

From Matter to Materials and Life

Thomas Stöhlker and Andreas Stierle

PROGRAM MML: *From Matter to Materials and Life*

Research on the structure, dynamics, and function of matter, materials and life

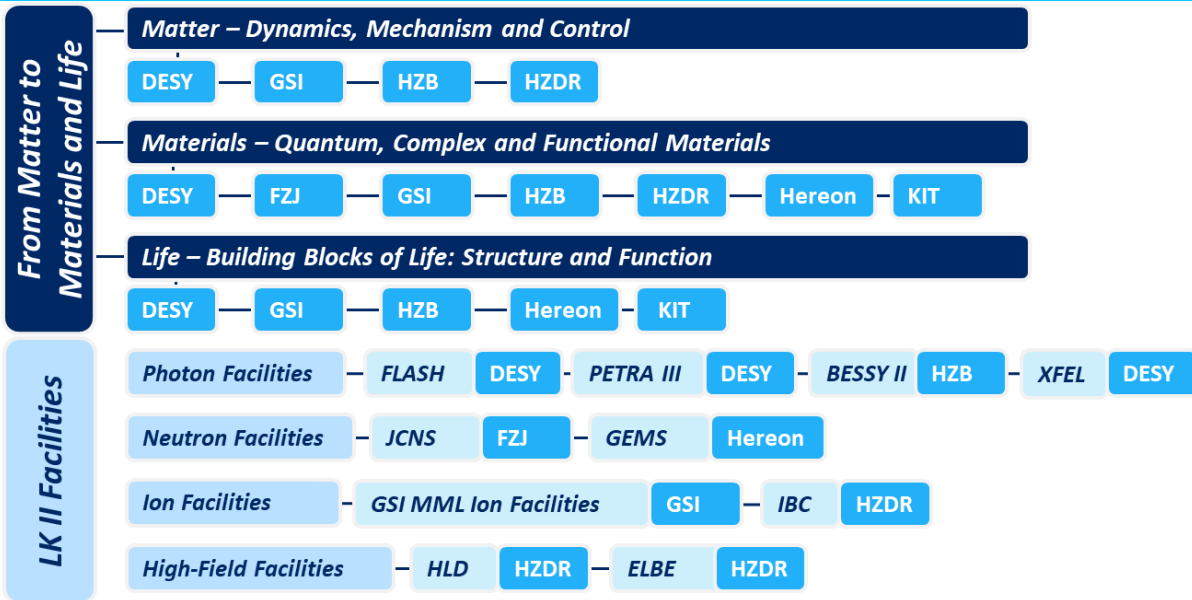
Mission Shaping and enabling forefront research with large-scale facilities

- Unique insights into properties of matter, materials, and life, inaccessible on conventional laboratory scale;
- providing access / support for an interdisciplinary national and international user community;
- essential contributions to solving major challenges ranging from energy to health.



From Matter to Materials and Life

The Topic Structure of the Program



Photons



Neutrons



Ions



High EM Fields



User support



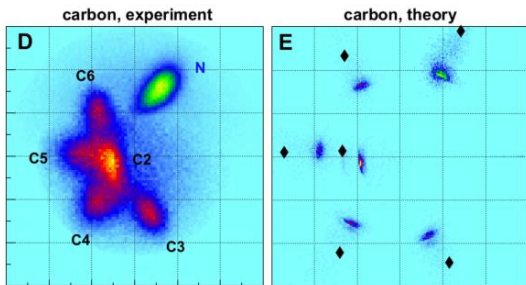
Matter: Dynamics, Mechanisms, and Control

Scientific focus: Fundamental aspects of the structure and dynamics of matter and its interaction with light

Selected Highlights 2022



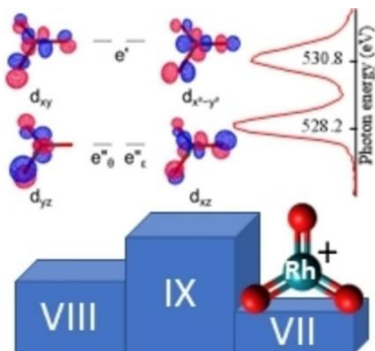
Single-molecule imaging via XFEL-driven Coulomb explosion



R. Boll et al., Nature Phys. **18**, 423 (2022)



The highest oxidation state of rhodium



M. da Silva Santos et al., Angew. Chem. **134**, e202207688 (2022)



Refractive index of extremely supercooled water



C. Goy et al., J. Phys. Chem. Lett. **13**, 11872 7 (2022)

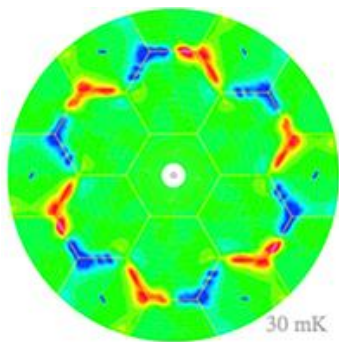
Materials: Quantum, Complex and Functional Materials

Scientific focus: Investigation of complex (multi-functional) materials for new applications

