PETRAIV. NEW DIMENSIONS

A sustainable accelerator?

Sustainability at PETRA IV.

Andrea Klumpp 16.12.2024



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DESY Sustainability D6 – Staff unit to the directorate

Our team



Denise Völker Head of D6



Frank Merker Technical monitoring



Kathrin Schulz Research funding Specialist for BMBF Civil construction Support FLASH



Eva Leistner Technical monitoring



Andrea Klumpp Sustainability in **PETRA IV**. project



What is sustainability at DESY

Broad approach with focus on energy efficiency

Science

- Science case supports sustainability goals
- High number of beamlines
- Innovation and technology transfer

Personnel

- Sustainable career development
- Keep knowledge on campus and attract best talents



Infrastructure

- Reuse of infrastructure
- Energy saving technologies
- New building concepts and materials

Supporting processes

- Key infrastructure of Science City Bahrenfeld
- Cooperation in campus security, safety, enviromental protection and mobility

Management

- Transperent to employees and stakeholders
- Documentation of processes and decions
- Boost socio-econimic impact (education, employment...)

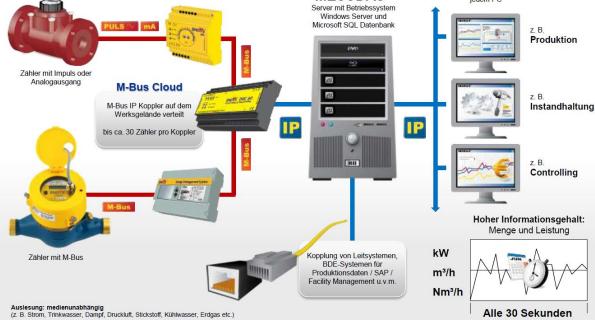


Energy approach

Energy monitoring system

Detailed, unified meter marking, centralized data collection and analysis, meters directly connected to database

- For Electricity, Water, Heat, Cooling
- → Enables for user-based/sourcerelated accounting, identification of efficiency potentials and therefore more awareness



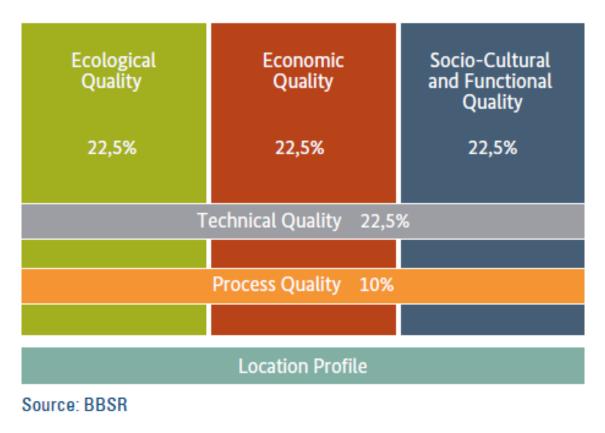






Civil construction

LCA for buildings



Main Criteria Groups of the BNB System

National certification system for sustainable building (BNB):

- Consideration of the whole life cycle of the building (LCA)
- Ecological, economic, socio-cultural and technical qualities are rated equally
- End of life and recycling are included
- BNB silver for all new buildings at **PETRA IV.**
- New experimental hall with equivalent criteria



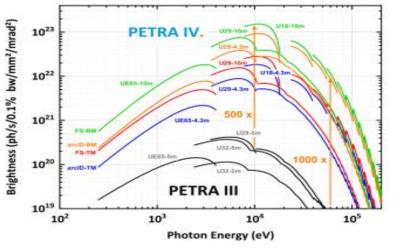


PETRA IV

Upgrade PETRA III : PETRA IV.



What is the benefit of the upgrade?

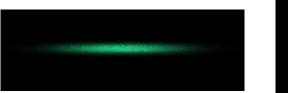


Spectral brightness of PETRA IV (H6BA lattice) compared to PETRA III [1]

Brilliance increase by →500 x (hard X-rays) →1000 x (high-energy X-rays)

PETRA IV. brilliance at 100 keV higher than for 10 keV at PETRA III today!!

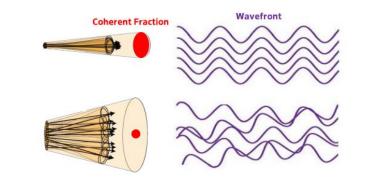
Photon source size –ideal imaging capabilities





Comparison of the beam emittance for PETRA III (left) and PETRA IV (right)

	PETRA III	PETRA IV
Horizontal	1300 pm rad	20 pm rad
Vertical	10 pm rad	5 pm rad



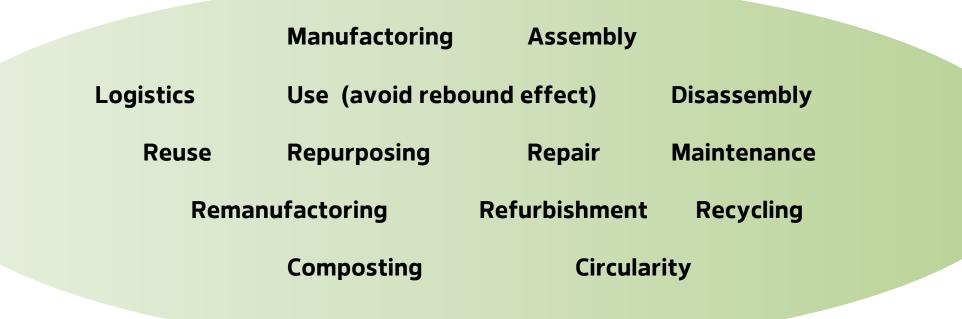
Coherence of the emitted light for PETRA III (bottom) and PETRA IV. (upper figure)



Design 4 Sustainability

Design 4 sustainability? – Design for:







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Innovate solutions

- Rethink how to provide the benefit
- Anticipate technology change
- Optimise or integrate functions
- Integrate natural systems



SUSTAIN

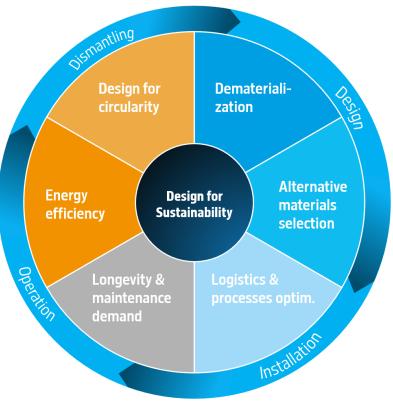
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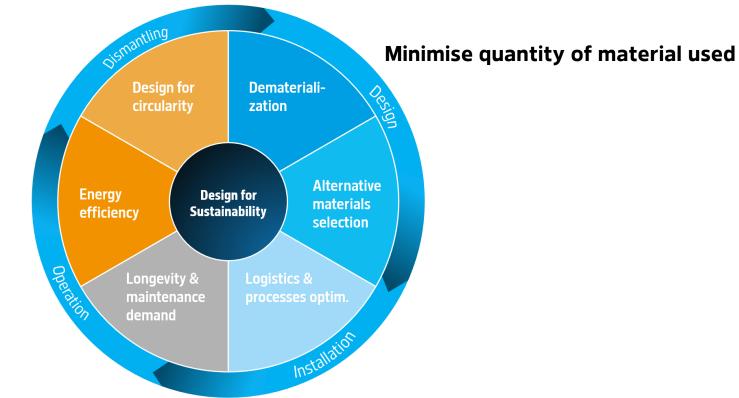
SUSTAIN ABLE DESY.





