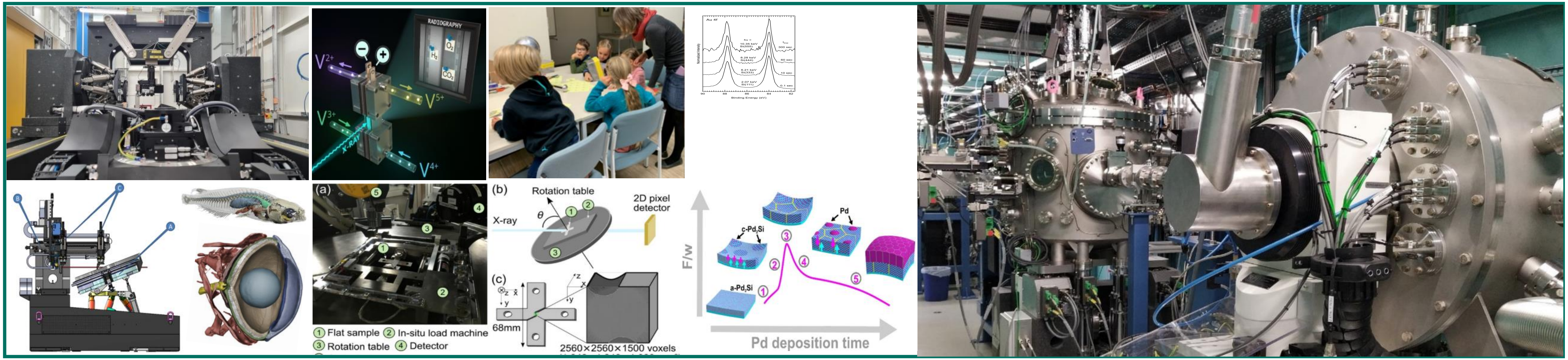
Proposed integration of MML@KIT into DTS in PoF V – First Draft

Tilo Baumbach, Clemens Heske



Detector Technology and Systems (DTS)

"Develop advanced detector technologies & systems to convert multidimensional data into information for scientific discovery"

ST1 – **Sensing and Detecting Technologies**

"Realize intelligent and compact granular detectors with high space and time resolution"

ST2 – **Quantum Technologies**

"Establish highly pixelated quantum sensors with ultimate energy resolution"

ST3 – **System Technologies**

"Build sustainable detector systems and cope with drastically increasing data rates"

ST4 – **Multidimensional Methods and Data Processing**

"Integrate advanced detector systems into multidimensional modalities for scientific discovery"

Detector Technology and Systems (DTS)

KIT's proposal for integration of MML@KIT into the ST-Structure of DTS

ST1 – Sensing and Detecting Technologies

- Sensors
- High-Z sensors – growth and characterization
- Electrical and Photonic Integrated Circuits (ASICs) and on-detector Intelligence
- 3D and Interposer Interconnection & Packaging

ST2 – Quantum Technologies

- Quantum Sensors and Production Technologies
- Scalable Readout for Superconducting Quantum Devices
- Quantum Sensor Applications

ST3 – System Technologies

- Intelligent Data Acquisition
- Novel Engineering Techniques, Advanced Materials, Cooling
- X-ray Optics XT-OPT
- Detector System Concepts & Demonstrators
- Detector and System Simulation

ST4 – Multidimensional Methods and Data Processing

- Distributed High-throughput Readout Systems
- Developments for serial, *in situ, in vivo, operando Applications*
- AI-supported Multidimensional Data Analysis

DetecTABL: Research Infrastructures for Detector Deve… ation Beamlines & Labs

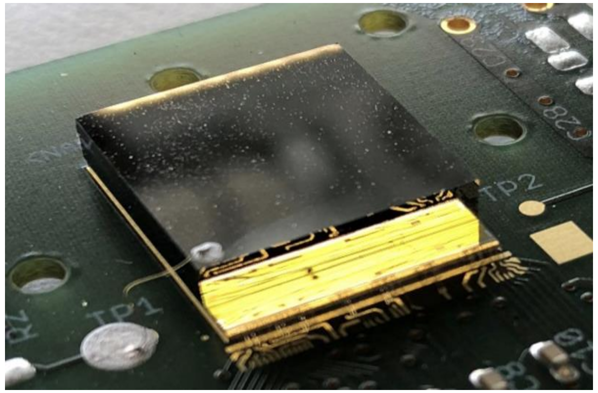
- Interconnect and Packaging Facilities
- Quantum Sensor Production Facilities
- Assembly Facilities
- Test and Application Labs & Beamlines

Detector Test X-ray Lab
Characterization Methods for Defect Analysis
Beamlines for Performance Test and Application

ST1 – High-Z Sensors

- **High-Z detectors based on CdZnTe/GaAs (collaboration with U-Frei …)**

- **Goal: Development of CdZnTe/GaAs sensor technologies from crystal growth towards detector production**:
  - **Growth of CdZnTe**
    - Partner in the OptiBeams proposal in the HORIZON-INFRA-2024-TECH-01-01 call - coordinated by DESY FLASH
    - Cooperation with PSI for the growth of 75 mm diameter CdZnTe crystals
  - **Technology for pixel detectors**
    - Work on flip-chip bonding in cooperation with IPE
  - **Production of TPX3 (TPX4) and Eiger (PSI) detectors**
    - Production of detector modules with different thicknesses from 0.5 up to 3 mm for covering X-ray energies from 30 up to 300 keV
    - Development of large-area detectors



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U-Frei – MML – MT

ST1 – High-Z Sensors

- **Research on Perovskites**
  - New class of semiconductors: Perovskite semiconductors (promising photovoltaic materials)
  - Perovskite materials are a promising alternative regarding availability, toxicity, and low production costs, compared to conventional high-Z materials like CdZnTe or GaAs

- **Crystal growth from solution and the melt of $CsAgBiBr_6$ and $CsPbBr_3$**
- **Intensive material characterization:**
  - (topography, XDL, SIMS, I-V, DLTS, ...)
- **Detector technology:**
  - Development of planar technology (surface preparation, contacts, bonding)
- **Development of a growth process**:
  - Deposition directly on electronics (solution, 3D printing, ...)
- **Production of detectors:**
  - using Timepix3 and Timepix4 with High-Z sensor based on perovskites semiconductors

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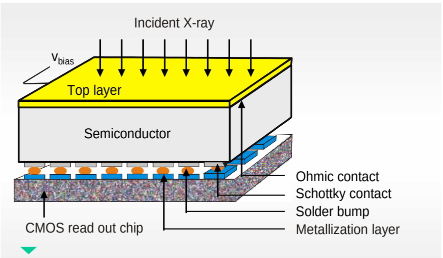
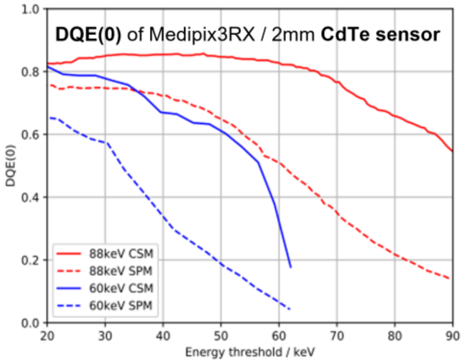
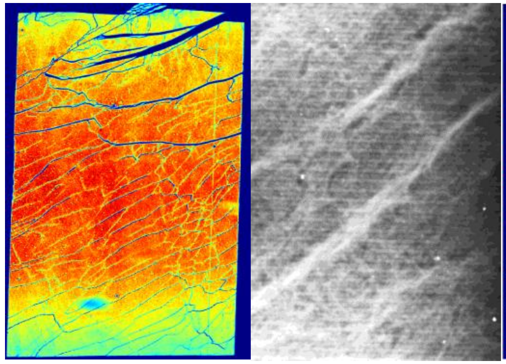
ST1 – Sensor & Detector Characterization

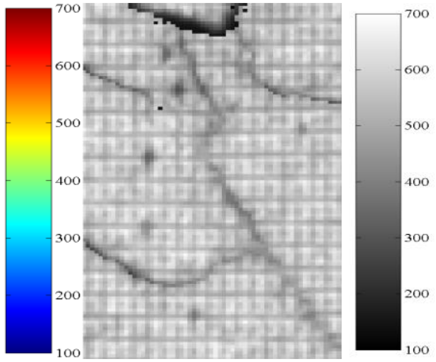
- **Sensor Materials Characterization**
  - Crystal perfection / defect characterization of perovskites and conv. high-Z sensor materials by X-ray topography, 2D rocking curve imaging, 3D diffraction laminography, …, & SIMS, I-V, DLTS in collab. with U-Frei
- **Non-destructive Testing**
  - Testing flip-chip interconnections by X-ray absorption laminography …
- **Characterization of Detector System Performance**
  - Timepix3 and Timepix4 with High-Z sensor based on perovskite semiconductors → key parameters of full detector assemblies, e.g., energy and spatial resolution, flux-dependent linearity, stability, charge-sharing, …

