

Up dates from LISA

Prof. Dr. Bridget Murphy

Institute for Experimental and Applied Physics
Ruprecht Haensel Laboratory
Kiel University

DESY

TU Dortmund



@ DESY

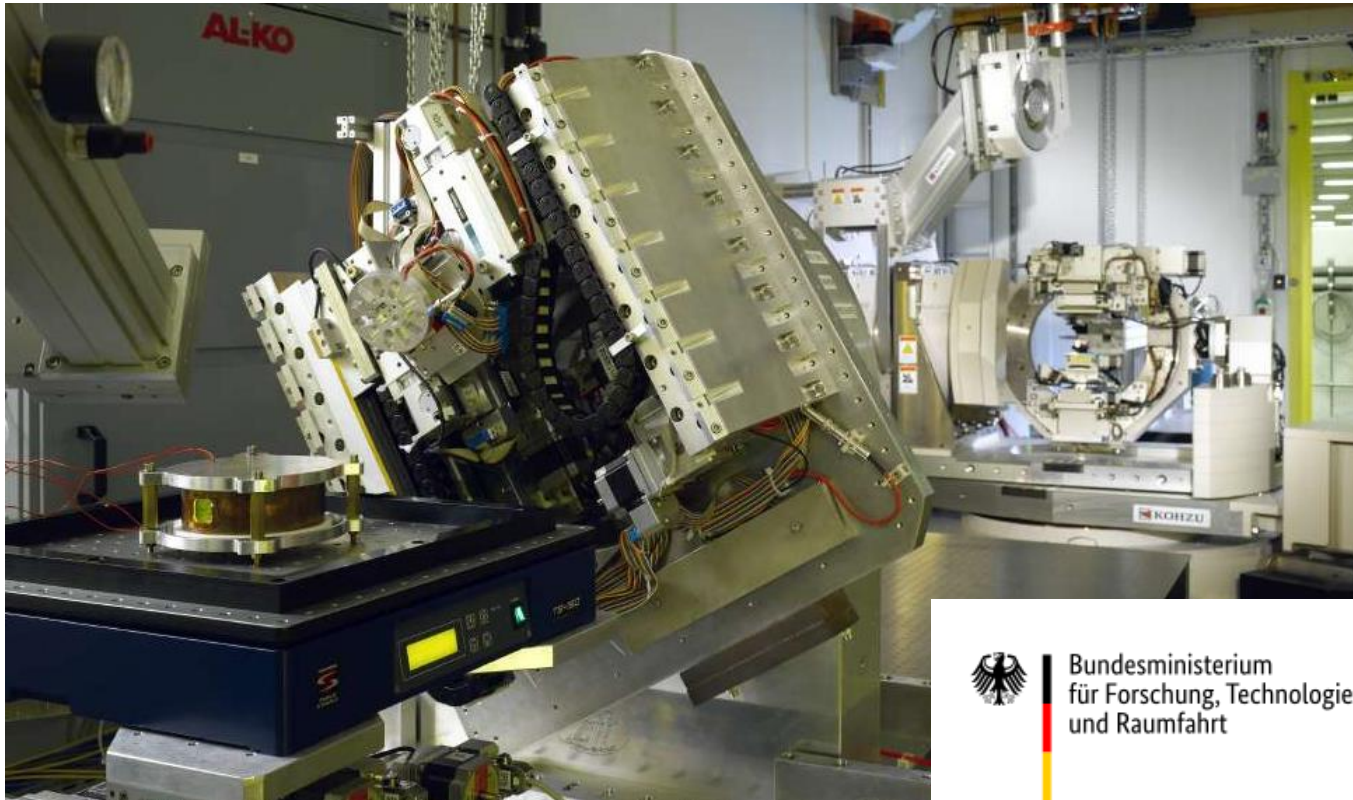
Regina Hinzman, Anjali Aggarwal, Zeynep Isik Dursun

Kiel University

Prashant Hitaishi
Julia Kobus
Philipp Jordt
Ali Ashtiani
Ajit Seth
Sunil
Otto Lipmann
Nicolas Hayden
Rabia Quamar
Olaf Magnussen
Matthias Greve
Jochim Stettner

Svenja Hövelmann
Jonas Warias
Lukas Petersdorf
Ella Dieball
Sven Festersen
Rajendra Giri
Andrea Sartori
Benjamin Runge
Annika Elsen
Christoph Lemke
Hiromasa Fujii

Liquid Interface Scattering Apparatus (LISA)



Murphy et al. *J. Synchrotron Rad.* **21** (2014).



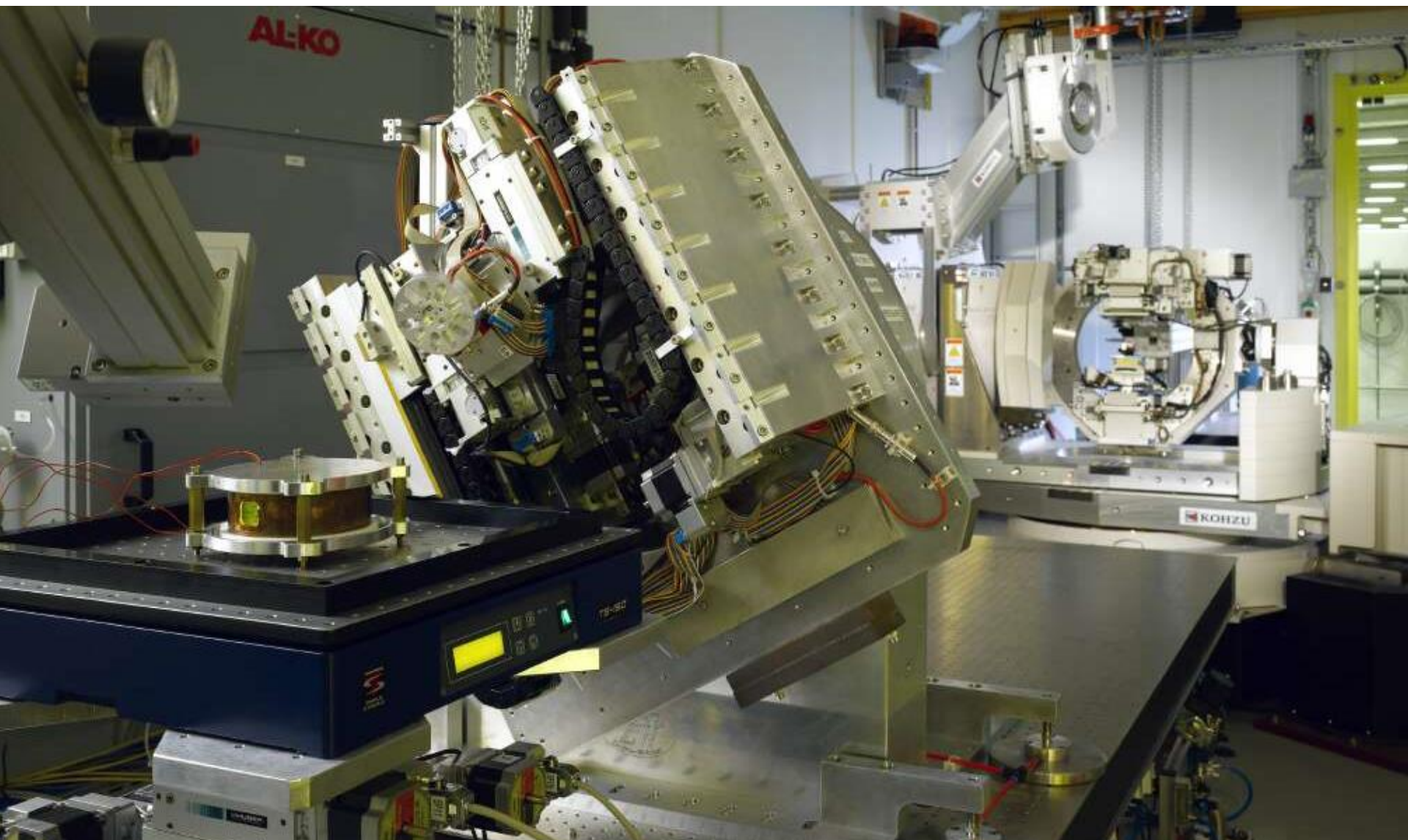
Bundesministerium
für Forschung, Technologie
und Raumfahrt