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SUSTAIN

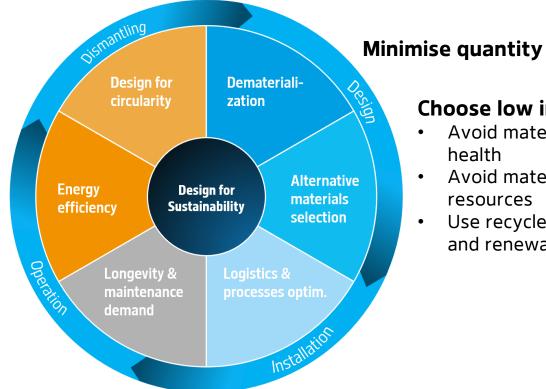
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Minimise quantity of material used

Choose low impact materials

- Avoid materials that damage ecology or
- Avoid materials that deplete natural
- Use recycled, reclaimed, waste by-products and renewable resources



SUSTAIN

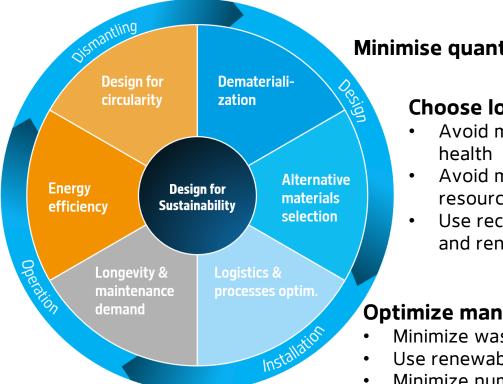
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Optimize manufactoring and logistic

- Minimize waste energy use in production
- Use renewable and carbon-neutral energy
- Minimize number of parts, materials and steps in production
- Reduce weight and volume of product and packaging



SUSTAIN

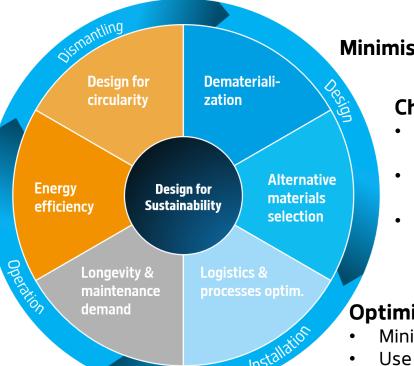
- Consider reusable packaging systems
- Use lowest-impact transport and source locally

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٠

٠



SUSTAIN

Maximise lifetime

- Design for durability
- Design for maintenance, easy ٠ repair, reuse and exchange
- Consider upgradable products and second life with different function

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Innovate solutions

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Minimize used impact

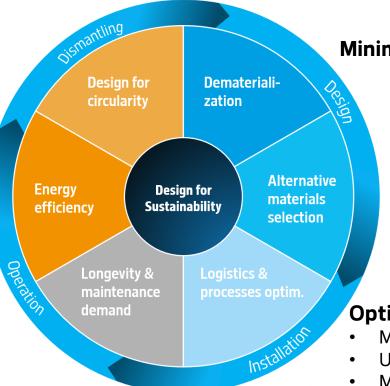
- Change behaviours and encourage lower impact consumption
- Reduce energy, water and material requirments during use
- Design for carbon-neutral or renewable energy

Maximise lifetime

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- Consider reusable packaging systems
- Use lowest-impact transport and source locally



SUSTAIN ABLE DESY.

Optimize end-of-life

- Design for easy disassembly, component reuse and recycling
- Integrate with used-product collection models
- Design for safe disposal and biodegradability

Minimize used impact

- Change behaviours and encourage lower impact consumption
- Reduce energy, water and material requirments during use
- Design for carbon-neutral or renewable energy

Maximise lifetime

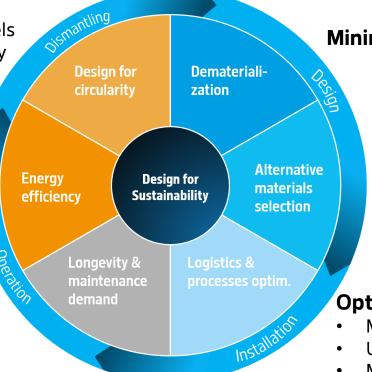
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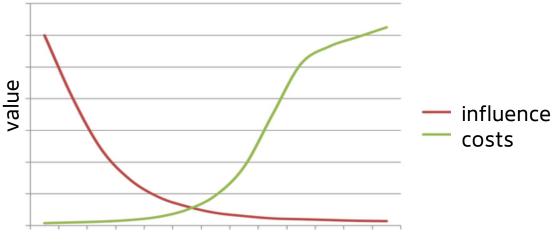


- Consider reusable packaging systems
- Use lowest-impact transport and source locally

How to ...