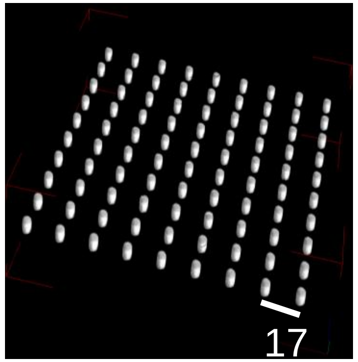


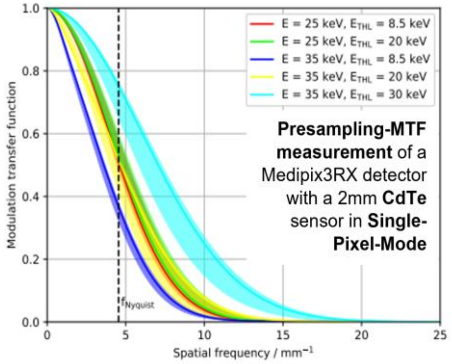
GaAs detector array with flip-chip bonding between detector layer and read-out chip







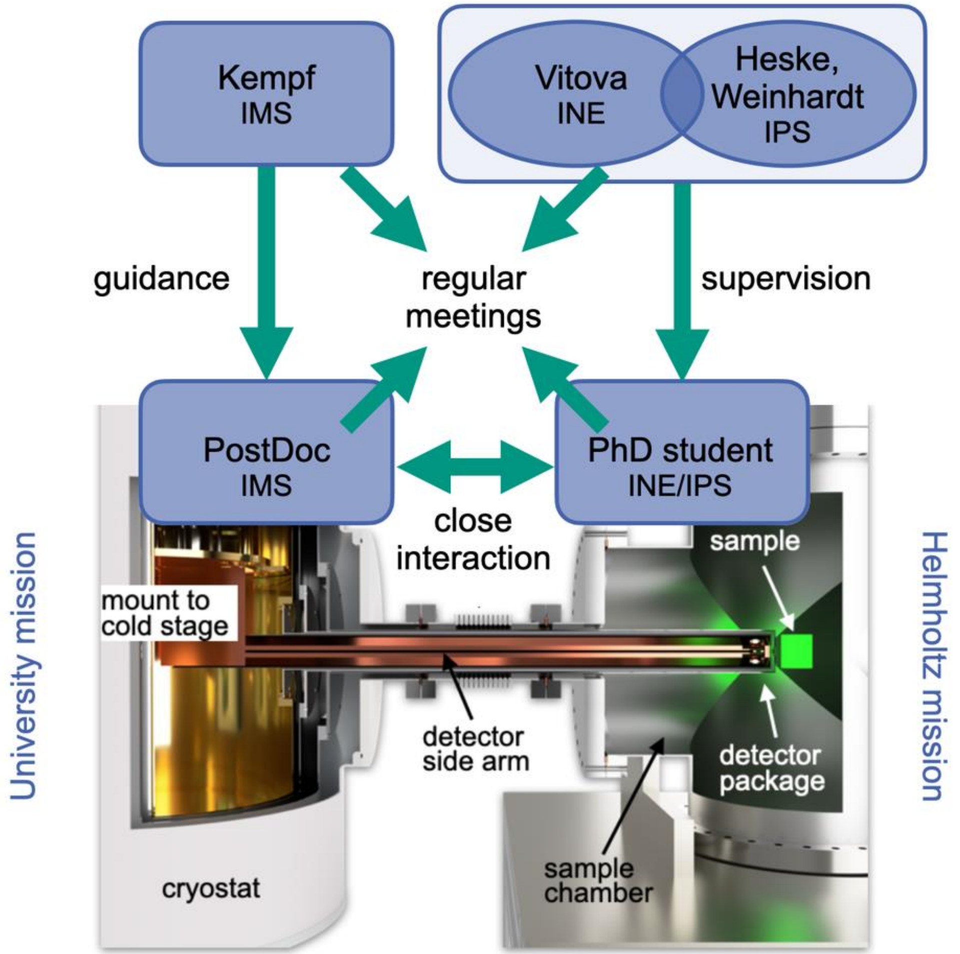




ST2 – Quantum Sensor Applications

QUASY - Quantum Sensor Platform for Synchrotron X-ray Spectroscopy

- **Magnetic Microcalorimeters – MMCs**
- For various beamlines in the IPS Spectroscopy Cluster
- Energy resolution **orders of magnitude better** than for conventional EDX detectors



Collaboration with S. Kempf (IMS), T. Vitova (INE)

ST3 – X-ray optics

- **Integrating Optics and Detectors in powerful Detecting Systems**
  - Integration of high-Z Single Photon Counting Detectors (SPCDs) and Bragg-Magnifiers (BMs) for dose-efficient high-resolution imaging
  - Compared to conventional high resolution imaging:
    - Efficient noise suppression
    - Improved (spatial) frequency-dependent OTF
    - Gain in DQE, particularly at the high frequencies defining the resolution up to above two orders of magnitude
    - → Higher image contrast at µm resolution
    - → Substantial increase of dose efficiency

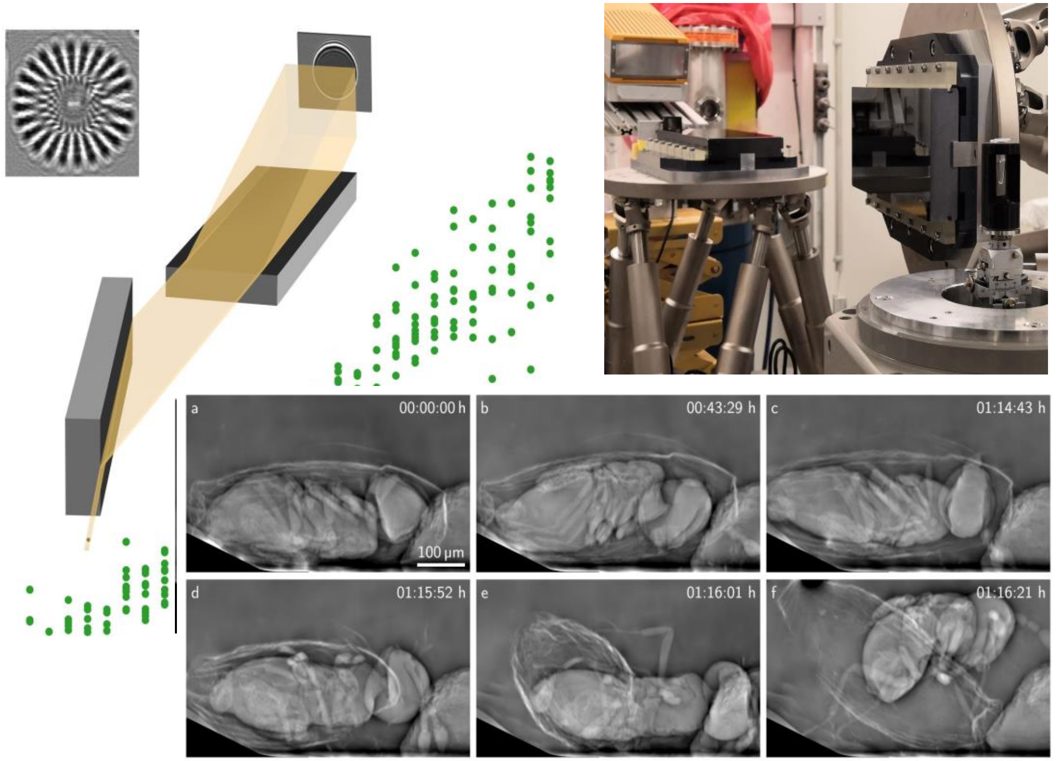


Illustration of dose-efficient coherent near field imaging with 1 µm resolution based on SPCDs (of <100 µm resolution): Scheme and instrumental realization of magnifying by asymmetric crystal optics the X-ray image subsequently detected by a SPCD (here a GaAs LAMBDA-detector); application example *in vivo* cine-radiography – here a behavioral study of parasitoid wasps in their host.
R. Spiecker et al., Optica 2023