Selected Highlights 2022



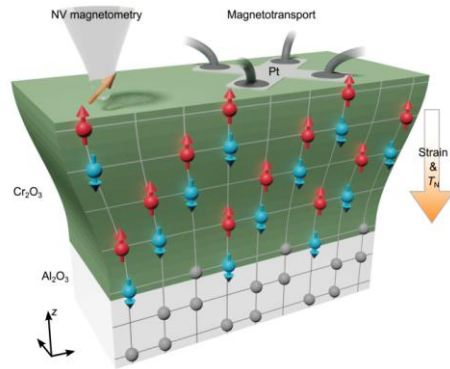
Chiral quantum state detected



W. Schweika et al., Phys. Rev. X **12**, 021029 (2022)



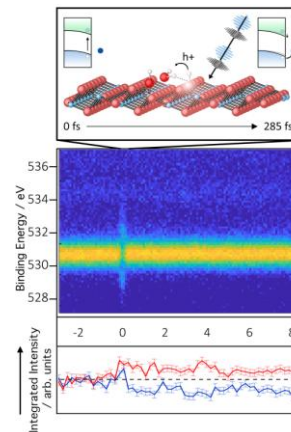
New flexomagnetic effect



P. Makushko et al., Nat. Commun. **13**, 6745 (2022)



Decoding ultrafast surface dynamics



M. Wagstaffe et al., Phys. Rev. Lett **130**, 108001 (2023)

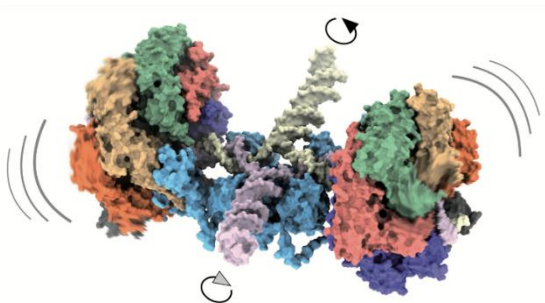
Life Science: Building Blocks of Life – Structure and Function

Scientific focus: Decoding of complex biological structures and processes for next generation of new drugs and particle therapy

Selected Highlights 2022



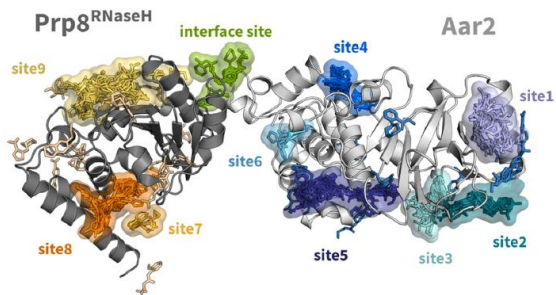
Mechanism of an ATP-driven molecular motor



J. Wald et al., Nature **609**, 630 (2022)



Large-scale crystallographic fragment screening

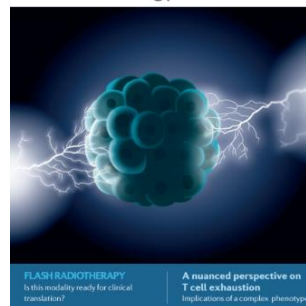


T. Barthel et al., J. Med. Chem. **65**, 14630 (2022)



FLASH radiotherapy

nature reviews
clinical oncology



M.-C. Vozenin et al., Nat. Rev. Clin. Oncol. **19** 791 (2022)

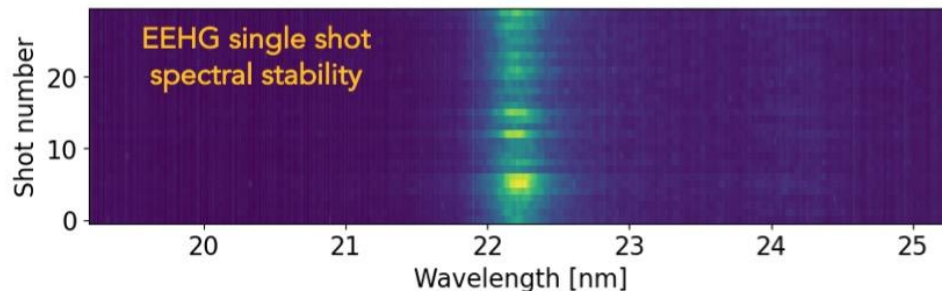
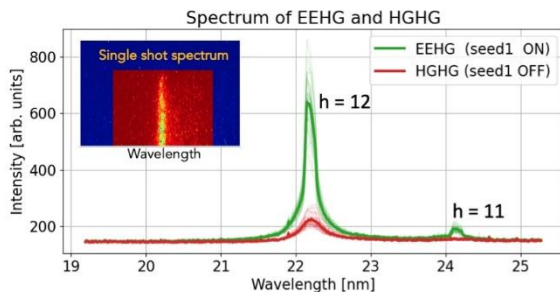
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Senate Recommendations: Overview