FAIR data workflows and tools

- Use Case 6 X-ray reflectivity

Liquid Interface Surface Apparatus (LISA) at P08



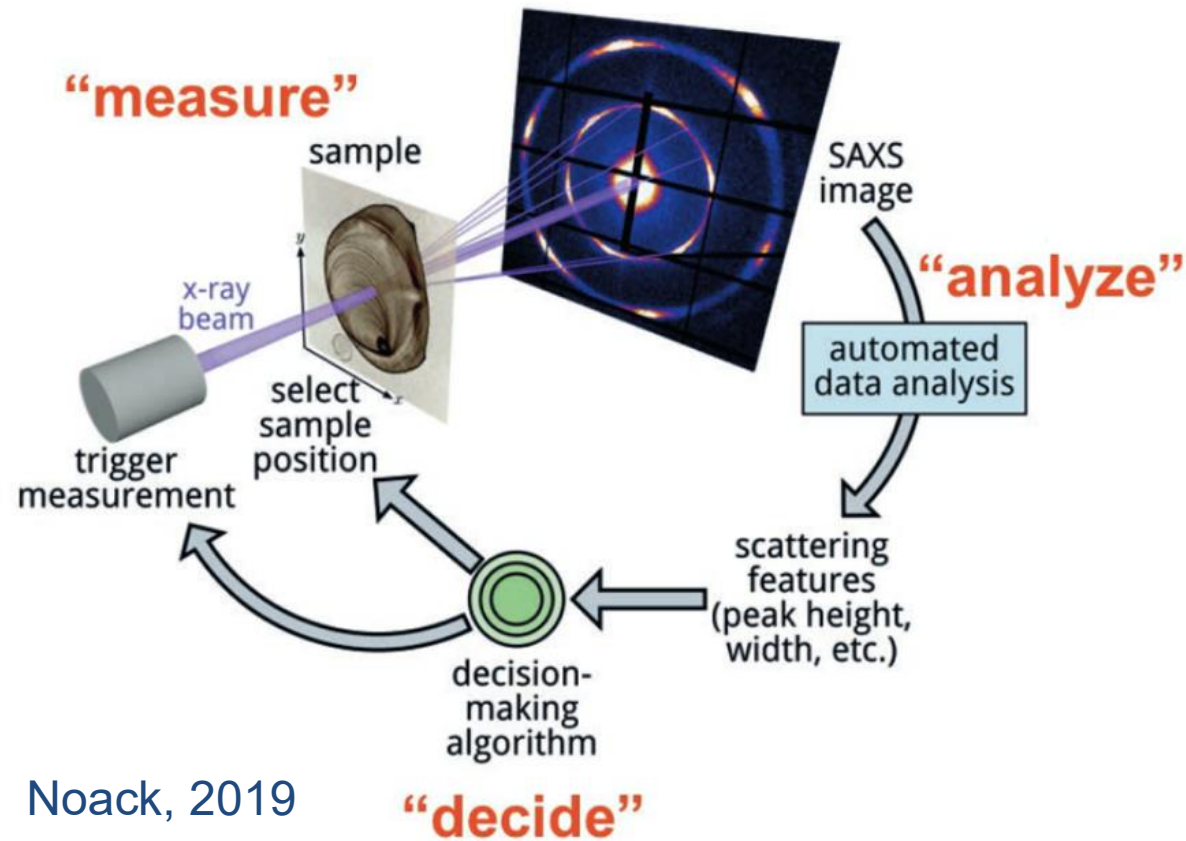
Double crystal beam
tilter in Bragg geometry:

- Studies of liquid-liquid and liquid-vapour interfaces
- X-ray reflectivity without sample movement
- Grazing incident diffraction
- High precision beam positioning

FASTER

Fast feedback mechanism and autonomous experiments in synchrotron and neutron science

Dr. Sinul



- develop autonomous and closed-loop experiments
- develop fast real-time data analysis methods
- Implementing intelligent decision-making algorithms
- Advancing automation and experimental control systems

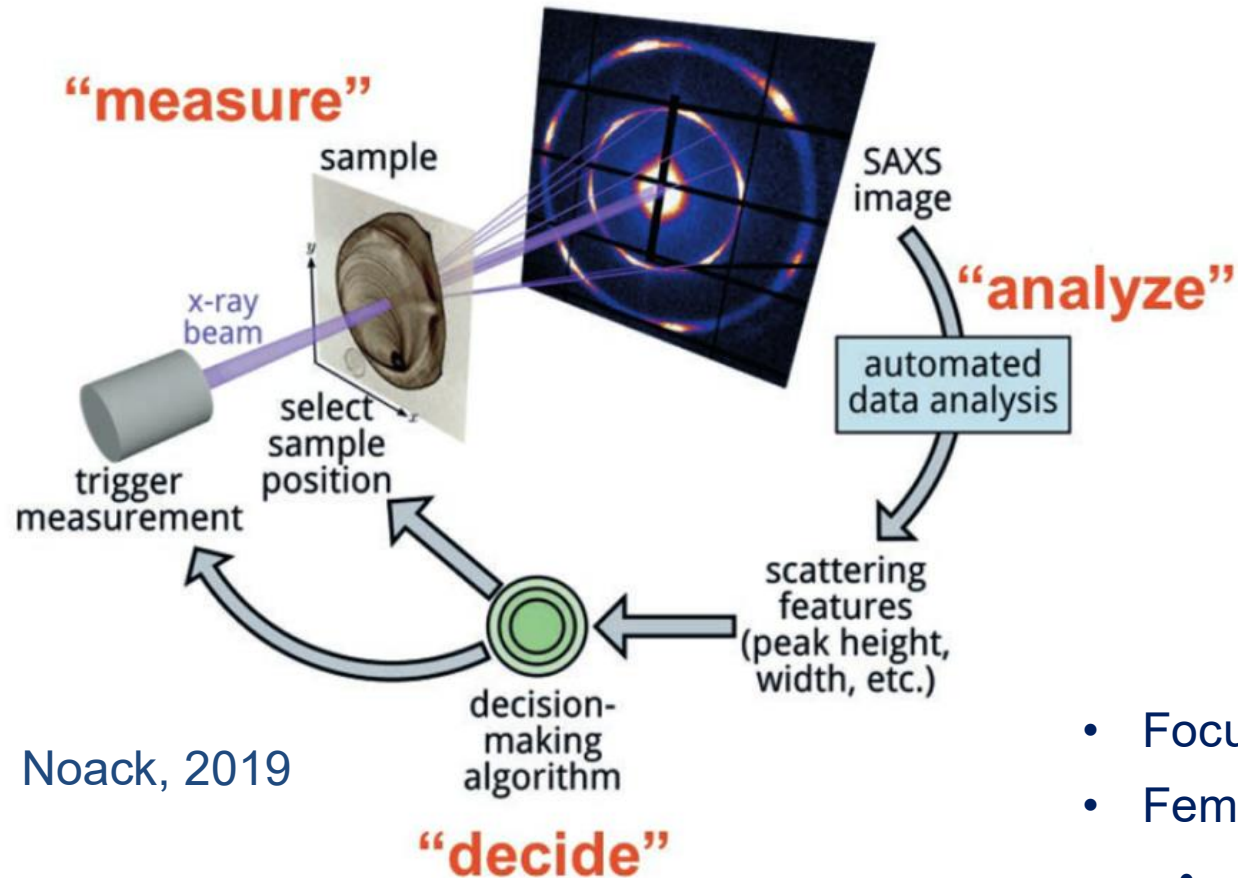
- Synchrotron
- Neutrons
- Accelerators
- Industry