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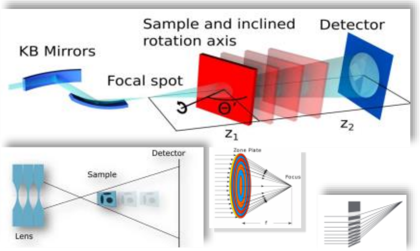
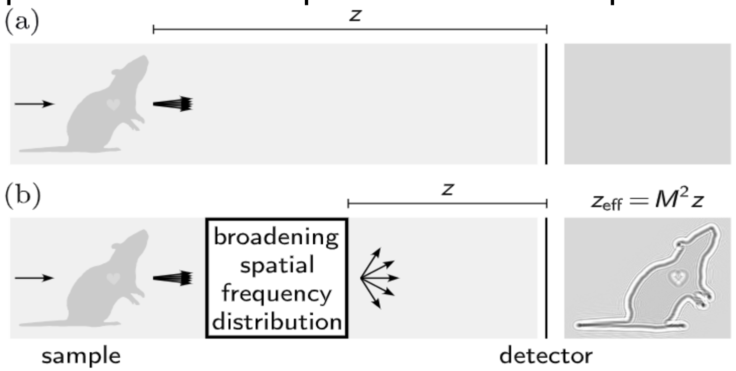
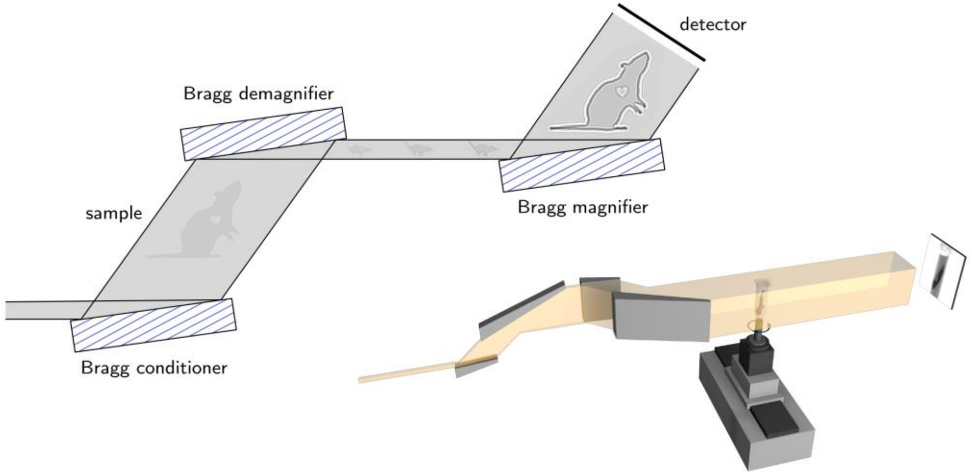
ST3 – X-ray optics



Combination of SPCDs and Coherent Bragg Optics provides massive phase contrast amplification





R. Spiecker et al, under review

- **Integrating Optics and Detectors to powerful Detecting Systems**
  - **Integrating Bragg-*De*magnifier Technology and SPCDs to enable compact realization of holographic phase contrast imaging outperforming beamlines even with kilometers-long wave-field propagation distances**
    → drastic contrast amplification even for low spatial frequencies
    → dose-efficient phase contrast at large fields of view
  - **Dose-efficient holographic phase-contrast applicable to larger objects**
    → radiation sensitive objects, (bio-)medical diagnostics
  - **Combination with novel compact brilliant X-ray sources**
    → new options for bio-medical imaging

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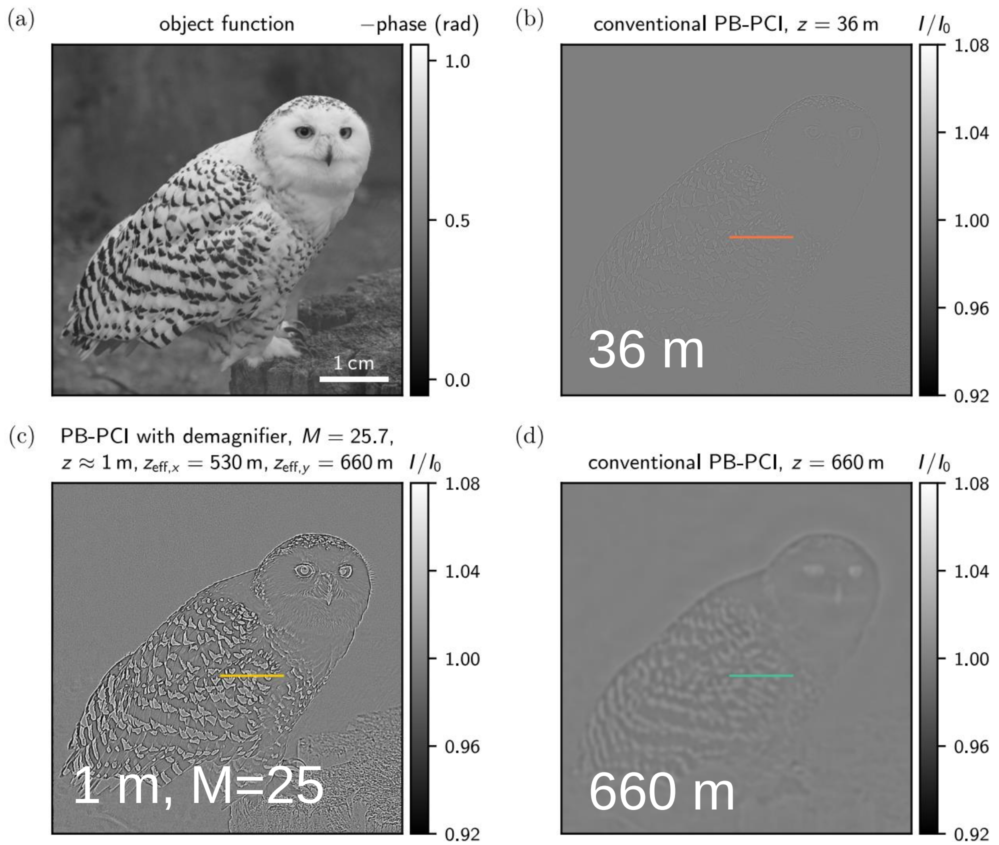
ST3 – Detector and System Simulation

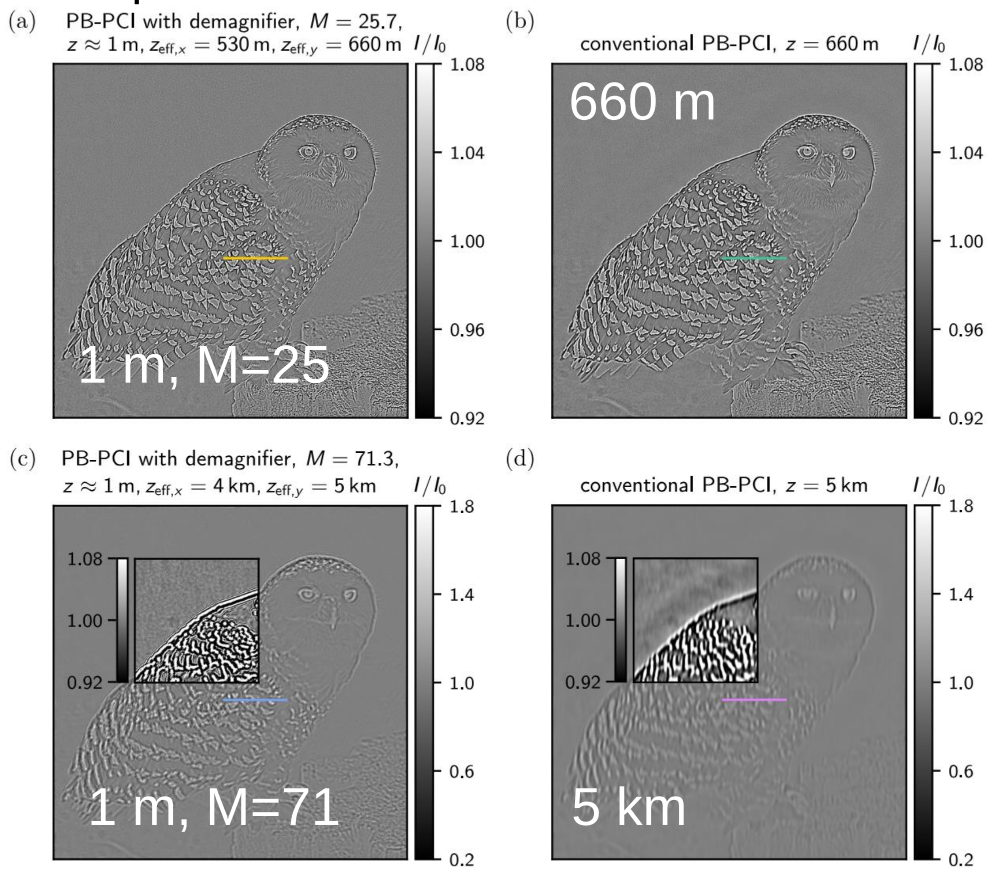
SPCDs combined with coherent X-ray optics will outperform even kilometers-long beamlines

for P23 **PETRA III,** but assuming symmetrical source



SPCD+**BM** SPCD, **no BM**

Comparison for **ESRF EBS** conditions at BM18

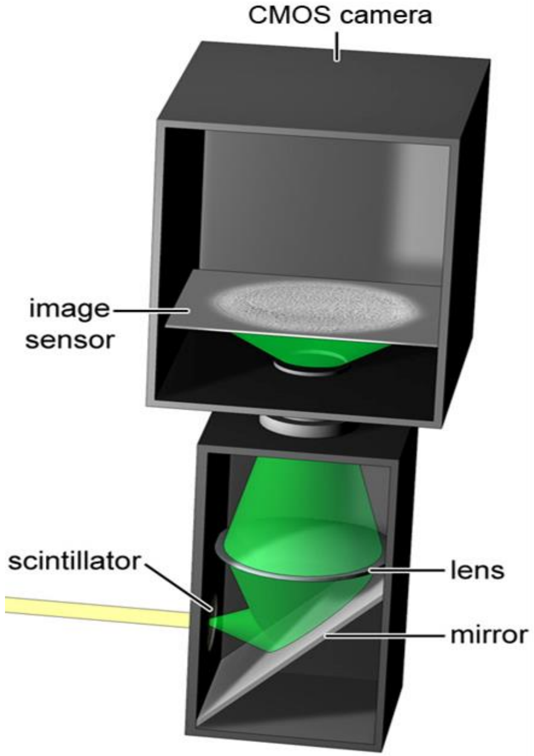


SPCD+**BM** SPCD, **no BM**

ST3 – Detector and System Simulation

- **High-fidelity simulation of detecting systems**
  - Optical Transfer Function (OTF) / Modulation Transfer Function (MTF) / Detective Quantum Efficiency (DQE)
  - Dose efficiency
  - Photon-energy dependence of direct and indirect converting X-ray detection systems …
  - … and their involved components (X-ray optics, converting sensor, light optics, read-out electronics, …)