Recommendation	Page/Appendix
Make clear what the major challenges are that MML can address with their facilities and competence, and where the Helmholtz Association is going to play a leading role	17
Strengthen the commitment to THz methodology and science even more to become a world leader in the ongoing "THz revolution"	18
Improve coordination between materials and instrument researchers and scientists at large-scale facilities	19
Continue to support the Helmholtz mission and Helmholtz scientists by providing new measurement capabilities at large-scale facilities for users	20
Pursue outstanding, scientifically broad-based life science in the first stage of the program as proposed, ensuring that the valuable coherence of the biological research is maintained during PoF IV through joint meetings	21

Large-Scale Infrastructures (LKII): Substantial Achievements

sFLASH: FIRST Echo-Enabled HG LASING



PHOTONS

FIRST BEAM ON TARGET ON DEC. 12, 2022, WITH 3 BEAMLINES IN OPERATION

- proton beamline from cyclotron (45 MeV; pulsed)
- target-moderator-reflector (TMR) unit
- cold methane moderator
- three experimental stations in operation

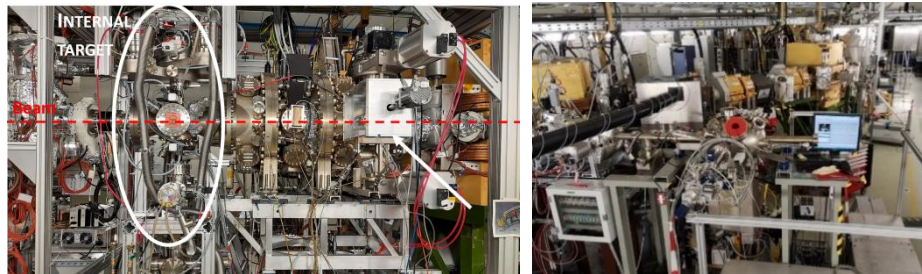


NEUTRONS

Large-Scale Infrastructures (LKII): Substantial Achievements

CRYRING@ESR IN FULL USER OPERATION

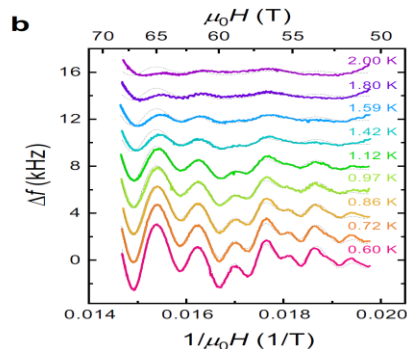
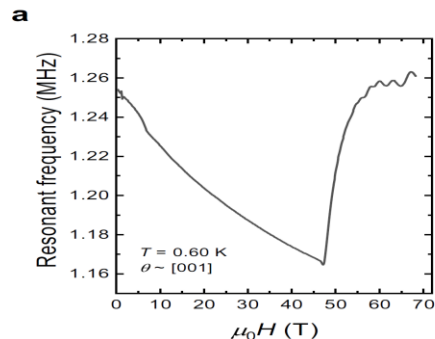
IONS



- Atomic and astro-physical reaction studies for stored highly charged ions at low energies;
- Ion solid interaction as a function of potential and kinetic energy;
- Sputtering and surface processes;
- Interaction with 2D materials.

USER OPERATION AT HLD

HIGH FIELDS

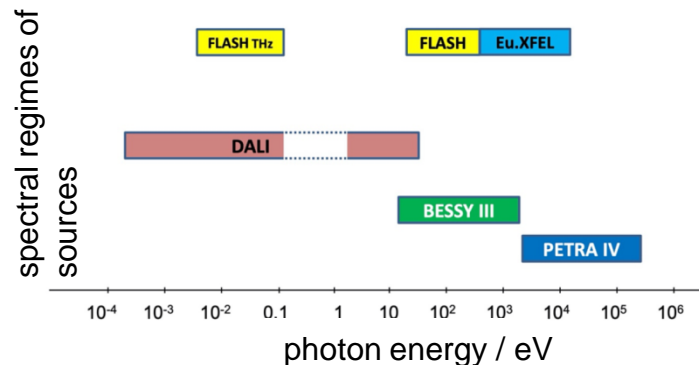


- Typical user experiment by British group;
- YbB_{12} is unconventional, so-called Kondo insulator;
- Above about 47 T metallic state;
- Quantum oscillations allow comparison with band structure and comparison with oscillations in the insulating state.

Significant Developments in Research Infrastructures

- Maintain and enhance world-leading capabilities for forefront science;
- Coherent upgrade plans for large-scale facilities shaping national and European strategy plans.

Joint Helmholtz Photon Science Roadmap (PETRA IV, BESSY III, DALI, FLASH2020+)



Complementary X-ray energy regimes (BESSY III and PETRA IV) and operation modes for VUV/soft x-ray experiments (DALI and FLASH2020+).