Noack, 2019

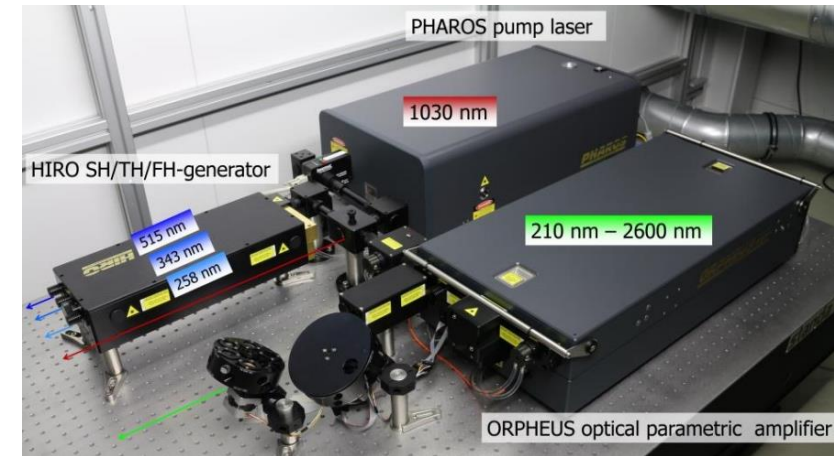
FASTER

Fast feedback mechanism and autonomous experiments in synchrotron and neutron science

Dr. Sinul



Noack, 2019



- Focus on Pump-probe methods
- Femtosecond laser and Nanosecond laser at P08
 - XRR
 - Reciprocal space mapping

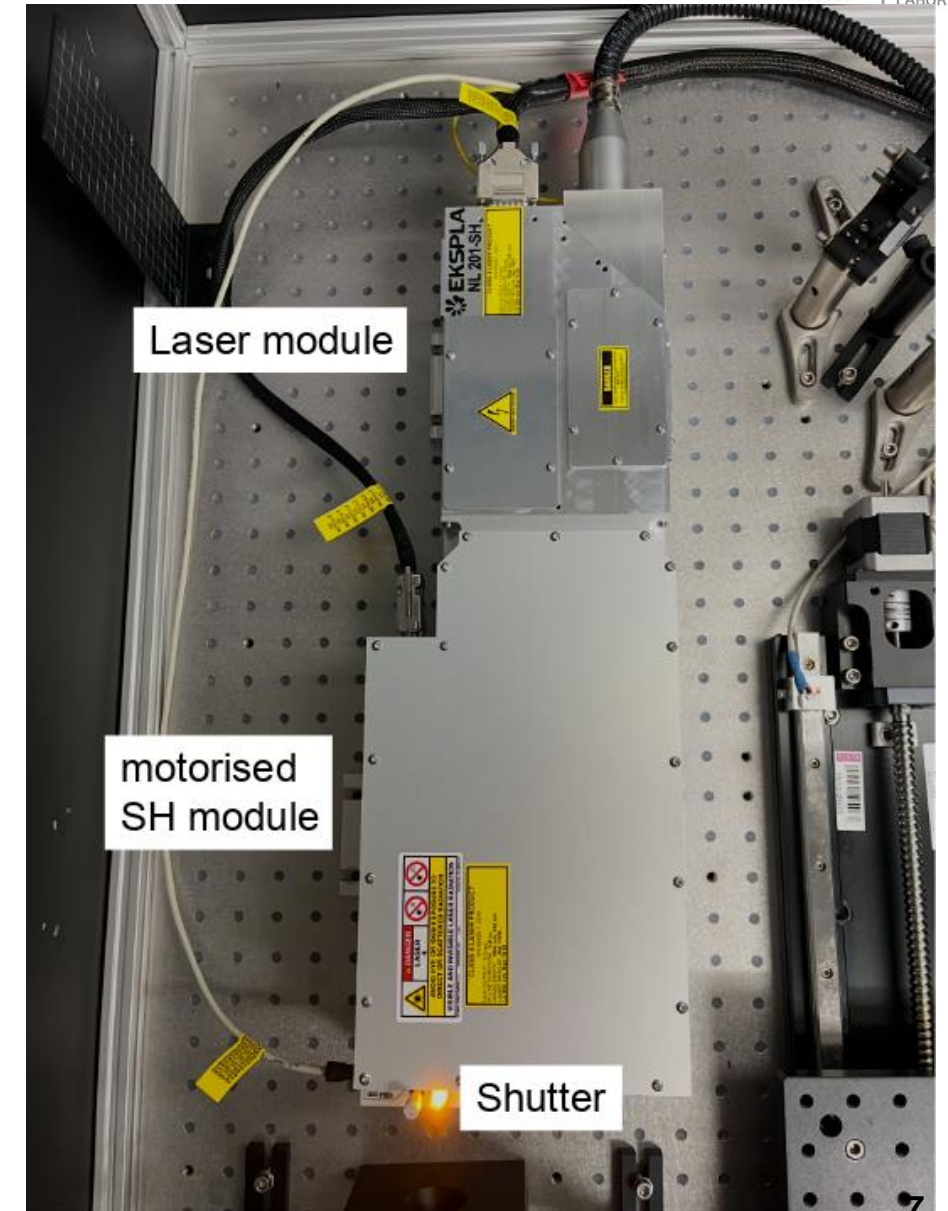
EKSPLA ns laser commissioning at LISA

Dr. Svenja Hönelmann

General specs:

- Q-switch nanosecond laser NL201 from EKSPLA
- Wavelength fundamental: 1064 nm
- Wavelength 2nd harmonics: 532 nm
- Frequency: 1 Hz – 2.2 kHz
- Pulse length: 4 – 8 ns
- Optimised for 2.5 kHz rep. rate.
- Max. pulse intensity 1064 nm: 2.3 mJ
- Max. pulse intensity 532 nm: 0.9 mJ
- External trigger: optimal time difference between gate in and sync in trigger pulse: 95 μ s

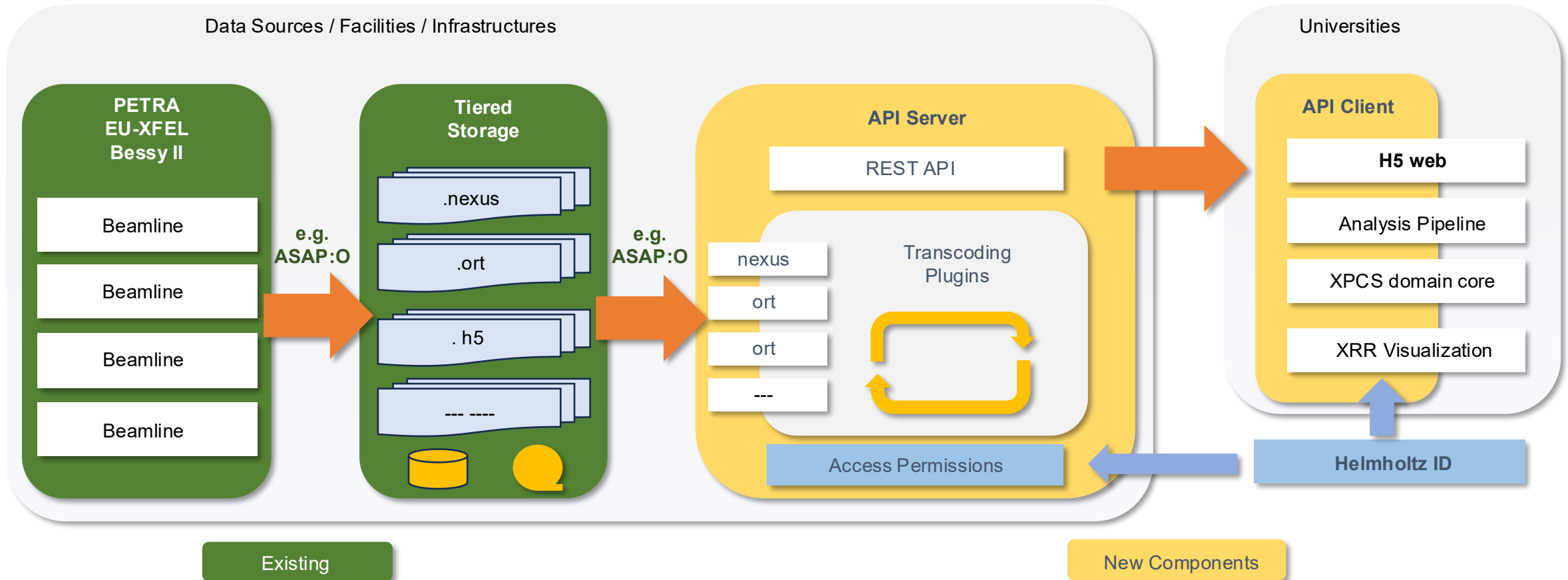
Successfully commissioned during beamtime: 11.2025



PHOTONIC

Photon Science - Harmonized Online Tools for Open, Navigable, Interactive Computing

Dr. Ajit Seth



Selective Data Access (Slice) with Tiled

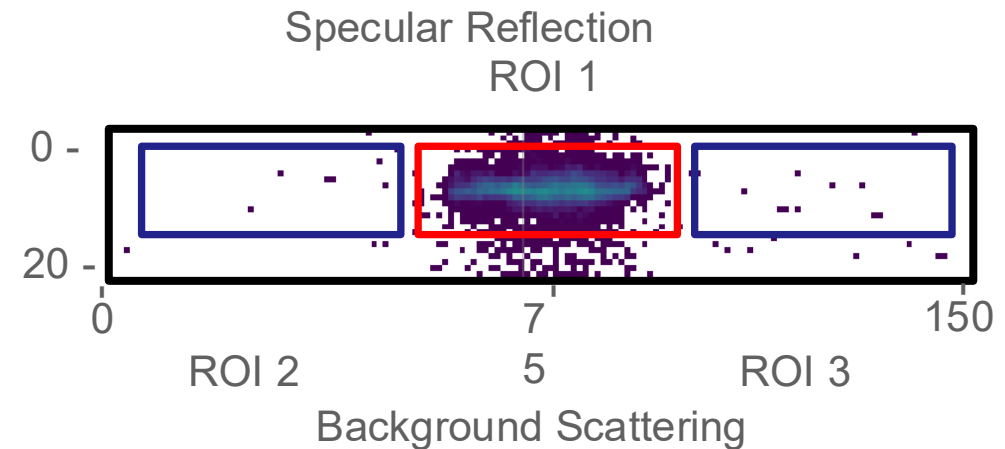
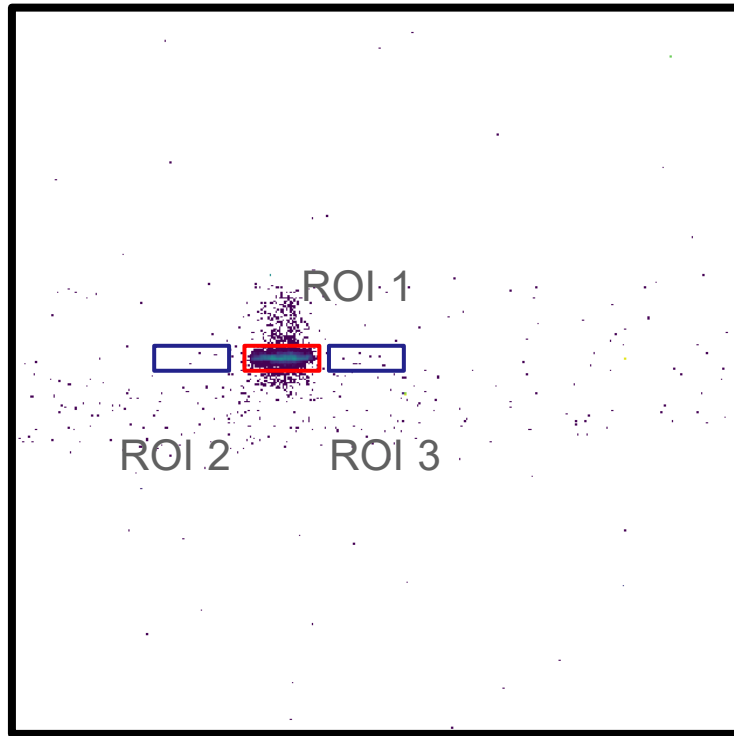
Tiled for XRR

Enables structure-aware data access,

- allowing clients to request only the slice or region of interest needed for analysis.