Simulating properties of a high-resolution indirect X-ray camera system



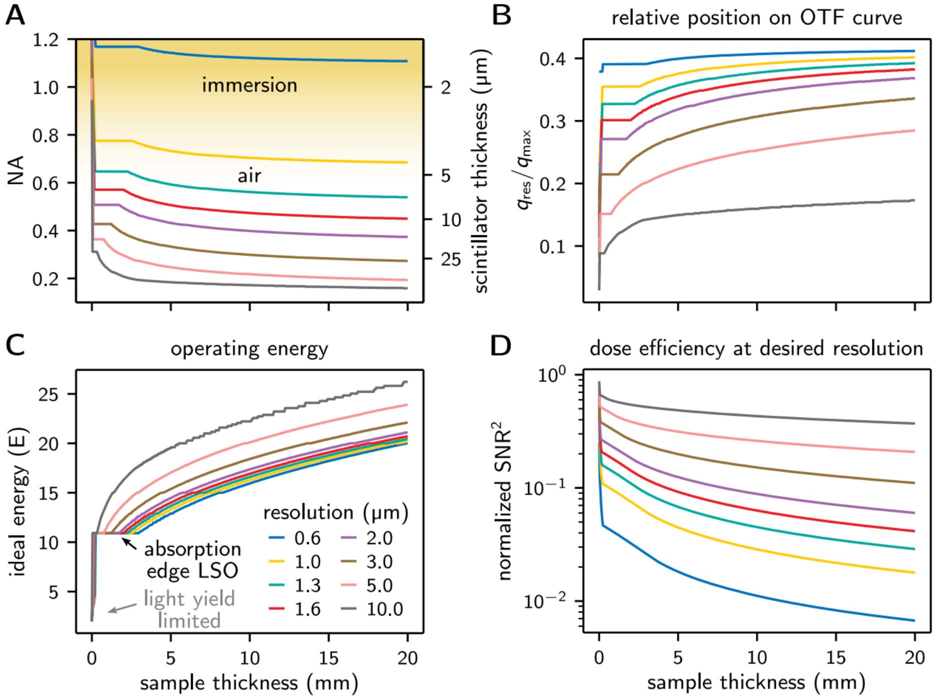
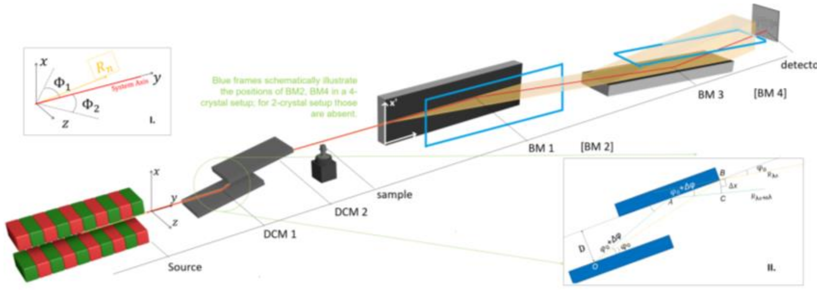


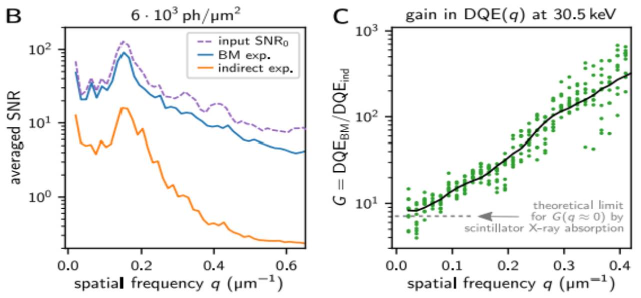
Fig. S4. Optimized parameters for the indirect system and an LSO scintillator for different sample thicknesses (material: soft tissue) and resolutions. **A** Optimized numerical aperture over sample thickness for different resolutions. We indicate that for high NA, objectives with immersion liquids are necessary. **B** Spatial frequency q_{res} that corresponds to the desired resolution in relation to the spatial frequency q_{max} where the OTF of the objective becomes zero. **C** Optimal operating energy. A lower limit is given by the light yield of the scintillator per absorbed X-ray photon (gray arrow). The absorption edge of LSO determines an optimal energy of 11 keV for thin samples (black arrow). **D** Resulting normalized SNR^2 at the desired resolution, which is an upper estimate for the dose efficiency compared to an ideal detector. The legend shown in C is valid for all panels.

ST3 – Detector and System Simulation

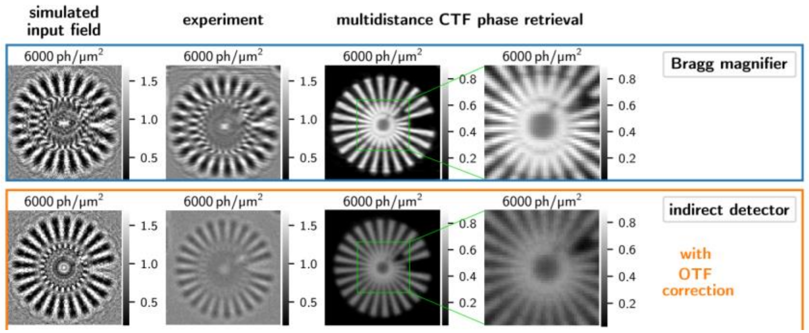
- **High-fidelity simulation of complete DAQ systems**
  - **Simulation of image formation from source via optics, including source blur, optics, detector OTFs / MTFs / DQE, …**
    - Ray tracing
    - Near field / far field image formation …
    - X-ray Microscopy, grating interferometry image formation
    - Image formation in shift-variant systems (e.g., Bragg Magnifier technology)
    - Generative AI models to simulate large image data sets
    - AI to close the reality gap of simulation
    - 4D process simulation of complete experiments (digital twin of beamline and samples) – and their influence on the data acquisition of the detecting system



Ray tracing for non-coplanar crystal arrangements



Comparison of SNR and DQE of detecting systems



Comparison of image formation of detection systems

ST4 – Multidimensional Method and Data Analysis

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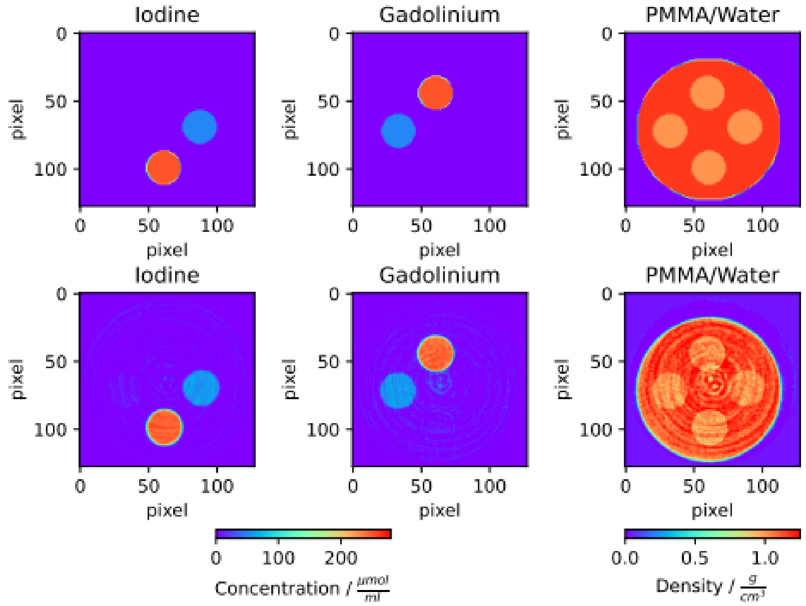
- **Systems Integration of novel Detectors:** Integration in versatile X-ray imaging pipelines (Hard- and Software) at synchrotron beamlines and X-ray tube-based laboratory setups
- **Dedicated method developments based** on novel detectors and combinations with optics & smart analysis
  - Dose-efficient phase contrast imaging, hierarchical imaging, serial CT, Cine-tomography, MHz-imaging …
  - Spectroscopic X-ray imaging with machine learning based material decomposition …
  - Rapid RIXS: On-the-fly component integration from undulator to optics and soft x-ray photon detection systems
- **Application Tests:** Quality measure for imaging properties evaluating exemplary applicability in life science, materials research, …
- **MT-DTS-ST4 connects to other Helmholtz Programs and Research Fields**



Material-specific spectroscopic CT-slices of a test phantom. Top: ground-truth, bottom: measurement, Medipix3RX with 2mm CdTe in charge-summing-mode