Nationale Strategie zur Weiterentwicklung beschleunigerbasierter Nutzereinrichtungen für die Forschung mit Photonen und mit hohen elektromagnetischen Feldern („Helmholtz Photon Science Roadmap“)

Sven Kiele, Jan Lüning, Bernd Rech, Sebastian M. Schmidt, Barbara Schramm, Christian G. Schroer, Olaf Schwarzkopf, Edgar Weckert

Helmut Dosch, Forschungsbereichs-Koordinator
Ilja Bohnet, Forschungsbereichs-Beauftragter



Coordinated with

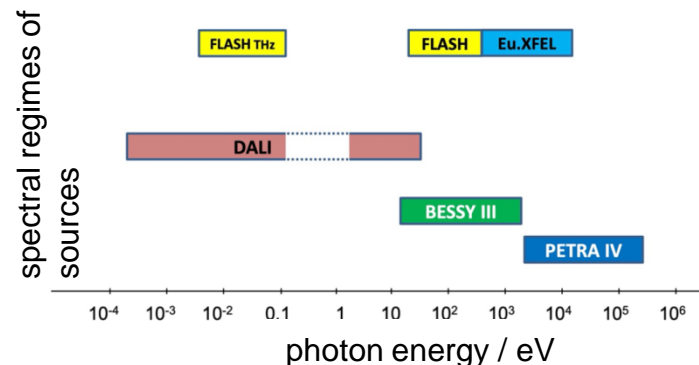


Significant Developments in Research Infrastructures

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Joint Helmholtz Photon Science Roadmap

(PETRA IV, BESSY III, DALI, FLASH2020+)



Complementary X-ray energy regimes (BESSY III and PETRA IV) and operation modes for VUV/soft x-ray experiments (DALI and FLASH2020+).



- **PETRA IV:** Proposal finished → ready to go, project start mid 2024
- **BESSY III:** CDR Phase → construction start 2029/30
- **DALI:** CDR in final stage

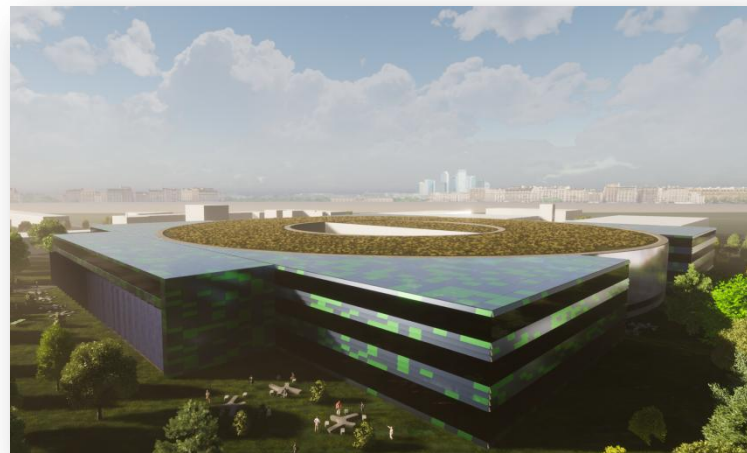
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Significant Developments in Research Infrastructures

- **BESSY III Pre-CDR submitted to FIS commission**
 - Cost projection: 976 Mio €
 - **Overall assessment „outstanding“** in written review
 - „BESSY III will certainly play a central role in the scientific areas explained in the document.[...] USPs are the facility's leadership as a key enabler of metrology with SR.“
 - „Envisaging BESSY III not only as a synchrotron source but as a more complete research infrastructure [...] is also an excellent choice“
 - „The local expertise at BESSY, in science and in all core technologies, is among the best in the world.“
 - **Recommendation for full application** of the FIS commission
 - Confirmation anticipated by Helmholtz Members' Assembly on April 25th & Helmholtz Senate on June 20th



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Significant Developments in Research Infrastructures

- **PETRA IV project proposal ready for submission**
 - Cost projection: 1541.8 Mio €
 - **Overall assessment** in written review
 - *“The new accelerator technology will enable new scientific research opportunities.”*
 - *“For the Helmholtz Association, and especially for the field of matter, the project is considered to be of great strategic importance.”*
 - *“PETRA IV will be one of the best top light sources world wide and thus the place for top research.”*
 - **Recommendation for full application** of the FIS commission
 - Helmholtz Members' Assembly on April 21st, 2020: PETRA IV is part of the Helmholtz Roadmap for Research Infrastructures (published in June 2021).



Recommendation	Page/Appendix
Develop a TDR for PETRA IV and a CDR for BESSY III as part of overall prioritized plans for MBA upgrades to these facilities.	23
Develop a CDR and a TDR for DALI infrastructure as part of ELBE upgrade	24
Ensure that synchrotron beamlines have sufficient levels of scientific and technical support for the user community.	25
Exploit the full range of capabilities for research with neutrons addressing the grand challenge issues in many areas targeted by Helmholtz.	26
Put the HIBEF facility at the European XFEL in operation during the first few years of the PoF IV period.	27
For GSI: perform the FAIR Phase-0 in accordance not only with nuclear physics, but also with the MML developments.	28
For IBC at HZDR: introduce cutting-edge technologies and/or science that will take it to a leadership position in ion beam technology and applications.	29

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Summary and Outlook

- A multitude of research highlights achieved
- COVID-19, basically all MML facilities in user operation.
 - 2022, reduction in protective measures against Corona.
- Sustainable operation: Pushing for Mail-in and Remote-access user operation: funding from the Helmholtz Association for beamline demonstrator.
- National/European strategies for Photons, Neutrons, and High Magnetic Fields.