Start as early as possible



design phase or time

Our Roadmap

- Analyze the starting point and/or current status
 - Legal requirements (VDI, ...)
 - How do others do? (eg. industry)
 - LCA (collecting information and experiences)
- Discussions with developers and technicians
 - > How to include sustainability in existing processes
 - Find examples for projects
- Develop of strategies and ideas
 - Stakeholder, approaches, possible projects
- In cooperation with developer and technicians: developing a training programme for physicians and technicians



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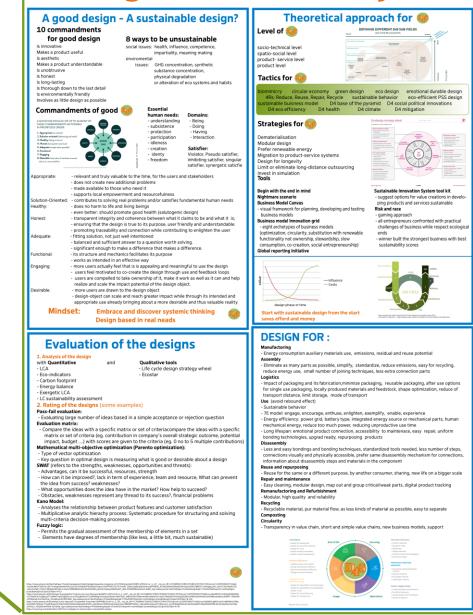
First steps at DESY



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Design for sustainability

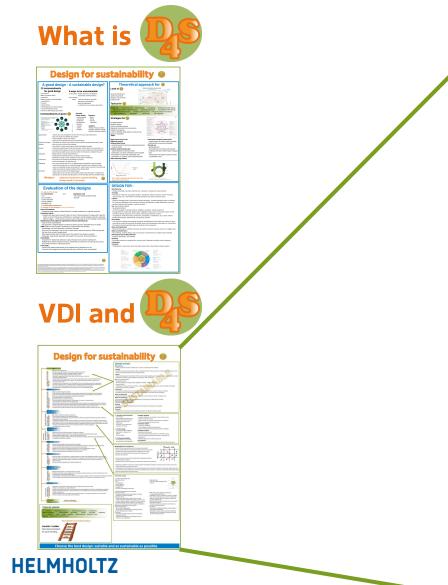


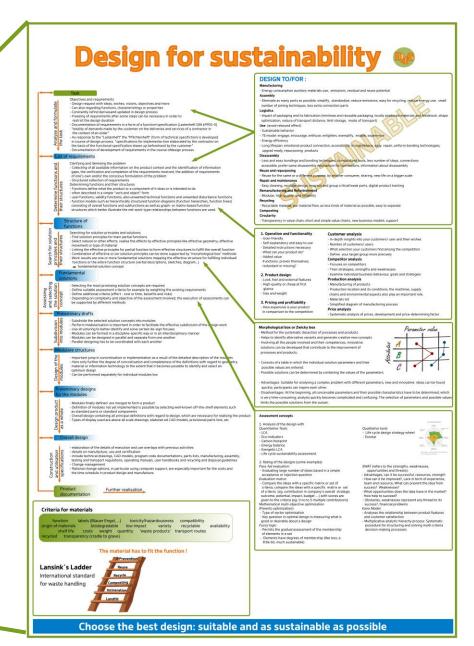




First steps at DESY









First steps at DESY









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Life Cycle Assessment







Why we need accounting - Groundwork for any sustainability or CSR strategy

- Comply With Regulations and laws (50001,...) - Development of more sustainable instruments and components

Methodes

- LCA Standardised (14040:2006 and 14044:2006, DIN EN ISO 14040, 500001 ...) Procedure for recording and evaluating environmentally relevant processes - Cross-media consideration: All relevant potential harmful effects on the environmental media soil, air and water must be taken into account all environmental impacts are considered.
 - for the carbon footprint and water footprint, only one environmental impact is considered in each case (calculation methods are based on the LCA method)

Material and energy balances differ from life cycle assessments in that they relate to a specific period (often referred to as the balance sheet year) and are not based on the causation principle (what material and energy flows has the product caused over its entire life cycle?) Due to their methodological proximity, it is not always possible to make a clear distinction between life cycle assessments and material flow analyses. Put simply, material flow analyses tend to focus on the quantities and paths of a system's substance, material and energy flows. Life cycle assessments, on the other hand, also analyse and evaluate the environmental impacts associated with these flows

Sustainability accounting for research facilities

More - ABC-analysis: multidimensional cradie-to-grave LCI for material and energy flows - CML-methode: multidimensional cradie-to-grave impact analysis for material and energy flows (14 categories) - CO2-accounting one dimensional cradle-to-gate impact analysis for directe and indirecte GHG

Society

- Politicians...

- Eco-indicator 99 one-dimensionally aggregated cradle-to-grave impact analysis for material and energy flows (9 categories

How to do LCA 1. Definition of goal and scope of investigation

Goal and - Laws Optimization of processes and Recipient technology Decision suppor -Definition starting point Scope





Scopes for accelerator facilities (talk 15.02.2024 Jean-Luc Revol

3. Impact assessment (LCIA)

Selection of indicators and models: Human toxicity, Global Warming Potential, Ecotoxicity, Acidification, Eutrophication Classification: assigning Life Cycle Inventory to defined impact categories Impact Measurement: finally calculate all equivalents and sum up in overall impact category totals

Tools

- LCA with Simulation program: GaBi, Open LCA, SimaPro, Sphera, Ecochain, Earth Shift Global, iPoint, Pré sustainability, ... and Data base: ProBas, ELCD, ÖKOBAUDAT, Literature research (LCA's for materials like rare earth elements, for technical components like electro motors....) Technical monitoring (energy, fresh water, heating, cooling...)

Laws and standards

- ISO 14001: Environmental Management System: ISO 14001 defines the criteria Environmental Management Systems have to comply with. It ensures that environmental impacts are being measured and improved.
- ISO 14021: Environmental Claims and Labels: ISO 14021 defines how specific environmental claims have to be and how they have to be formulated and documented. ISO 14040:2006: Life Cycle Assessment Framework: ISO 14040:2006 defined the principles and framework of a Life Cycle Assessment. Many parts of this article are based on ISO 14040:2006.

ISO 14044: The Update: ISO 14044 replaced earlier versions of ISO 14041 with ISO 14043.

ISO 14067: Quantifying carbon footprint: ISO 14067 defines how the carbon footprint of products is quantified during a Life Cycle Assessment. ISO 50001: Efficient Energy Management: ISO 50001 defines Energy Management Systems

- employees for Campus Normalization

user, publications or measure time for research infrastructure (machine, tunnel...)