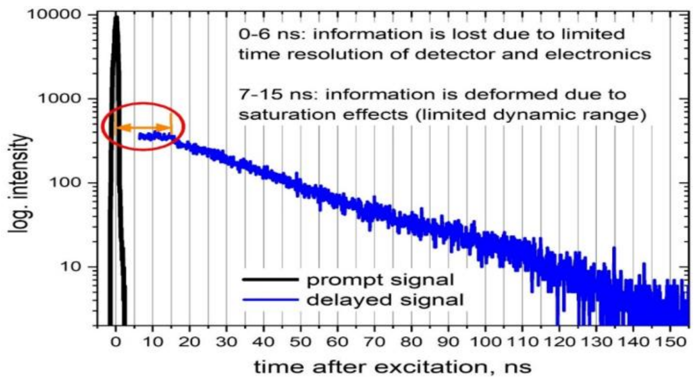
PhD-thesis Marcus Zuber

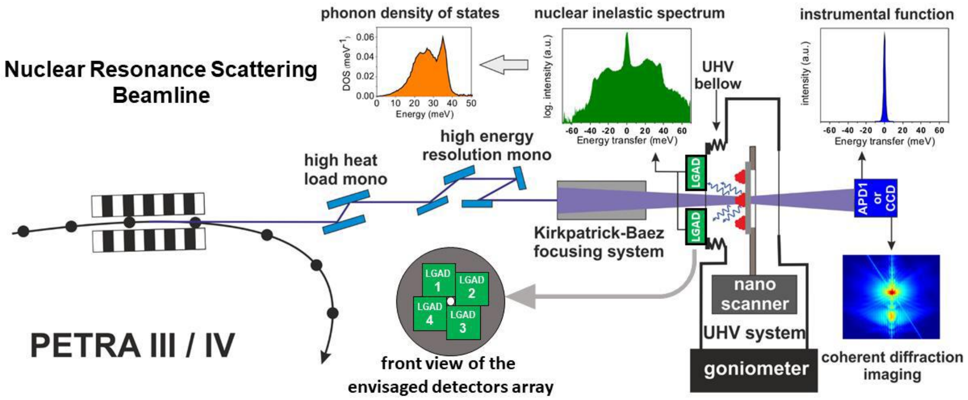
ST4 – Multidimensional Method and Data Analysis

Advanced multidimensional synchrotron method developments trigger new detector developments

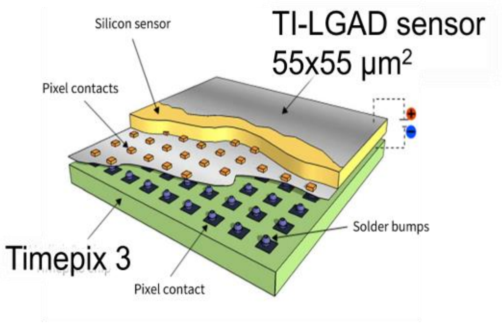
- Example: Advanced Nuclear Resonant Scattering for Phonon Studies of Nanostructures for dead-time reduced data acquisition

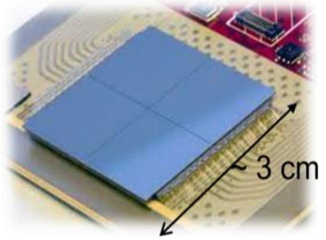
Current detector



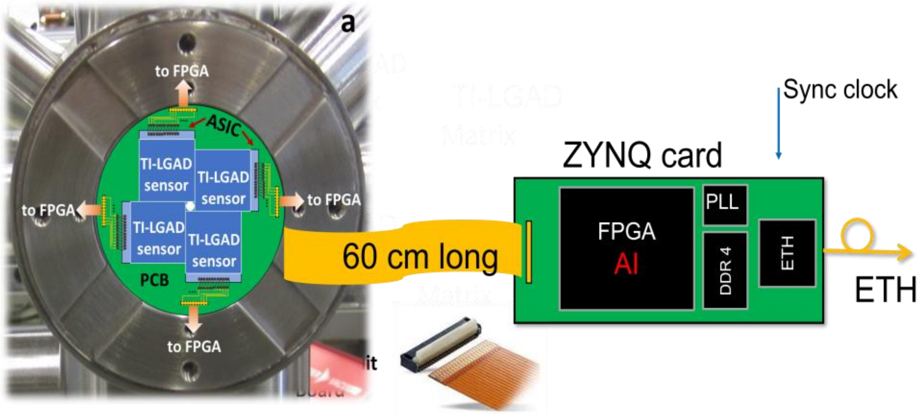


- Based on new detector concepts of **Trench-Isolated Low-Gain Avalanche Diode TI-LGAD technology**





Timepix 3 bonded to standard pixel sensor developed at CERN



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KIT-CS – MML – MT

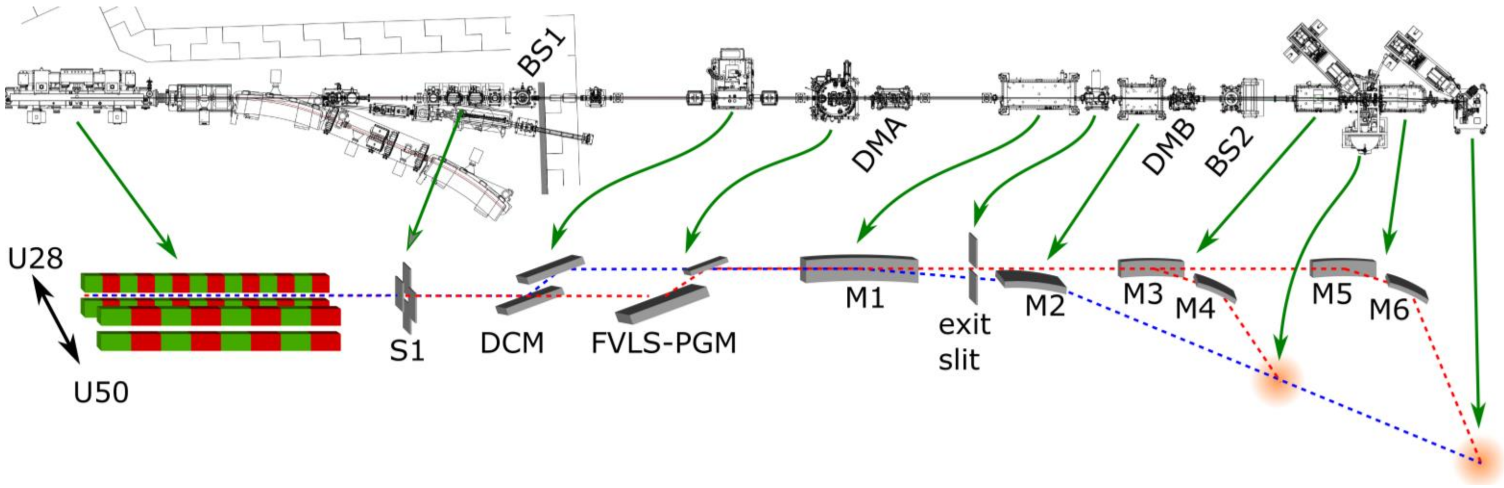
ST4 – Multidimensional Method and Data Analysis

Development for serial, *in situ*, *in vivo*, *operando* Applications

Advanced multidimensional synchrotron method developments trigger new detector developments

- High dose efficiency and short exposure times towards *operando* soft x-ray detection systems
- Combination of powerful optics (e.g., gratings) and pixel array detectors
- On-the-fly component integration from source (undulator), mono-chromator, and focusing optics, to sample, analyzer optics, and soft x-ray photon detection systems

Example: The X-SPEC Beamline at the KIT Light Source

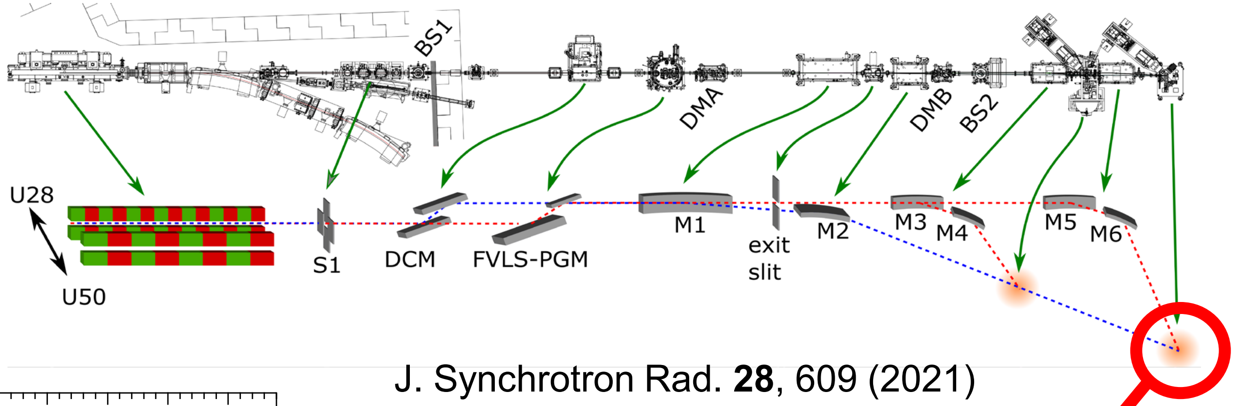


J. Synchrotron Rad. **28**, 609 (2021)

ST4 – Multidimensional Method and Data Analysis

Rapid resonant inelastic soft x-ray scattering (rRIXS) maps at X-SPEC

- Novel high transmission soft x-ray spectrometer detection system
- Reduces time for a RIXS map from tens of minutes to tens of seconds