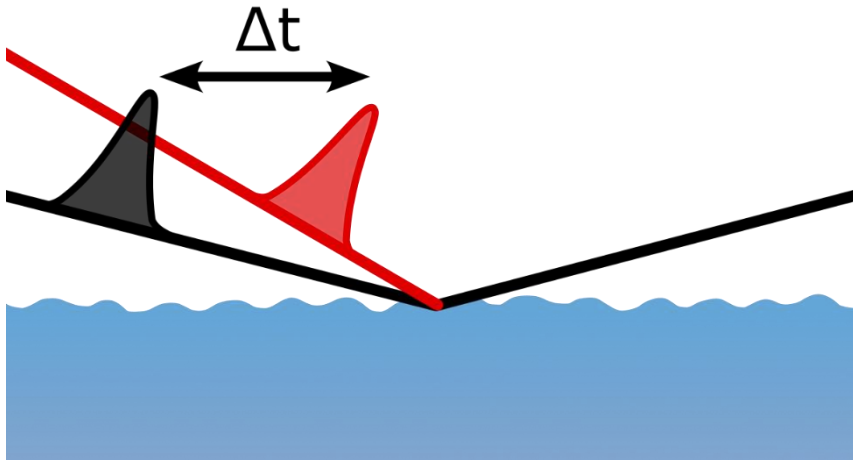
By transferring selected subsets instead of complete datasets,

- Tiled reduces data movement and accelerates remote visualization workflows.

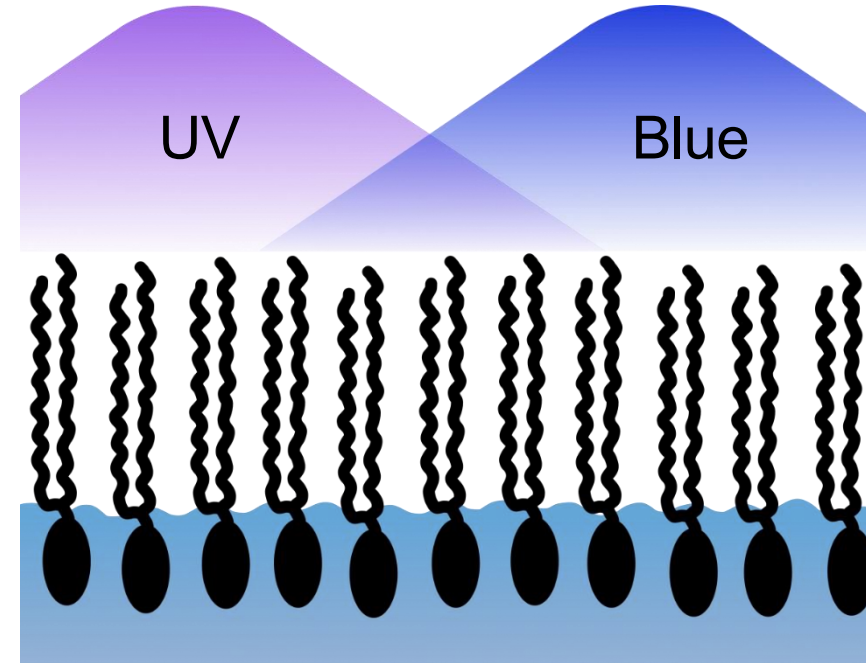


- Initial beam localization & adaptive ROI definitions.
- Automated pre-scan absorber optimization (LISA absorber wheel).
- Dynamic centroid tracking along the scan coordinate.
- Dynamic binding and coordinate-based slicing of motor positions from metadata to tag the 2d detector frames via Tiled.
- FAIR Data compliance through collaboration with DAPHNE4NFDI. 9