 Choosing of supplier in procurement - Strategical decision (Can we do this science or shouldn't we do) Which changes has large impact which less - Definition of start point for improvement

OA - Not internationally standardised

- Methods can vary greatly depending on the issue at hand, the research interest and the analysis system Records substance and material flows associated with specific products

processes, services or entire areas of need, such as construction and housing, mobility or nutrition - Raw materials or resources, different types of energy, water, emissions

to air. land, or water by substance

Critical volumina: multidimensional cradle-to-grave LCI (pollution of air and water, waste, energy consumption) Cumulative energy expenditure: one-dimensional cradle-to-gate LCI for energy expenditure

- Cumulative energy expenditure: one-dimensional cradie-to-gate LCI for energy expenditure - MIPS: one-dimensional aggregated cradie-to-grave LCI for material flows and service units - Method of ecological scarcity: one-dimensional aggregated gate-to-gate LCI for material and energy flows

UBA impact indicators: multidimensional cradle-to-gate impact analysis for material and energy flows in different categories

Indicators Greenhouse Gases (GHG): Carbon dioxid (CO2), Methane (CH4), Nitrous oxide (N2O). Ozone (O3)

Chlorofluorocarbons (CFCs and HCFCs), Hydrofluorocarbons (HFCs), Perfluorocarbons (CF4, C2F6, etc.), SF6, and NF3

Water footprint Reduced LCA: which factors are important for us? Complete LCA: including all ecological and socio-economical impacts

Models Cradie-to-grave: - Analyze a product's impact along the 5 product lifecycle steps - Cradle is the inception of the product with the sourcing of the raw materials

- Grave being the disposal of the product - Transportation is mentioned as step 3, but can, in reality, occur between all steps
- Only assesses a product until it leaves the factory gates before Cradie-to-gate: is transported to the consumer
- Common in environmental product declarations (EPD) Cradle-to-cradle: - Circular Economy - Variation of cradle-to-grave, exchanging the waste stage with a recycling process
- To reduce complexity, only one value-added process in the Gate-to-gate: production chain is assessed

2. Life cycle inventory (LCI)

- Input/Output flows Technical monitoring for electricity, water heat, cooling Ouestionnaires - Use of averages Use of flow models in order to miss nothing

4. Evaluation

Identifying significant issues based on our LCI and LCIA phase Evaluating the study itself, how complete it is, if it's done sensitively and consistently - Conclusions, limitations, and recommendations



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Life Cycle Assessment

Life Cycle

It starts with the design

"LCA is a tool for the analysis of the **environmental** burden of **products** at all stages in their **life cycle**"

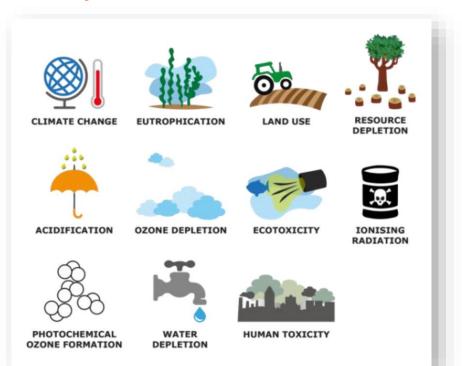
+ Social

+ Governance



What is being considered:

Not only Greenhouse Gases



I Source: European Commission, Joint Research Centre, Cristobal-Garcia, J., Pant, R., Reale, F., et al., *Life cycle assessment for the impact assessment of policies*, Publications Office, 2017, <u>https://data.europa.eu/doi/10.2788/318544</u>

First GWP calculations for magnets have been done. Now a complete LCA for a power supply is ready!



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Life Cycle Assessment

Basics

WHAT'S THE ENVIROMENTAL IMPACT OF THE PRODUCT?



Why ask?

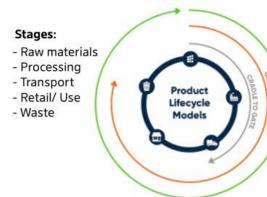
Management Make sustainable decisions

Product Development Develop sustainable products Sales & Marketing

Prove sustainable claims Supply Chain

Find better suppliers

What is the "Life Cycle"



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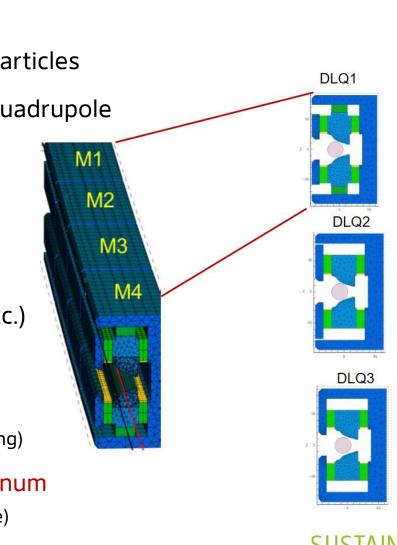
Ökobilanz (LCA) - Vollständiger Leitfaden für Einsteiger - Ecochain - DE

Examples

Bending magnets for PETRA IV.

Permanent magnet-based dipoles with transverse and longitudinal gradient

- Dipole magnets change the direction of moving charged particles
- H6BA lattice: DLQs combine the function of a dipole and quadrupole magnets to save space
- Soft iron poles and yoke; SmCo magnets
- Thermal shims for temperature compensation
- Modular concept, unification across the 3 DLQ types as much as possible (yoke, block size, mounting, shimming etc.)
- **144** DLQs of each type to build, i.e. ~**2000** modules
- Energy savings: nearly 2.87 GWh/year (calculated with 6500 h operation time per year; without cooling and heating)
- For all electromagnets in PETRA IV nearly 6.4 GWh per annum (6500 h operation time)

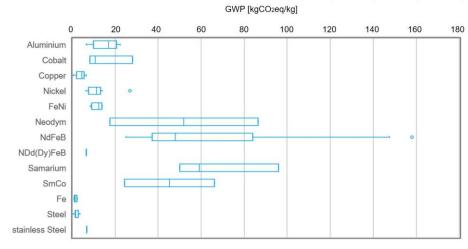




Global warming potential

Literature research

- Round about 100 papers
- Different regions, techniques, data bases, calculation programs
- Cradle to gate LCA's
- Dependend on material more or less publications (Cu more than 20, Sm 3)
- Good overview to judge the values is shown in the picture



Justment of values

н (A) Global Warming Potential (kg CO₂-eq/kg) Li Be N 0 F Ne 7.1 122 15 Na Mg AI CI Si P S Ar 8.2 к Zn Ge Br Kr Ca Co Ni Cu Ga As 5,710 8.1 33.1 2.4 1.0 1.5 8.3 6.5 2.8 3.1 205 170 0.3 3.6 Rb Nb Mo Tc Cd Xe Sr Zr Ru Pd Sn Sb Те Ag 196 3.2 15.1 1.1 5.7 3.0 12.5 2,110 3,880 102 17.1 12.9 21.9 Cs Ba Та W Os Pt Po At Rn Hf Re Ir Au Hg TI Pb Ri La-Lu* 0.2 131 260 12.6 450 4,560 8,860 12,500 12,500 12.1 376 1.3 58.9 Fr Ra Rf Db Sg Bh Hs Mt Ac-Lr

*Group of Lanthanide	La 11.0	Ce 12.9	Pr 19.2	Nd 17.6	Pm	Sm 59.1	Eu 395	Gd 46.6	Tb 297	Dy 59.6	Ho 226	Er 48.7	Tm 649	Yb 125	Lu 896
**Group of Actinide	Ac	Th 74.9	Pa	U 90.7	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr