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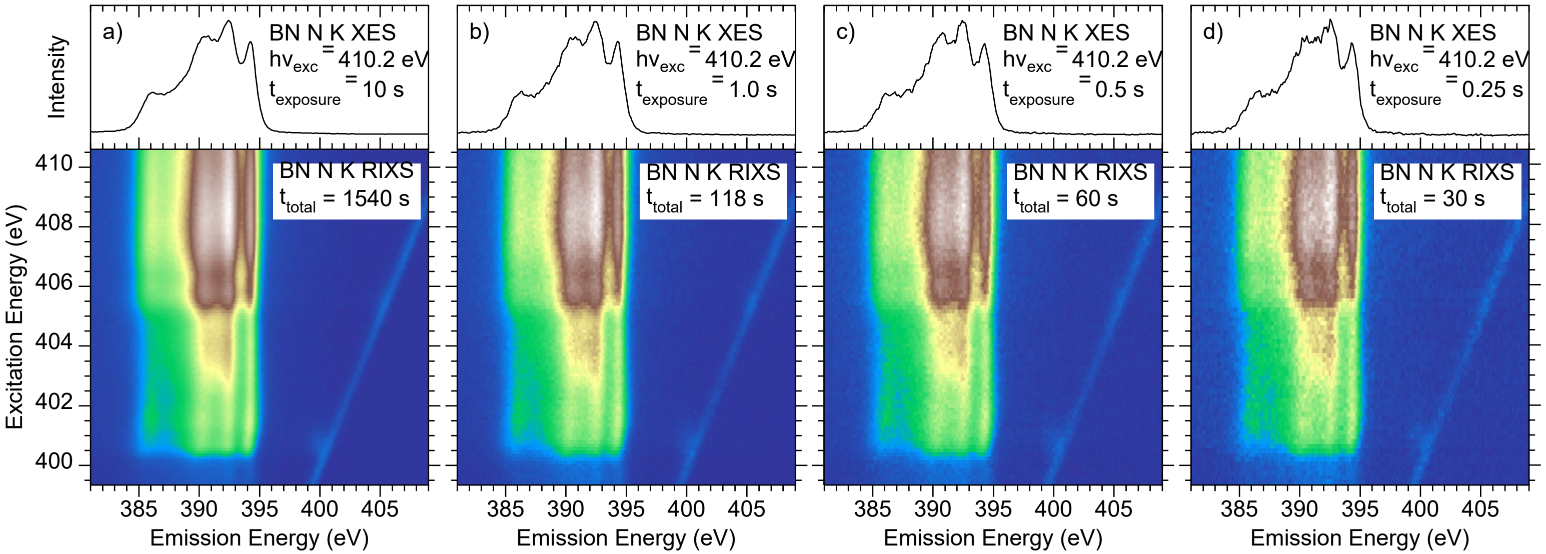

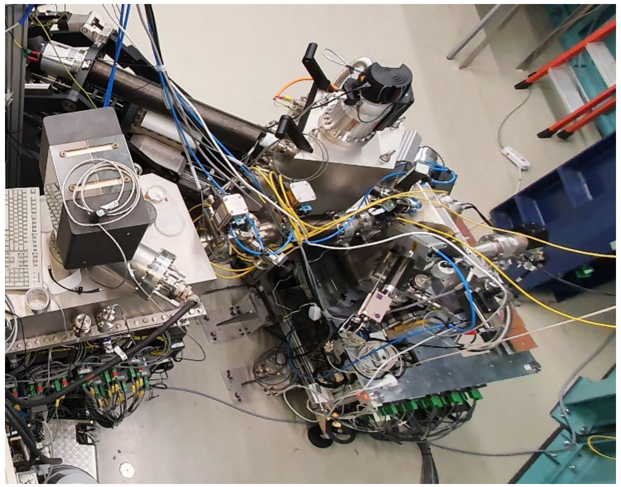

ST4 – Multidimensional Method and Data Analysis

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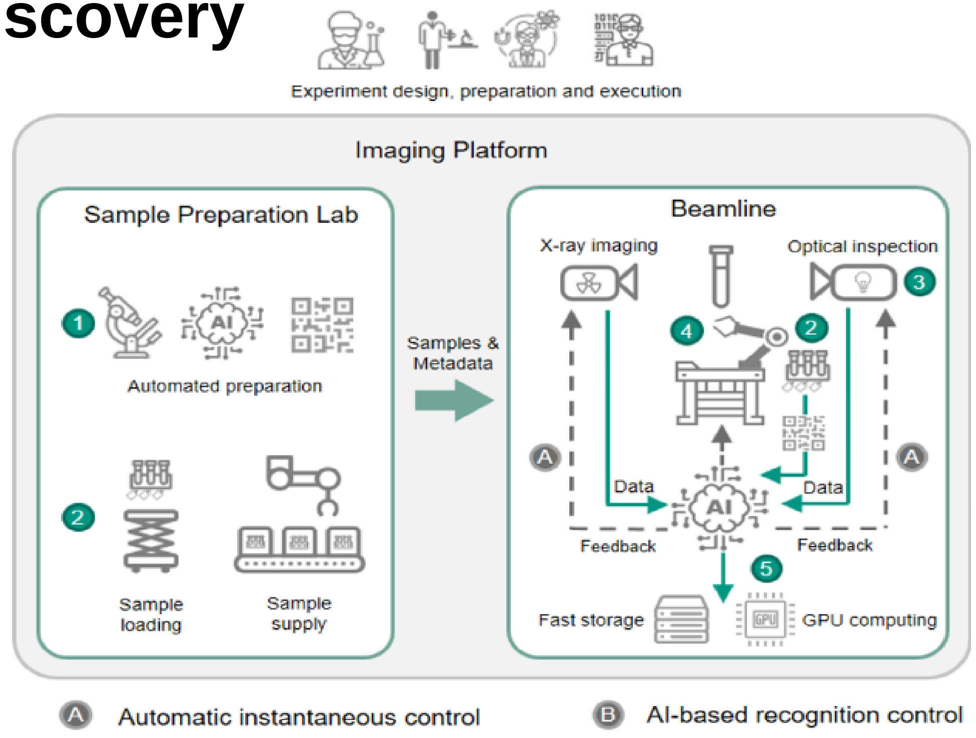
- **Integrate Autonomous Data Acquisition and Smart Data Analysis into multidimensional modalities for scientific discovery**
- **Development for serial, *in situ, in vivo, operando* Applications**
  - **Autonomous data acquisition**
    - Autonomous system calibration
    - AI-supported controlling of DAQ process
    - Immediate data reconstruction during measurement and remote visualization
    - Detector-image based continuous quality assurance of the DAQ process



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05K22VKA – SMART-Morph
KIT-CS – MML Collaboration

ST4 – Multidimensional Method and Data Analysis

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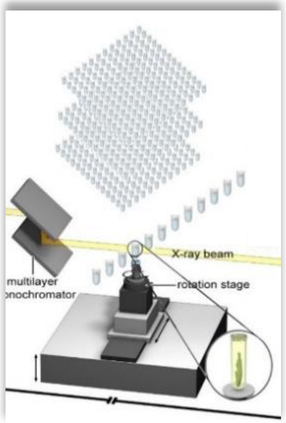
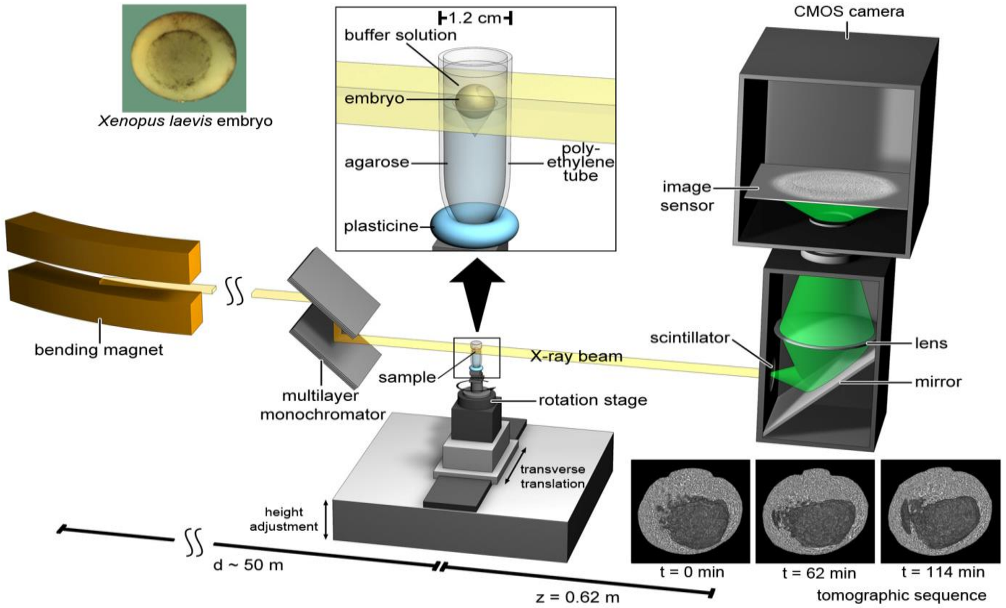
- **Development for serial, *in situ, in vivo, operando* Applications**
  - **System implementation for Imaging, Spectroscopy, and Scattering methods**
    - Smart robotics for autonomous sample handling
    - Integration of smart *in situ, in vivo*, *operando* environments