2 examples of Light-induced dynamics at liquid interfaces



- Laser pump – X-ray probe dynamics
- Ions at the interface

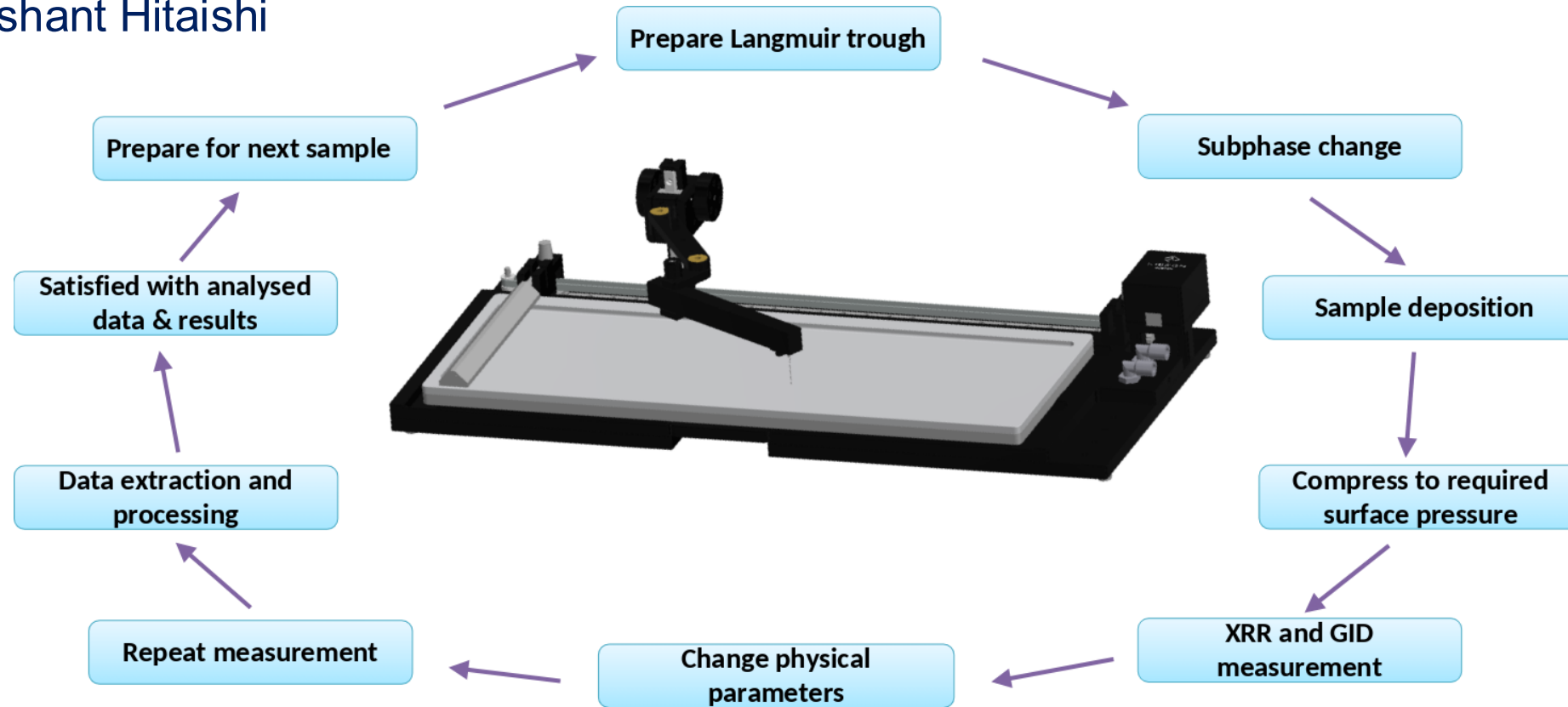


- Structural changes in lipid membranes

UPRALS

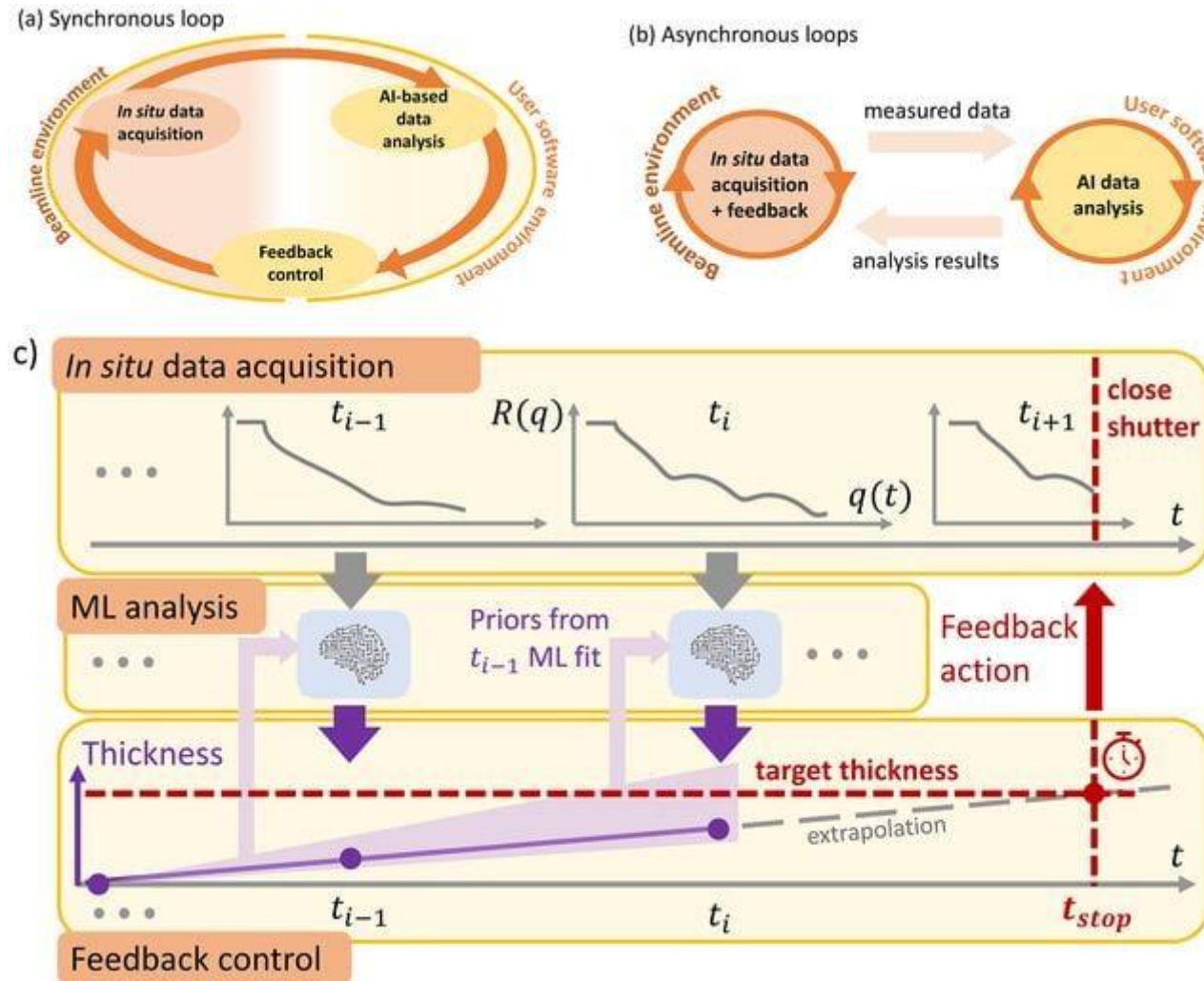
Unleashing the power of automation in reflectometry at liquid surfaces

Dr. Prashant Hitaishi



Achieving **reproducibility** and **precision** remains a major challenge in studying liquid surfaces