Life Cycle Assessment of Metals: A Scientific Synthesis Philip Nuss1*, Matthew J. Eckelman www.plosone.org 1 July 2014 | Volume 9 | Issue 7 | e101298

- Large spreading in values
- Permanent magnetic material from LCA for electromotors
- Accuracy of values only makes sense in integers
- GWP for SmCo should be calculated by GWP from the incredencies



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Calculation of the Global warming potential



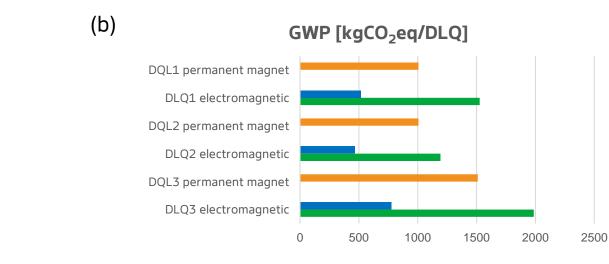
		DI	_Q1	D	LQ2	DLQ3		
Material	GWP [kgCo2eq]	amount	GWP	amount	GWP	amount	GWP	
AI	16	20	320	20	320	30	480	
pure iron	2	112	224	112	224	168	336	
FeNi	11	1,21	13	1,21	13	1,81	20	
SmCo	27	16,47	445	16,47	445	24,70	667	
Steel	2	2,42	5	2,42	5	3,63	7	
Sum for material		152	1007	152	1007	228	1510	

Permanent magnetic design

(a)

	DL	.Q1	DL	.Q2	DLQ3		
Material	GWP [kgCo2eq	amount	GWP [kgCo2eq]	amount	GW [kgCo2eq]	amount	GWP [kgCo2eq
Copper (Cu)	4	34kg	134	31kg	124	50kg	200
Steel	2	189,6kg	379	170,6kg	341	287,6kg	575
Sum for material		224 kg	515	202 kg	465	338 kg	776
power consumption per year (6500h)	0,410 ¹	8255 kW	3384	4355 kW	1795	7215 kW	2967
power consumption per year (6500h)	0,03 ²	8255 kW	248	3095 kW	131	7215kW	217
Sum GWP (n)			3900		2260		3743
Sum GWP (e)			763		596		993

Electromagnetic design



DQL1 permanent magnet

GWP [kgCO₂eq/DLQ]

DLQ1 electromagnetic DQL2 permanent magnet DLQ2 electromagnetic DQL3 permanent magnet DLQ3 electromagnetic Ω 500 1000 1500 2000

GWP for (a) material (electromagnets- blue and permanent magnets - orange) and (b) including estimated energy consumption (material + renewable electricity for 2 years - green)

Energy GWP from UBA for renewable electricity



Energy savings

1. Operation of magnets

- per cell 2 magnets from each kind, 72 cells in the ring
- $P=72x2x(P_{DQ1}+P_{DQ2}+P_{DQ3})\sim 440kW$
- Per year (6500 h operation time per year): 2.86GWh/year

2. Cable losses

- Each magnet needs an average cable length of 20m to the media shaft and 70m to the power supply
- Cable losses per magnet: DQ1~ 331,29W (120mm²=262,67W),DQ2 ~ 195,23W (120mm²=154,8W)
 DQ3 ~ 200,4W (120mm²=158,89W)
- $P=72x2 (P_{DQ1cable}+P_{DQ2cable}+P_{DQ3cable}) \sim 104,98kW (120mm^2=83kW)$
- Per year (6500 h operation time per year): 0.68GWh/year (120mm²=0.54GWh/year)



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Challenges in the use of permanent magnets

Beginning of life cycle: Mining and Processing

- Rare earths are mined and processed under destructive social and environmental conditions
- No alternative sources or certified mining and processing available

In operation

- Temperature fluctuations and radiation damages reduce the life span
- Magnetic field is not adjustable, so changes in trajectories can not be compensated
- Magnetic field can not be switched off (Safety aspects like maintenance)

End of life cycle: Recycling

• So far no industrial recycling chain

Workshop at DESY 6th-8th February 2023

https://indico.desy.de/event/35655/



Basis

Energy monitoring

Civil construction

LCA for technical

components

Infrastructure

Operation

Research

Finale

At work

"This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 101004730"





a) **Private, illegal minning in China**; <u>http://www.chinahush.com/2009/10/21/amazing-pictures-pollution-in-</u>

china/; 2009 - 2011 ChinaHush is licensed under a Creative Commons License *Copyright:* Lu Guang; b) **air pollution by heavy industries**; Quelle: china-digital-times *Copyright:* My Essentia com blog;

- c) In-Situ-Leaching; Quelle: Web-Page Bellona
- Copyright: Andrej Ozharovsky;
- d) Entrance to waste disposal for radioactive waste from REE production in Bukit Merah in Kledang mountains; built for 20 years storage of radioactive waste (14 Mrd years radioactive half-life); 1985 Copyright: Consumer Assciation Penang

Beitrag: <u>Collector</u> Lizenz: <u>Creative Commons (CC-BY-NC-SA) V.3.0</u>



Goal and scope definition



Goal and Scope What do we want to measure

- Why do we do the LCA For whom (audience)
- Define the product to measure Which parts of the life cycle? Which impact category (CO2, water,...)
- What do we exclude?

Ökobilanz (LCA) - Vollständiger Leitfaden für Einsteiger - Ecochain - DE

- Experience with LCA:
 - How to proceed?
 - Which indicators are useful?
 - Which programme fits best?
 - What can we learn from LCA?
 - What to look out for?
 - How much work is it?
 - What are the difficulties?
- Evaluation of the sustainability of the device
- Identify the sustainability potential of the device



Goal and scope definition



- Goal and Scope What do we want to measure
- Why do we do the LCA For whom (audience)

B Define the product to measure Which parts of the life cycle? Which impact category (CO2, water,...)

What do we exclude?