Pushing for the realization of the national roadmap for photon facilities (PETRA IV, BESSY III, DALI, FLASH2020+).

For neutrons: advancing the High Brilliance Neutron Source (HBS).



Photons



Neutrons



Ions



High EM Fields

In 2022, MML workshops (in presence) focused on the Research Topics

Next MML conference (in presence), University of Jena 27nd to 29th of Sept. 2023



APPENDIX

Implementation of Senate Recommendations (LKI): pages 17 to 21

Implementation of Senate Recommendations (LKII): pages 23 to 29

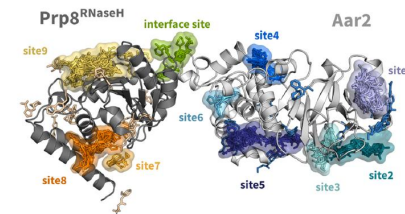
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Recommendations (1)

Make clear what the major challenges are that MML can address with their facilities and competence, and where the Helmholtz Association is going to play a leading role

MML In house research and with their largescale facilities are successfully developing their research and technical programs while quickly addressing emergent needs and new research directions

- **Fight against Epidemic Outbreaks**
 - Example of **Covid-19** (also part of the innovation pool project **FISCOV**)
 - Airborne Transmission of the SARS Coronavirus: IVF project **CORAERO**
- **Essential contributions** to the fields of Energy, Health and Materials Research
- **Essential contributions** to the European consortia **LEAPS** (photons), **LENS** (neutrons), **RADIATE** (ions), and **EMFL** (high fields)
- **Strong involvement** into **ARIE (Analytical Research Infrastructures in Europe)**; bringing together LEAPS, LENS, eDREAM, RADIATE, EMFL, LaserLab. In 2022, Jochen Wosnitza represented **ARIE** as spokesperson.



T. Barthel et al.,
J. Med. Chem. **65**, 14630 (2022)

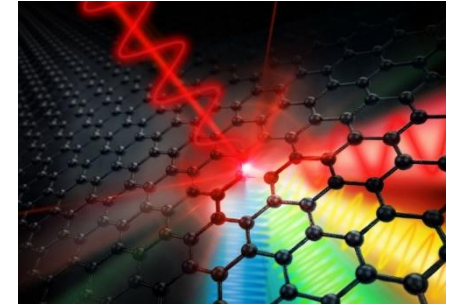
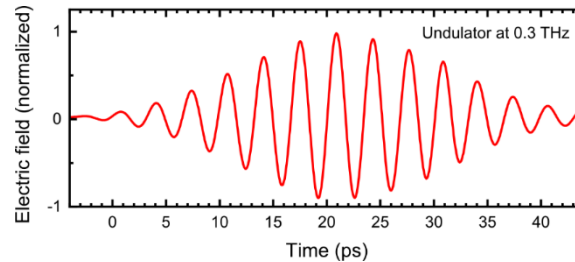
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Recommendations (2)

Strengthen the commitment to THz methodology and science even more to become a world leader in the ongoing "THz revolution"



THz sources: from ELBE to DALI



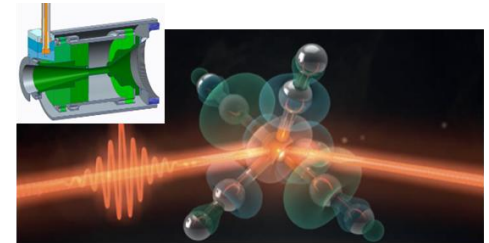
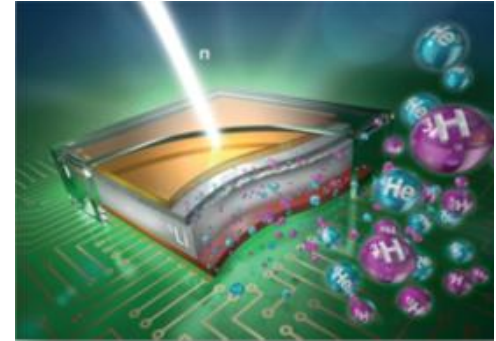
- **2021:** Preliminary CDR of **DALI** prepared and positively evaluated by HGF \Rightarrow recommendation of Senate to apply for inclusion on the National Roadmap for Research Infrastructures.
- Presently: Work on full CDR, with submission intended in summer/fall 2023; also design study and experimental test setups for crucial DALI components.
- Controlling non-equilibrium phenomena in matter with THz radiation coherently on a femtosecond scale: now at **ELBE**, in the future at **DALI** with 100 times higher pulse energy.