Towards high throughput



Towards autonomous *in vivo, in situ, operando* DAQ



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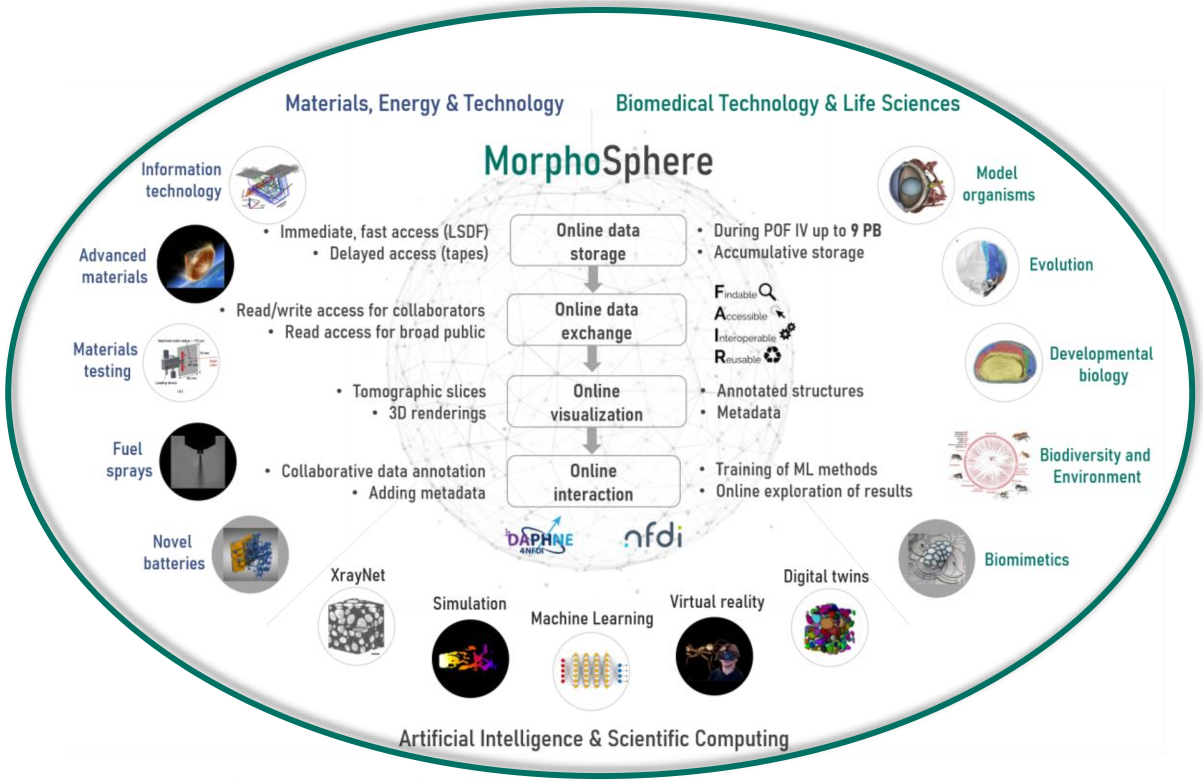
ST4 – Multidimensional Method and Data Analysis

Karlsruher Institut für Technologie

- **AI-Supported Multidimensional Data Analysis**
  - Develop Strategies for AI-based Big Data Analysis and Management
  - AI-based visualization and evaluation of massive amounts of 2D to 4D data
  - Artificial Intelligence for automated segmentation of 2D to 4D data for analysis
  - AI-supported correlation of multidimensional X-ray data and complementary metadata

Example:
MorphoSphere for digitized morphology



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Aktionsplan ErUM-Data
Von Big Data zu Smart Data: Digitalisierung in der naturwissenschaftlichen Grundlagenforschung

Supported by BMBF ErUM-Data Projects
05D23VK1 – KI4D4E and **05D23VK2 – KI-Morph**
KIT-CS – MML Collaboration

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ST4 – Multidimensional Method and Data Analysis

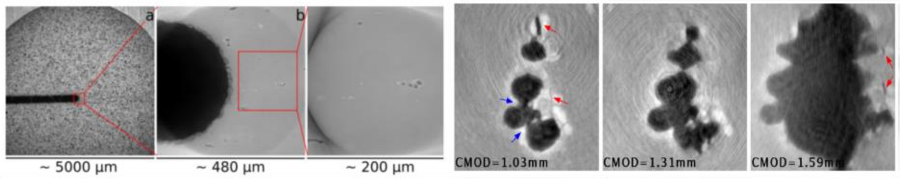
Karlsruher Institut für Technologie

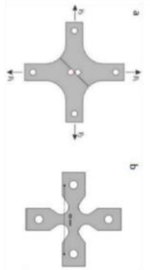
- **Integrate Autonomous Data Acquisition and Smart Data Analysis into multidimensional modalities for scientific discovery**

  - **Method Development for serial, *in situ, in vivo, operando* Applications**

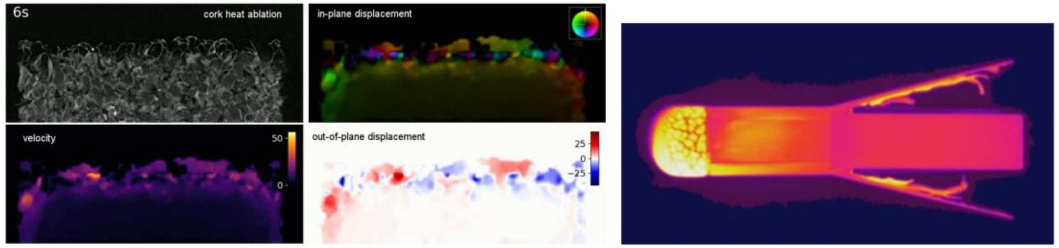
  Approaches

  - Serial tomography / laminography for large comparative studies
  - Hierarchical imaging, spectroscopic imaging
  - Ultrafast cine-radiography & tomography
  - *in situ, operando & in vivo environment*

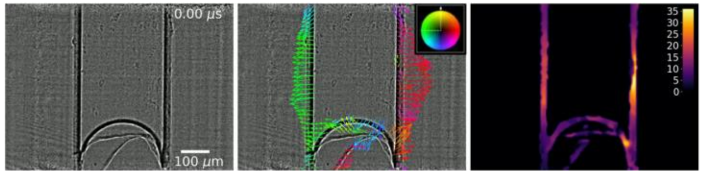


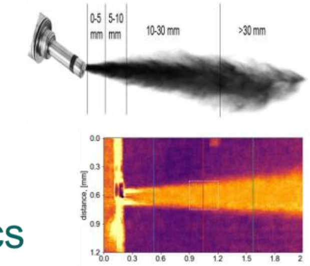


Hierarchical laminography of crack formation



Ultrafast CT of pyrolysis in heat shields for space crafts





MHz imaging for high speed microfluidics

Bundesministerium für Bildung und Forschung

Aktionsplan ErUM-Data
Von Big Data zu Smart Data: Digitalisierung in der naturwissenschaftlichen Grundlagenforschung

Supported by BMBF ErUM-Data Project **05D23VK1 – KI4D4E** and ANR-DFG Project **Lambda**

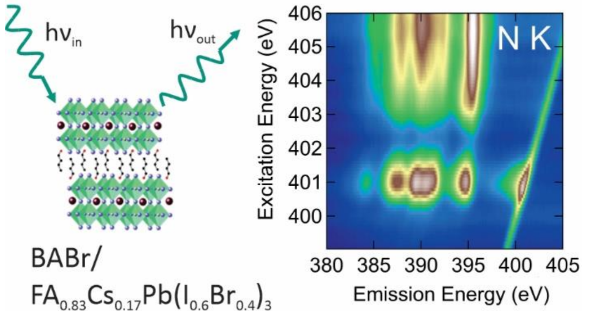
ST4 – Multidimensional Method and Data Analysis

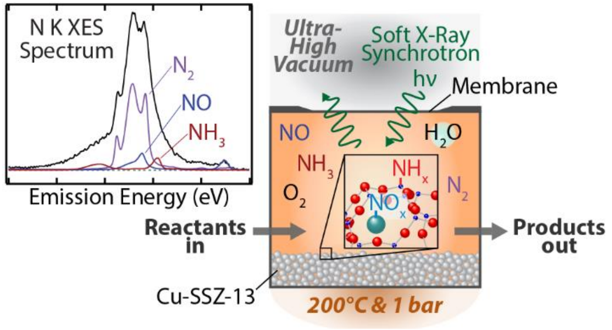
ST4 connects MT to other Programs and Research Fields