More than 4000 power supplies will be needed for PETRA IV

- Up to 3 power supplies have to be replaced weekly
- Hot-swap system also requires some devices
- Decision: A home-built and -designed power supply should be used
- Reasons: longer life, easier to repair, tailored to requirements

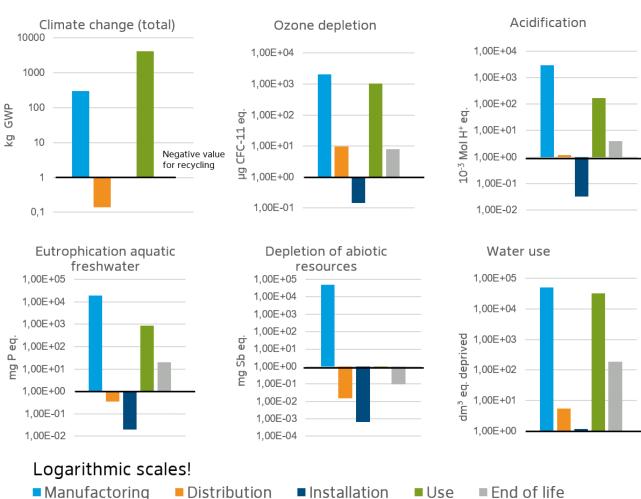




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LCA for a power supply

- Detailed Life Cycle Assessment of a power supply at PETRA IV
- More than 4000 power supplies for PETRA IV needed
- Included are extraction of material (mining, processing...), production, transport, operation, dismantling, recycling, disposal
- More than 1730 parts (approx. 400 capacitors and 280 resistors)
- The weight 22.6kg, P= 2.3- 4.5 kW, Pv_Standby= 50 W, service life: 20 years
- Energy consumption : 160.180 kWh



Biological inspirated Girder



- Inspired by corals
- Design a girder structure with high eigen-frequencies, a high stiffness, and a low mass
- Using topological optimisation program
- Casting the girder with casting iron

	Material	Weight	CO2 Footprint
ESRF ⁽¹⁾	Steel (S235 JR)	Approx. 6 ton +15% offcuts	7.8 tons CO ₂ eq/ton ⁽²⁾
PETRA IV	Steel (EN-GJS-600-3U)	5t no offcuts	4.4 tons CO ₂ eq/ton ⁽³⁾

(1) The Girders System for the New ESRF Storage Ring (cern.ch)

(2) OEKOBAU.DAT (oekobaudat.de) 1.125 ton CO2eq/ton

(3) co2-leitfaden.pdf (guss.de) 0.881 ton CO2eq/ton

Heritage from PETRA I

PETRA I tunnel reused for Petra IV.



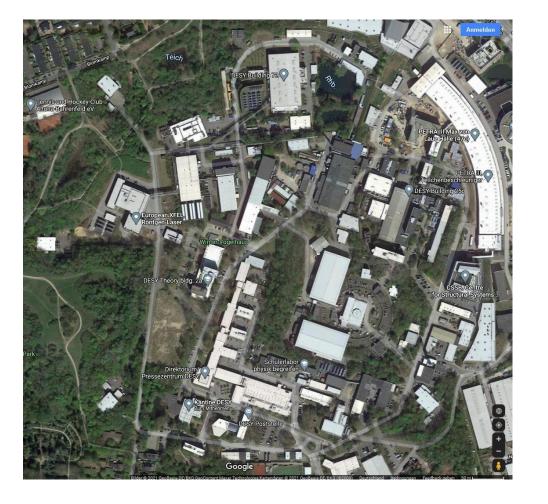
Basis

- Energy monitoring
- **Civil construction**
- LCA for technical components

At work

Infrastructure Operation

- Finale
- Research



PETRA IV Tunnel

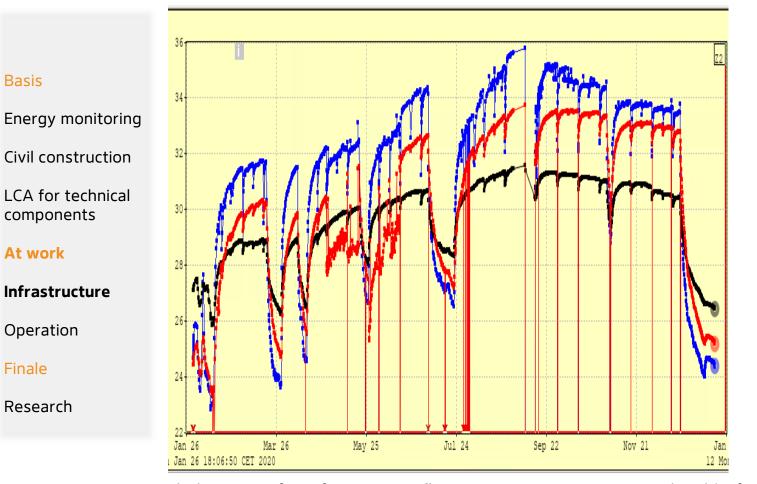
Outside the experimental halls the old PETRA I tunnel will be reused

- 6 old sections, 100 300 m long, in total ~1 km
- The old sections of the tunnel are below streets, buildings, a park.
- The tunnel is covered by 3 10 m of soil.



Tunnel temperature PETRA III

Heated and unheated sections



Tunnel Climatization today:

- Air (25° C) blown in every 300/600 m
- Cooling water inlet: 25° C

Temperature over one year

- Temperature difference between positions **up to 5°C**
- Operating schedule of PETRA clearly visible
- Summer and winter time visible

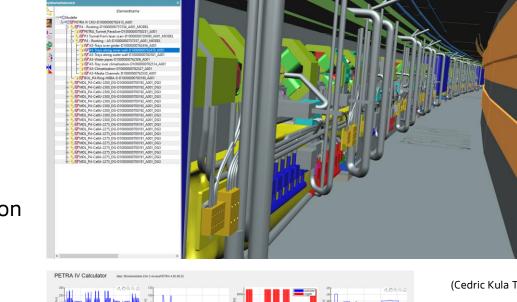


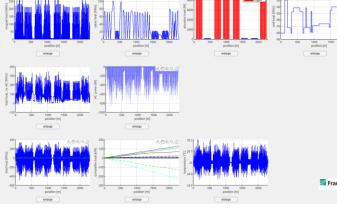
3D calculation of tunnel air and heat flows



Cooperation with Fraunhofer Magdeburg for CFD-simulation (fluid dynamic)

- **Digital Twin** of the tunnel in CAD (not yet completed) Single parts can be selected and hidden It can be rotated etc.
- A list with all consumer of electricity with their heat input (called Stromkreisliste)
- Including the cooling capacity and the position of air conditioners
- Fluid dynamical simulations:
 - Heat distribution also for corners and hidden places
 - Optimization for cooling and heating (in shutdowns)
 - Optimization of cabeling





(Cedric Kula TAC)

screenshot of the app and first test results (R. Zimmermann)