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Recommendations (3)

Improve coordination between materials and instrument researchers and scientists at large-scale facilities

- Scientists from the various centers work closely together in the innovation pool project **Materials Dynamics for Future Quantum Technologies: MaDQuant** and are active in Joint Labs.
- **Materials - Quantum, Complex and Functional Materials:** collaboration is promoted through **regular, cross-center and thematically oriented workshops**.
- Collaboration is strengthened by the **engagement in coordinated programs**, e.g. in the framework of SFBs and clusters of excellence.



X-ray scattering with pulsed-field magnet

Continue to support the Helmholtz mission and Helmholtz scientists by providing new measurement capabilities at large-scale facilities for users



Photons



Neutrons



Ions

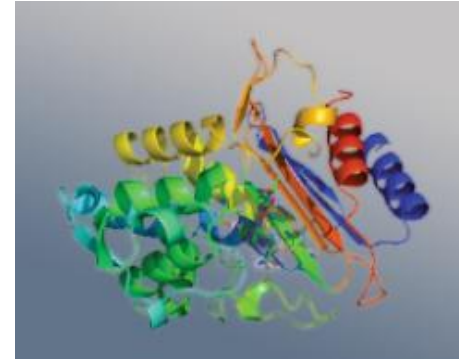


High EM Fields

- **Synchrotron and FEL sources:** further adaptation of capabilities to the needs of the user community is ongoing, including new beamlines (PETRA III – Ext., FLASH2020+, BEIChem/CatLab@BESSY II).
- **New magnetic-field beamline** (planned for ESRF) **and sample environment** at BESSY
- In 2021, **the HIBEF facility** (combination of the Facility Topics Photons and High Fields) **at XFEL** has been commissioned. 2022 dipole laser fully implemented.
- **Neutron facilities:** work is being carried out within the **Innovation Pool Project HBS** on the realization of an alternative, accelerator-based concept for neutron sources.
- **Ion facilities:** full user operation of the **new ion storage ring CRYRING@ESR**.

Pursue outstanding, scientifically broad-based life science in the first stage of the program as proposed, ensuring that the valuable coherence of the biological research is maintained during PoF IV through joint meetings

- In the topic Life, collaboration between the scientists involved is promoted through **regular, cross-center and thematically oriented workshops**.
- Participating centers work closely together in the **cross-research area innovation pool project FISCOV**, in which the large research infrastructures are used for research **in fight against Covid-19**.
- **CCA Structural Biology and Biological Processes & Radiation Research:** substantial contributions



Recommendations for the program-associated large-scale infrastructures (LK II)



Photons



Neutrons



Ions



High EM Fields

Associated Large-Scale Infrastructure (LK II): Photon Facilities

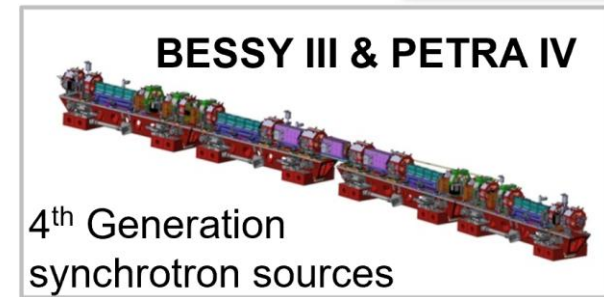
Develop a TDR for PETRA IV and a CDR for BESSY III as part of overall prioritized plans for MBA upgrades to these facilities.

PETRA IV

- Important milestones toward a **PETRA IV TDR**:
 - Updated design of the new storage ring magnet lattice (xxxxx)
 - Portfolio of beamlines and experimental stations finalized
 - Planning of additional infrastructure and new user services completed
 - Funding proposal close to completion

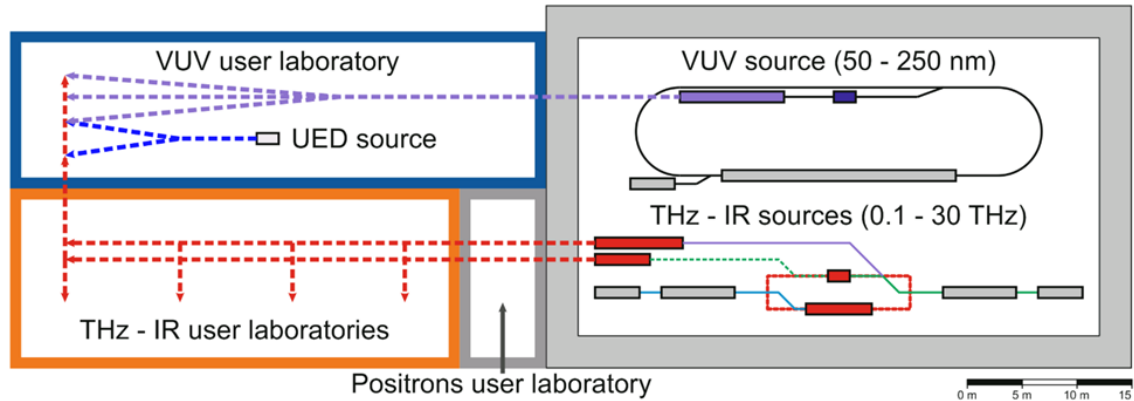
BESSY III: Based on expert workshops and advice by PAC/SAC

- In the reporting year, a preliminary CDR (Pre-CDR) for BESSY III was completed and submitted to the FIS Commission of the Helmholtz Association.