Autonomous experiments enabled by machine-learning-based online data analysis

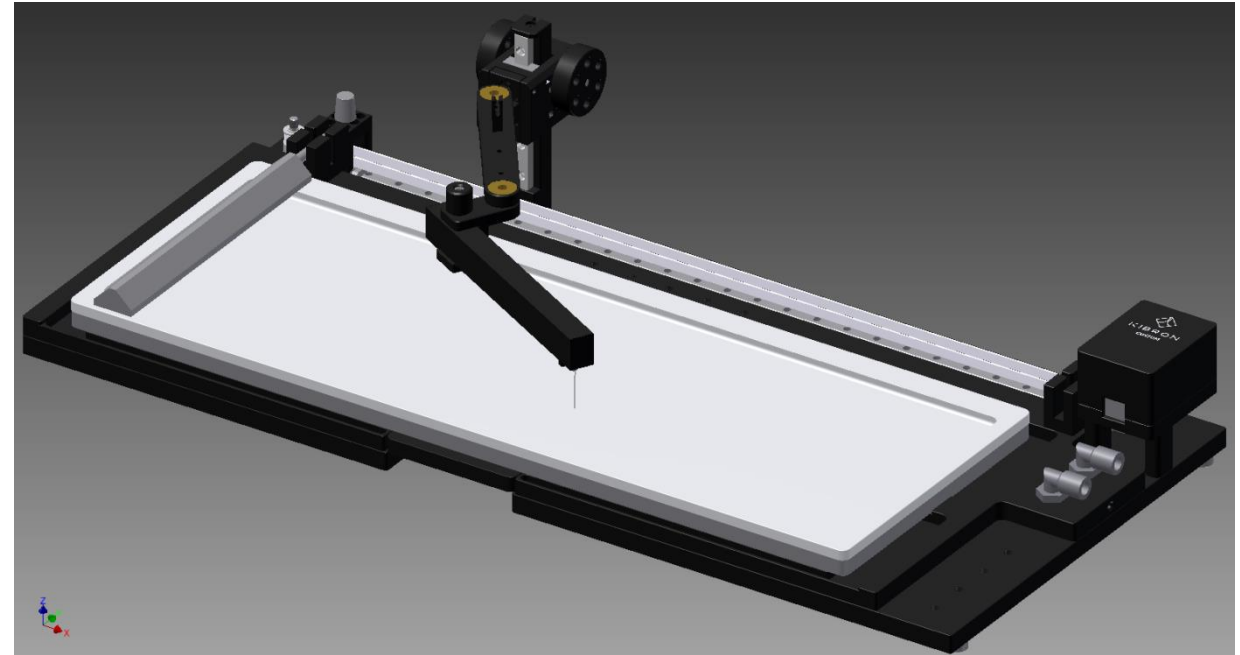


Investment for automation

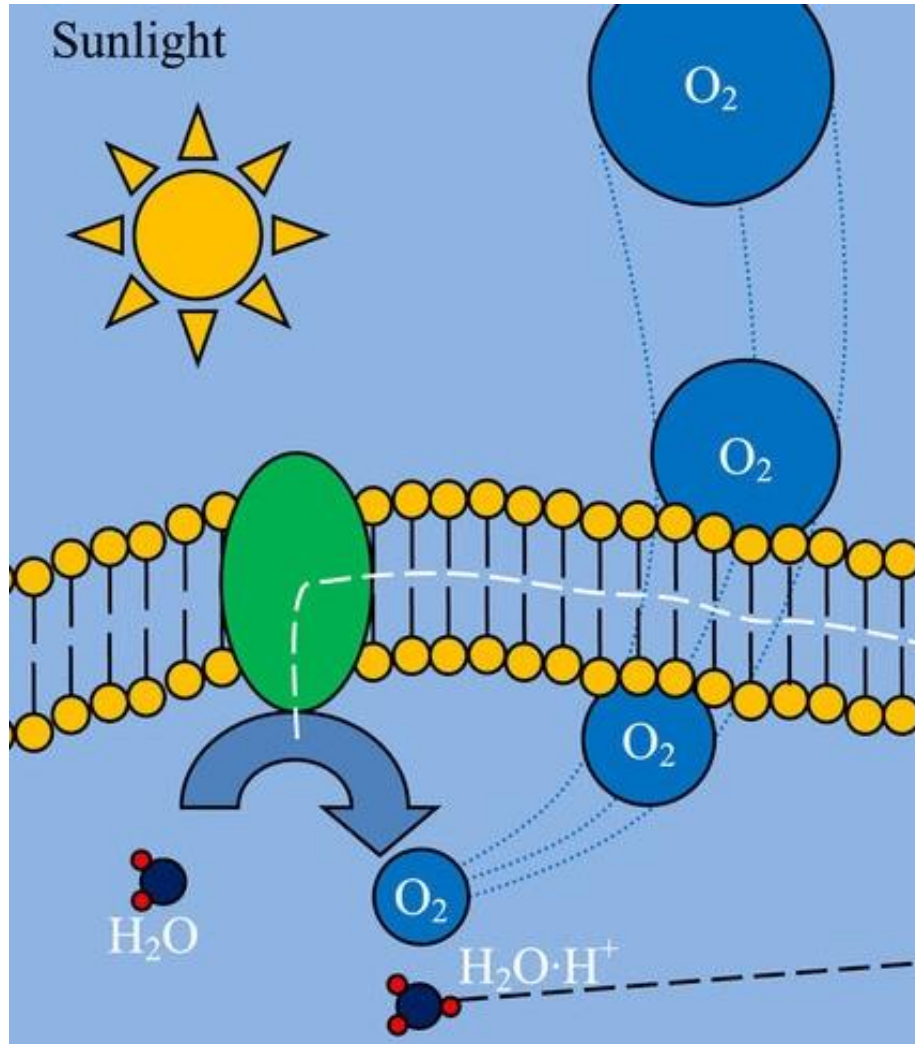
Kibron trough Commissioned

Specifications (Kibron trough):

- Trough dimension: 500 mm (L) x 155 mm (W)
- Easy trough exchange
- Single and double barrier operation modes
- Tensiometer 3-point calibration process
- Completely software-controlled
- Python-based API/supporting libraries available
- TANGO servers developed at P08, DESY
- 1D Diamond lenses from JJ X-ray
- Beamstop and guard slit optimisation
- Automated subphase exchange

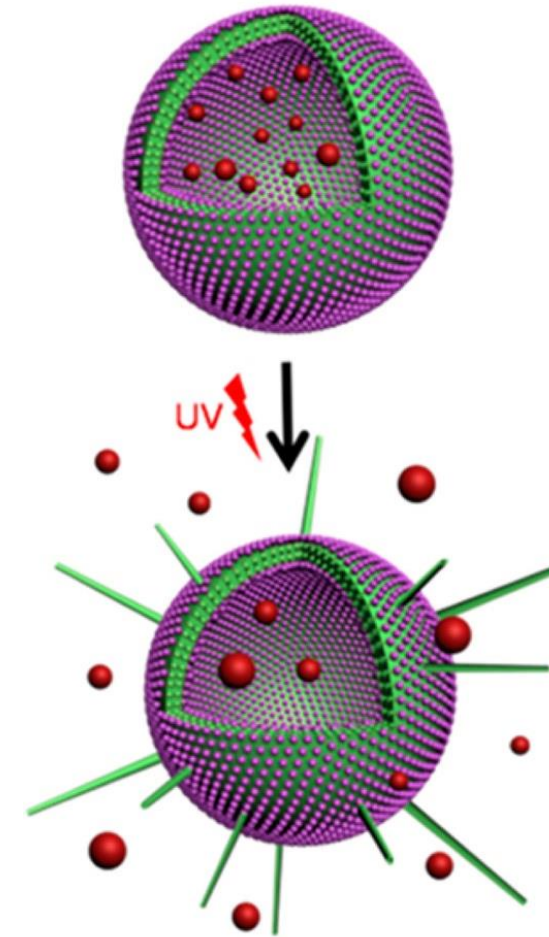


Photosynthesis



Psaltis et al., *APL Photonics*, **1** (2016).

Smart Nanocarrier

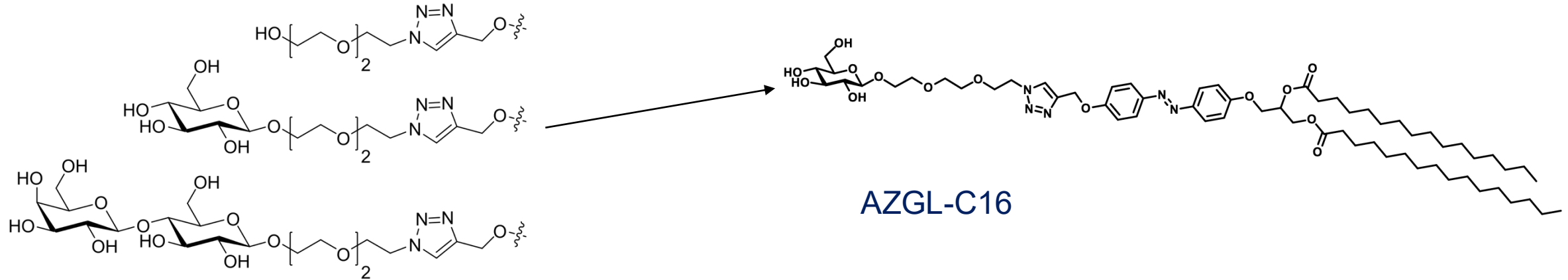
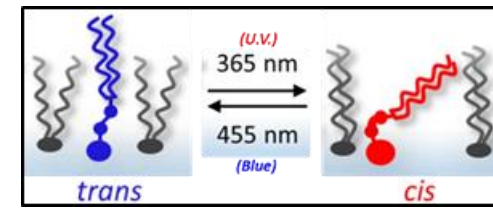


Zhao et al., *ACS Nano*, **8** (2014).