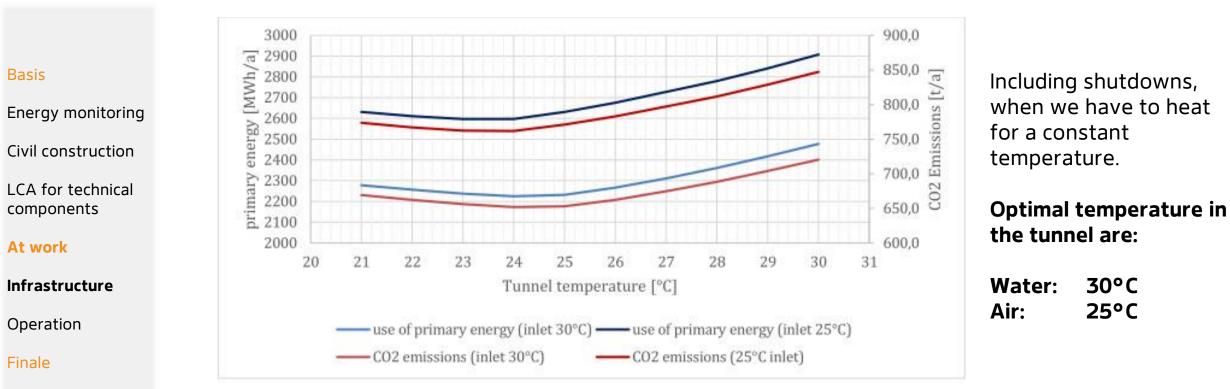
- Basis
- Energy monitoring
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At work

- Infrastructure
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- Research

Energy consumption for different tunnel temperatures





Research

Primary energy consumption and CO₂ emission for different tunnel temperatures and cooling water inlet temperatures with reference PETRA IV operation (T. Warnecke "Report on thermal parameters of PETRA IV")



Temperature vs. operation mode





Reference and alternative operation schedule and outdoor air temperature (T. Warnecke "Report on thermal parameters of PETRA IV")

> SUSTAIN ABLE DESY.

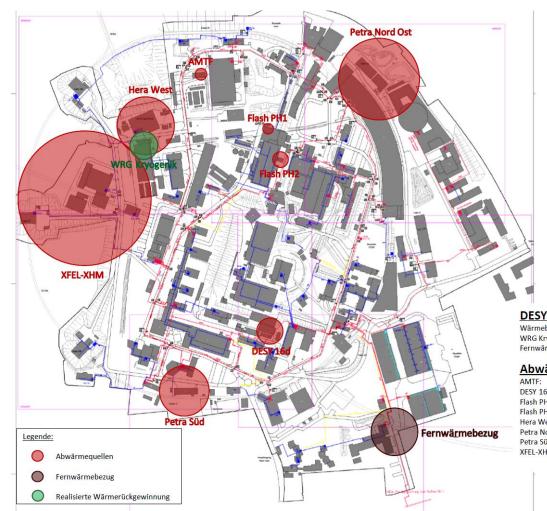
More ...

Waste heat usage



Potential at DESY Campus in Hamburg

- Currently heating is DESYs 3rd biggest CO₂ emission source
- Project with University of applied science in Hamburg (HAW) to identify potential
- Result: 129 GWh/y of waste heat available at a temperature level of 30°C - 40°C
- Possible CO₂ savings at DESY campus of about 4.000 tons/y
- Surplus can be used in neighborhood; if we get the 129GWh in use saving will be up to 40.000 tons CO₂/y



DESY Hamburg¹:

Wärmebedarf: 23,13 GWh WRG Kryogenik: 9,40 GWh Fernwärmebezug: 15,73 GWh

Abwärmequellen²:

 AMTF:
 3,86 GWh
 (22°C)

 DESY 16d:
 8,74 GWh
 (30°C)

 Flash PH1:
 3,77 GWh
 (30°C)

 Flash PH2:
 5,44 GWh
 (30°C)

 Hera West:
 19,6 GWh
 (29°C)

 Petra Nord OSt:
 26,8 GWh
 (30-38°C)

 Petra Süd:
 16,3 GWh
 (35°C)

 XFEL-XHM:
 44,9 GWh
 (34-38°C)

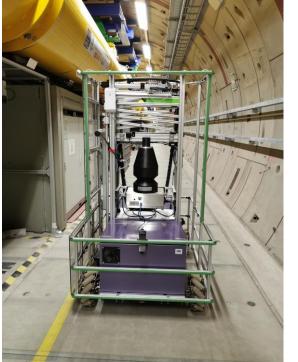
1: Daten aus dem Jahr 2019 (Zertifizierung TU Dresden). 2: Daten aus dem Zeitraum ab dem 01.04.2019 bis zum 01.04.2020.



Reliability in operation

Use of robotics and telepresence of experts







MARWIN3

MARWIN: Mobile Autonomous Robot for Maintenance and Inspection

 Routinely used for radiation measurements with the EuXFEL accelerator switched on

Project Proposal RobotiX: Robotics and Immersive User Experience

- Versatile platform based on MARWIN3 that provides
 - Multiple sensors
 - Multi-axis manipulators
- Immersive remote control interface using mixed reality technologies
- Project partners: Hochschule21, HAW, UHH, DESY





(Reinhard Bacher)

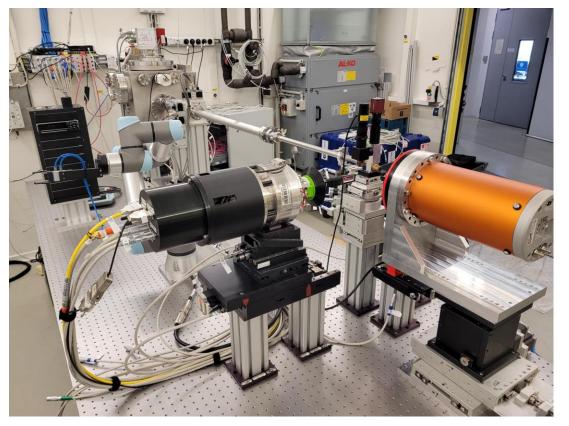
MARWIN2

Efficient use of beamtime – every photon counts



HiPhax: Highly automated pharmaceutical screening beamline for room temperature measurements

- Designed for high-throughput pharmaceutical screening at cryogenic temperatures and room temperature
- >1000 samples/24 h
- Goal: Fully automatic, Al- supported data collection
- Multicrystal samples holders (Si-chips) for highest throughput
- Robotic exchange of chips
- Hotel for chip storage
- Sample delivery format compatible with installation at SPB/SFX at EuXFEL



First successful test experiments in June/July 2022 at beamline P09 at PETRA III

HIR³X

Hardware installation of automatic sample changer: HIR3X milestone M1.1



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Petra IV. - Remote access – high-troughput MX

Petra IV. will enable remote access for mature and highly standardizes X-ray techniques

Prime example P11 beamline PETRA III:

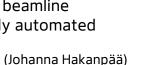
- Experienced users have the possibility to collect data remotely
 - No travel of persons, just sending samples
 - Access via remote session from internet browser
 - Guidelines for remote access (safety aspect)
 - Need to register for access

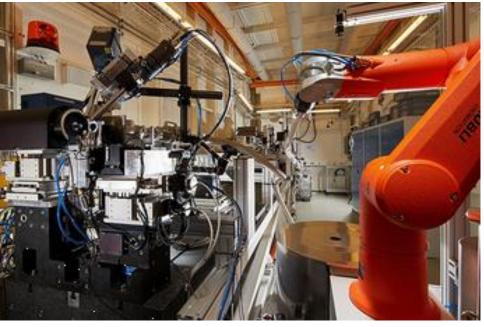
If all scheduled beamtimes would be remote (example):

- Users just from EU (only single P11 beamline)
- Ca. 17 tons CO₂ savings from flight travels / year (https://www.carbonfootprint.com)



sample changes





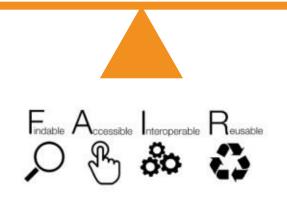


Keeping Data



- Academic tradition
- 'Good scientific practice'
- Sometimes mandated by law (USA)?
- Typically archive all 'raw' data for 10 years
- Including data known to be 'dud'
- A 'nice to have' or 'must have'

- Keeping raw data costs significant money (M€) and energy (MW)
- Keeping all data for lots of experiments becomes expensive very quickly
- Facility cost or user's own cost
- Sustainability?





Data on disk for 180 days after measurement

- (was :180 days after last access)> Data migrated to tape after 180 days
 - retention on site (dCache), dual tape copy
 - 4.5 PB ingested to GPFS in past 12 months
 - 6 PB/year archived to tape
 - 12 PB tapes/yr with dual copy (€20K/PB/10YR)
- Usage highly variable between instruments
- Time to analyse data often limits publication rate

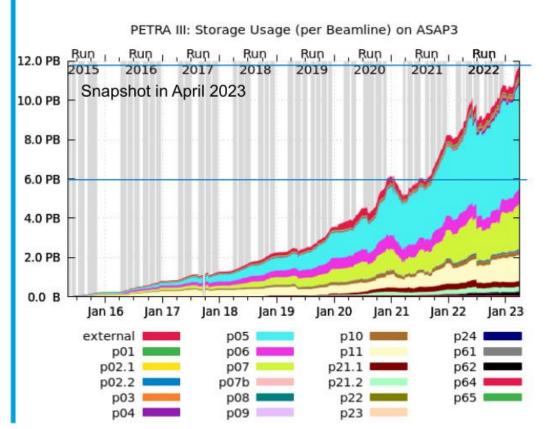
~2 years from measurement to publication

• Hardware typically has a 5 year lifetime Budget for regular replacement

Data management

Data policy

A snapshot of the status quo



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SUST SEMBLY ABLE

Projection for Petra IV. operation in 2028

Petra IV. science output should not be storage or compute limited

Peak total daily data generation will exceed 1PB per day based on actual peak 2021 GPFS usage

 Operation of any one instrument should not jeopardise operation High throughput of other instruments

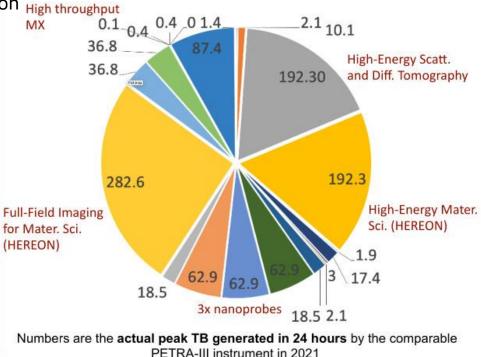
By 2028, detectors will be larger and faster:

- Planned 130 kHz detector with a frame size of 10 MP and dynamical range of 2 Bytes, would produce 2.5 TB/s
- Some individual instruments will produce >1PB per day
- Luckily, not at all instruments are data volcanoes
- Increase inevitable almost regardless of PETRA-IV project

Reality check:

- Some instruments at ESRF already produce 1 PB per day
- In 2022, EuXFEL operating only 3 instruments simultaneously has produced 7 PB in a week (=364 PB/yr)
- 1 PB/day * 5 big data instruments * 180 days = 900 P





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Peak daily data generated (in 2021)

Petra IV. will offer services for the complete data life cycle



Data management by the facility

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Integrated data capture

- Electronic log books
- Sample ID database

• Standard file formats



Integrated metadata harvesting

Infrastructure for data evaluation

- Central HPC resouces
- Sustainable and reusable software ecosystem
- Remote data evaluation
- Containerisation

(Open) data repositories and catalogues

- Raw data can be made open
- Searchable federated catalogues (with access control)

IGSN

- Common user Ids (AAI)
- DOI minting
- Place to put open results with process data



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Research for Sustainability

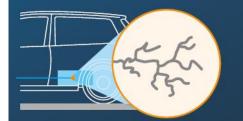
Petra IV. - Research for sustainability

Petra IV. enables research to tackle sustainability challenges and develop global solutions



Future trend: long-lasting solar cells and new batteries

Improve solar cell and battery materials: PETRA IV will make it possible to optimize the electronic structure of materials of solar cells and batteries. This can be accomplished by using atomic-level imaging and spectroscopy to follow the processes of energy transfer in specialised materials, so improved versions can be built from the ground up. This could enable longer lasting and more efficient energy generation and storage.



Deutsches Elektronen-Synchrotron DESY Notkestraße 85, 22607 Hamburg

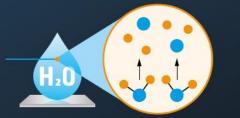


Future trend: plastic alternatives

Plastics as we know them are almost entirely derived from fossil fuels. Reasonable alternatives are on the doorstep: cellulose nanofibres derived from wood make for a sustainable version of our everyday plastics. However, the production of these fibres is still complex and time-consuming since the individual fibres are 10,000 times thinner than a human hair. Using the light from PETRA IV, the production process can be followed in much greater detail. Since PETRA IV will enable measurements to be made 100 times faster than before, the movement towards a market-ready alternative will also be faster. The cellulose fibres can also be used for textiles and packaging, as a matrix for construction composites.

Future trend: green hydrogen

Currently, the processes for generating hydrogen fuels are not sustainable, as they are most commonly produced using methane. By using PETRA IV to examine water-splitting reactions in nature and understand at the atomic level how they progress, we can develop more efficient processes by better understanding photochemical reactions – for example, how plants accomplish the same process, without the use of fossil fuels.





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