Associated Large-Scale Infrastructure (LK II): Photon Facilities

Develop a CDR and a TDR for DALI infrastructure as part of ELBE upgrade.



- **2020:** A preliminary CDR of the **DALI** project submitted for inclusion in the **Helmholtz Roadmap for Research Infrastructures** and positively evaluated by the Helmholtz Association in 2021.
- **Work has started on a CDR**, the submission of which (phase II in the Helmholtz Roadmap process) is planned for summer/fall 2023.
- **2023:** The official **inclusion in the Helmholtz Roadmap** will take place after a positive evaluation

Associated Large-Scale Infrastructure (LK II): Photon Facilities

Ensure that synchrotron beamlines have sufficient levels of scientific and technical support for the user community.

- **Close contact with the user community** is ensured through regular dedicated workshops,
- planning **new facilities or facility expansions** for our users.
- substantial **user support** needed for the expected **large amounts of data**.

But need for strengthening (more resources and personnel needed)

- data management /data handling,
- automation.
- remote and hybride access / mail-in.

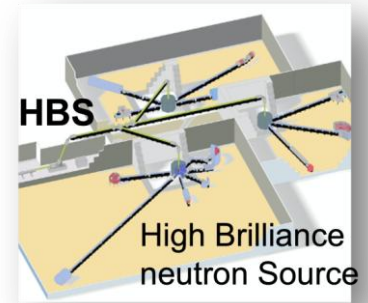


Temporary support (2023 – 2025): funding from the Helmholtz Association for demonstrator beamlines (ROCK-IT).



Exploit the full range of capabilities for research with neutrons addressing the grand challenge issues in many areas targeted by Helmholtz.

- Instrumentation and source development: **scientific and societal requirements and opportunities** are addressed at a series of workshops and conferences:
 - Instrument renewal program **MLZ2030**
 - Helmholtz contribution to the **European Spallation Source**
 - **HBS** project for a novel accelerator-driven neutron source
- Research with neutrons to solve urgent societal problems as presented by strategy paper of the **League of advanced European Neutron Sources LENS**
- The **Global Neutron Scientists (GNeuS)** Program trains a new generation of excellent neutron scientists

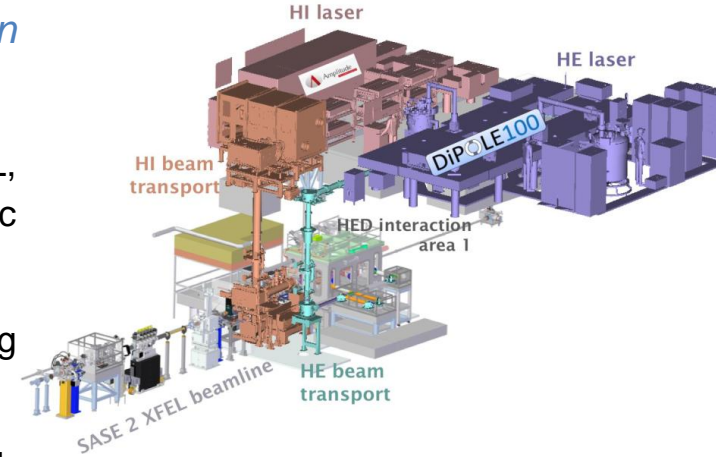


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Associated Large-Scale Infrastructure (LK II): High Field Facilities

Put the HIBEF facility at the European XFEL in operation during the first few years of the PoF IV period.

- In 2022 several **user experiments** at **HED/HIBEF** at EuXFEL, using Diamond Anvil Cells and ReLaX Laser (e.g., relativistic plasmas, laser driven shocks).
- **DiPOLE** laser fully implemented. User-supported commissioning and first **user experiments** in 2023.
- Realization of the **HIBEF beamline for materials research** experiments at the European XFEL" announced for 2022 was achieved, with the delivery of a pulsed capacitor bank to the HIBEF beamline" for high-field magnets. Commissioning in 2023.



MML researchers contribute to the EuXFEL instrumentation via the Helmholtz International Beamlines (HIB): **SFX** continues to contribute critically to the ongoing success of the **SPB/SFX** instrument through both funding and expert collaboration. For **hRIXS**, first user experiments performed in **2022**.

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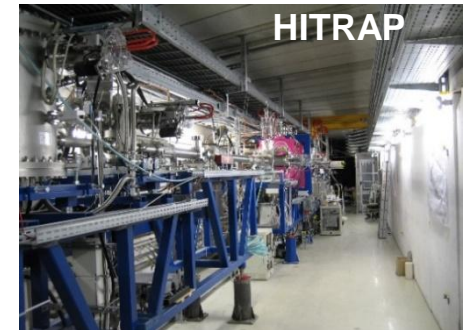
Associated Large-Scale Infrastructure (LK II): Ion Facilities

For GSI: perform the FAIR Phase-0 in accordance not only with nuclear physics, but also with the MML developments.