Energy technologies → characterize processes for **storage, conversion** … (photovoltaics, solar hydrogen, catalysts, batteries, electrolytes, …), understand degradation

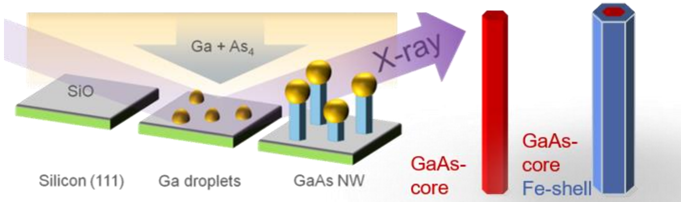
Information technologies → characterization of **growth and processing** of wafers, thin films, multilayers, nanomaterials, nanostructures → correlate structure and properties to understand multiferroics, photonics, quantum devices, high power electronics, …

Transport technologies → *In situ* and *operando* 3D defect recognition and 4D damage analysis



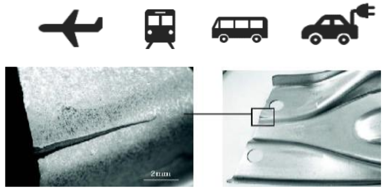


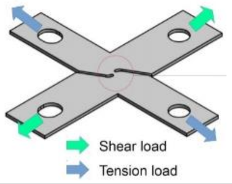
Example: Characterization of Structure and Dynamics of Materials, Devices, and Processes

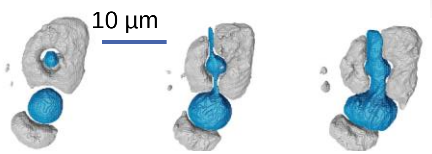


Goals

- Characterize structure and its evolution on micro, nano, and atomic scales
- Correlate structure, dynamics, and properties
- Determine *in situ / operando* changes of electronic and chemical structure during processing/operation







ST4 – Multidimensional Method and Data Analysis

ST4 connects MT to other Programs and Research Fields

Biomaterials & -technologies → morphology and bio-compatibility of biomaterials; tissue engineering, scaffolds, organoids; → bionics, bio-catalysis, food engineering …

Model organisms → correlate morphology and molecular data; determine gene functions & multigenic contributions to **development and disease** → Generate digital twins of biological systems (medaka, zebrafish, xenopus, … brain);

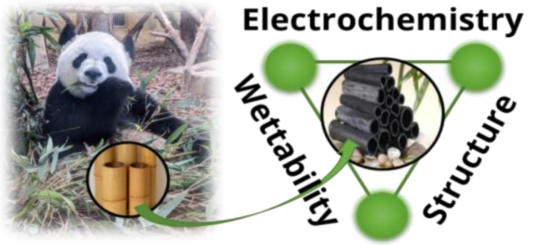
Biodiversity → Digitize morphological diversity, correlated with molecular & ecological data, including human impact → Focus on **indicator organisms for climate impact on biodiversity**, and models for environmental change on development → Identify morphological key features to determine evolutionary key events for diversification

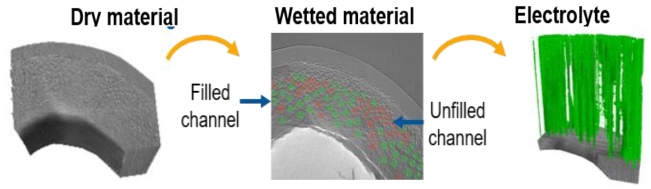
Example: Morphology of biomaterials, biological systems, and bio(technological) processes

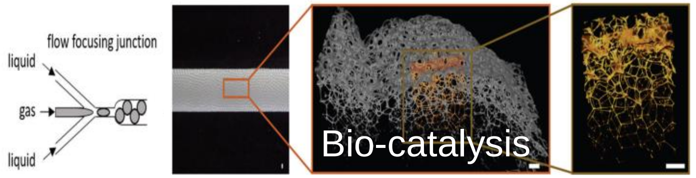
Goals

- Digitize morphology of large sample series
- Determine quantitative morphological / morphometric / morpho-dynamic information

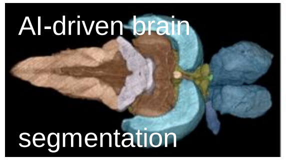
Bionics

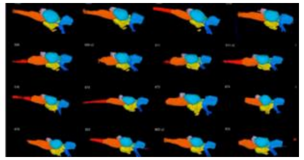






Model organisms

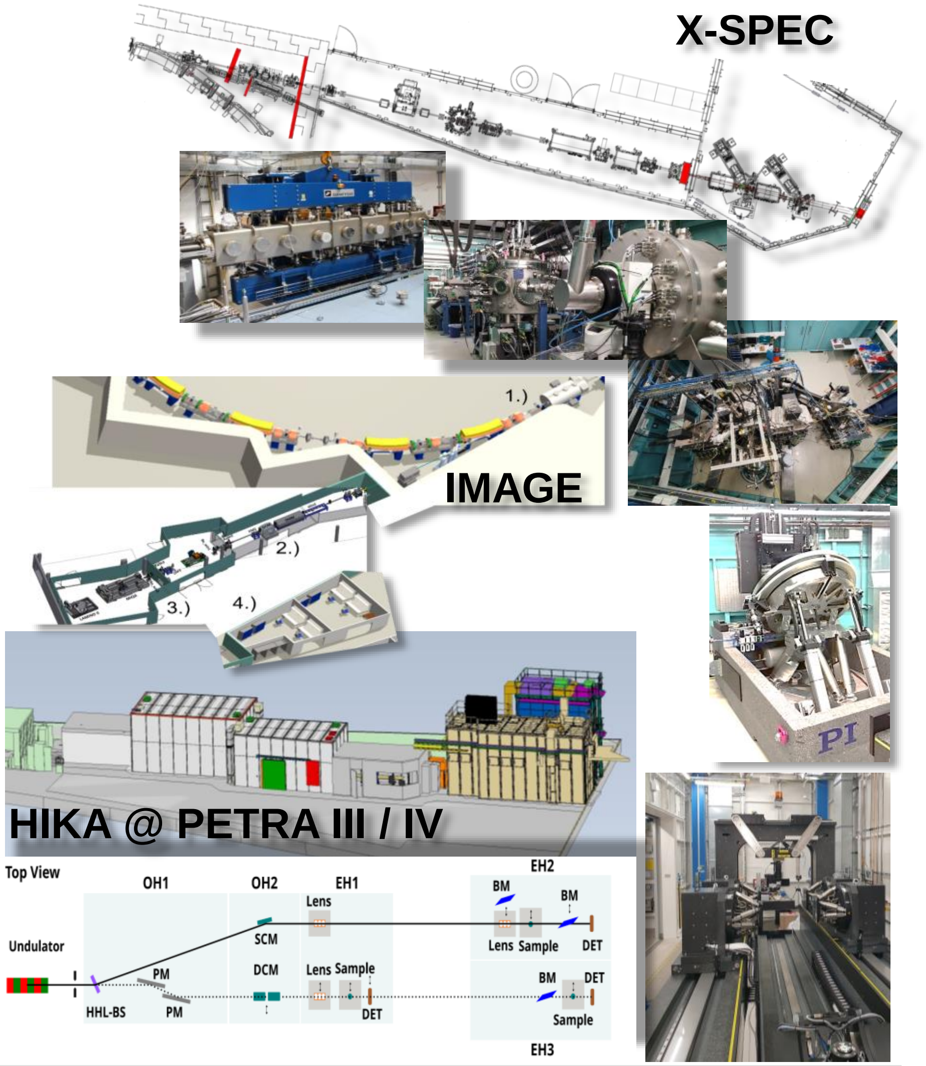




DetecTABL: Research Infrastructures for Detector Development, Test and Application Beamlines & Labs

Test and Application Beamlines & Labs

- **Beamlines for Characterization, Detection Performance Tests, Method & System Development for Multidimensional Data Modalities & Application**
  - **IPS Spectroscopy, Scattering & Imaging Cluster to convert multidimensional data into information for scientific discovery**
    - Multidimensional data acquisition & processing
    - High throughput, *operando, in situ & in vivo* data acquisition
    - X-SPEC for cutting-edge soft and hard x-ray spectroscopy development
    - IMAGE & HIKA: unique portfolio for laminography, hierarchical imaging, and serial tomography for large-scale comparative studies
  - **Methods Development & Application for**
    - Sensor characterization & detector performance
    - CL-CT-Det-Lab: Laboratory-based X-ray Development Platform for quality assurance of optics and detectors & method development
    - Synchrotron based sensor characterization, detector performance tests
    - Development of methods of multidimensional modalities and application to real-world challenges



Summary

Karlsruher Institut für Technologie

- Based on the results of MML, KIT proposes to strengthen MT-DTS by further contributions in ST1 – 3 and in a fourth subtopic, jointly with DESY
- ST4 will support system conception, design, characterization, and application
- KIT's beamlines and labs will extend the DTS "Research Infrastructures" portfolio → DetecTABL
- KIT's new activities in MT-DTS will contribute collaborations with other Helmholtz Programs and Research Fields