Since 2020/ 2021 new MML facilities in user operation:

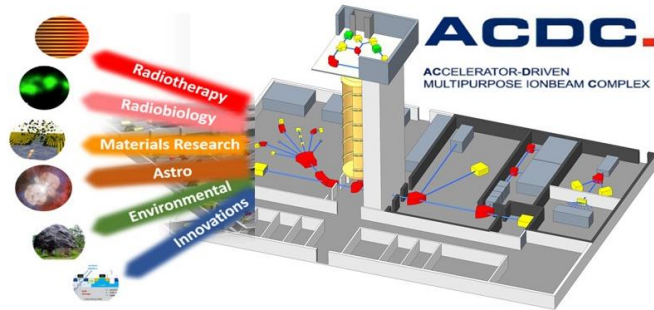
- **2020/2021: New ion storage ring CRYRING@ESR** (first FAIR facility) commissioned
- **2021: Proton microscopy PRIOR** in user operation
- **2021: New PHELIX laser beam line** (200 J; up to 10 ns) to high-energy ion-beam experimental area HHT
- **2022: CRYRING@ESR** in full user operation
- **2022: Commissioning of decelerator for trapping facility HITRAP**

50 % of the user beamtime at GSI in 2024/2025 is assigned to experiments in the realm of **MML**.



For IBC at HZDR: introduce cutting-edge technologies and/or science that will take it to a leadership position in ion beam technology and applications.

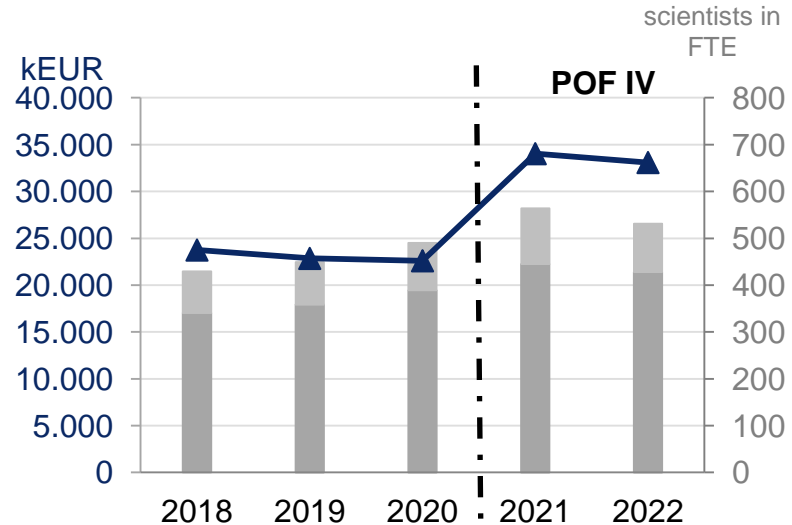
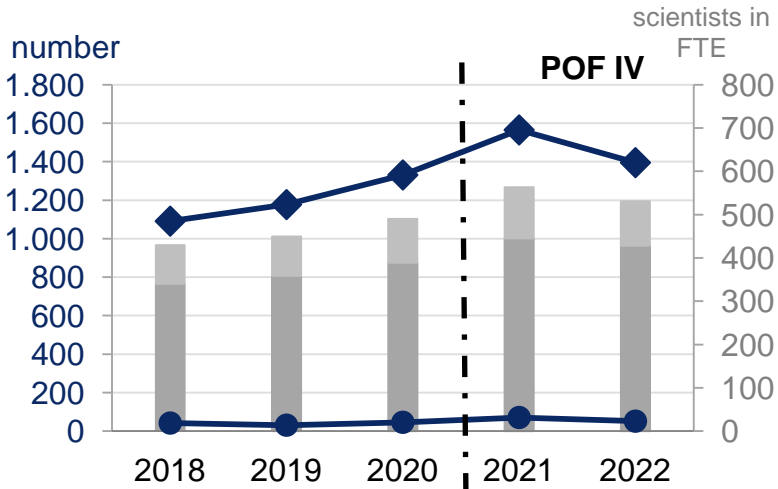
- **IBC** will strengthen its position as leading ion beam center in materials research
 - new analysis methods with highest lateral/depth resolution
 - low-energy ion doping and modification of 2D materials
- The **low-energy ion laboratory** commissioned in 2022/23 and enter user operation in 2024



- Strengthening of AMS, the **future IBC extension ACDC (Accelerator-Driven Multipurpose Ion Beam Complex)**
- Concept of the research infrastructure has been elaborated. A proposal for funding by the common Helmholtz infrastructure fund for strategic expansion investments can be submitted in 2024.

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Program development - Indicators



- number of core-funded scientists
- number of third-party funded scientists
- WoS-, SCOPUS or Open Research Europe indexed publications
- finished dissertations
- third-party funding