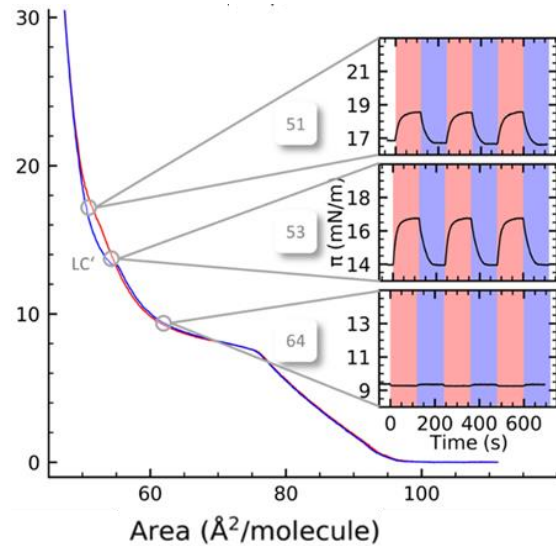
Synthetic azobenzene mimetics

Thisbe Lindhorst Group

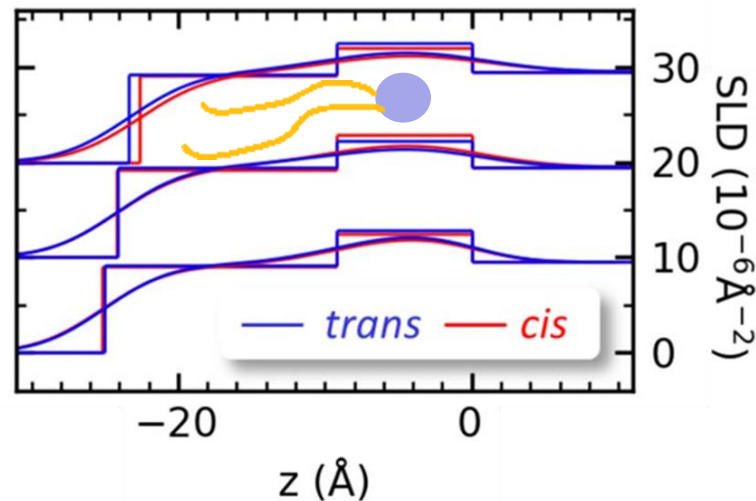
Franziska Reise, Michael Röhl



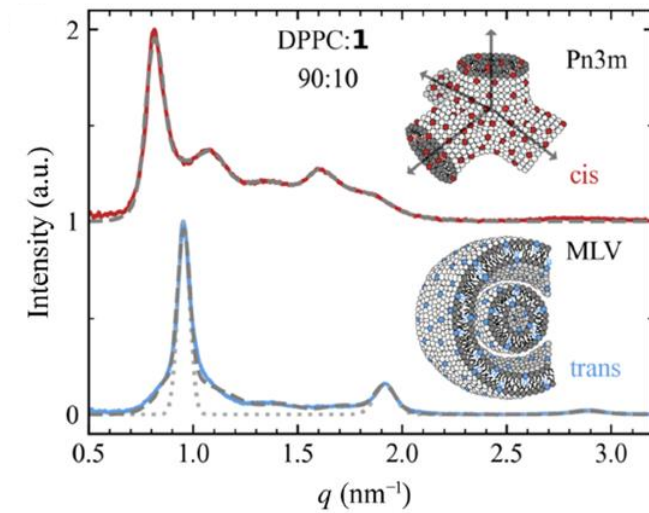
Lipid monolayer studies at air-water interface Multilamellar Vesicles (MLVs)



Reise et al., Chem. Eur. J. 24 (2018)

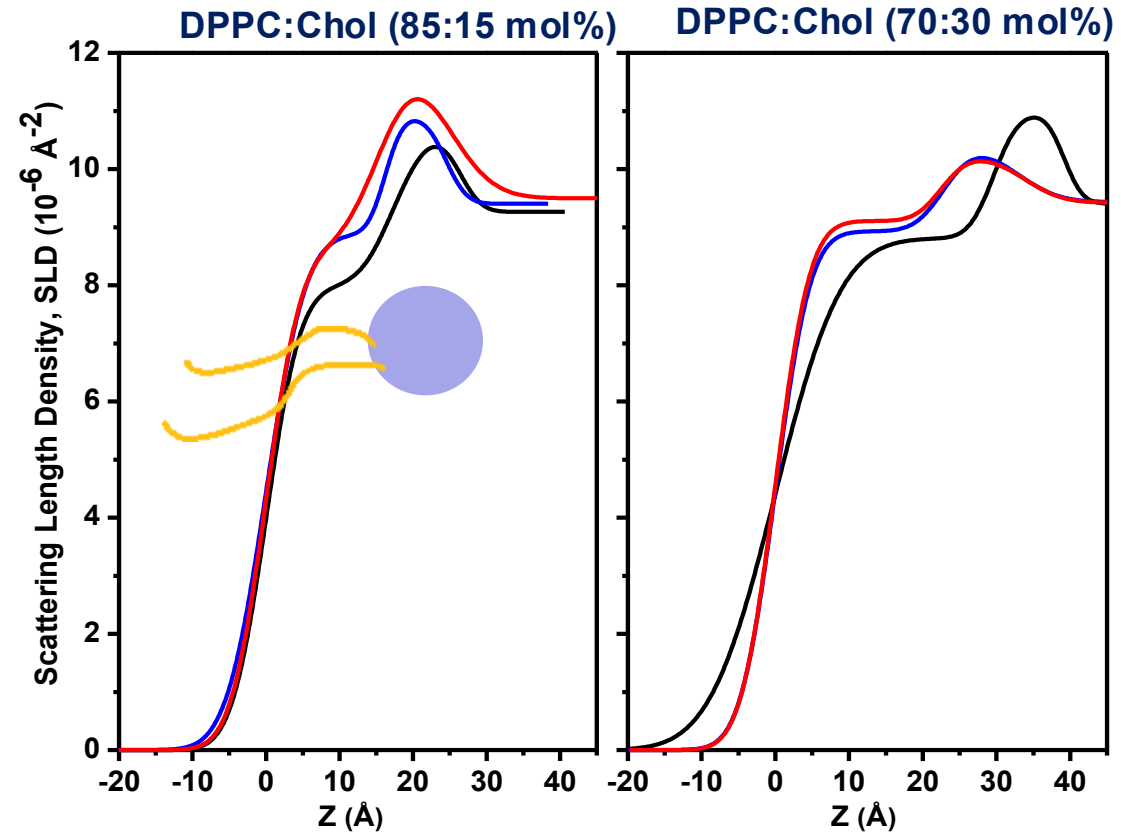
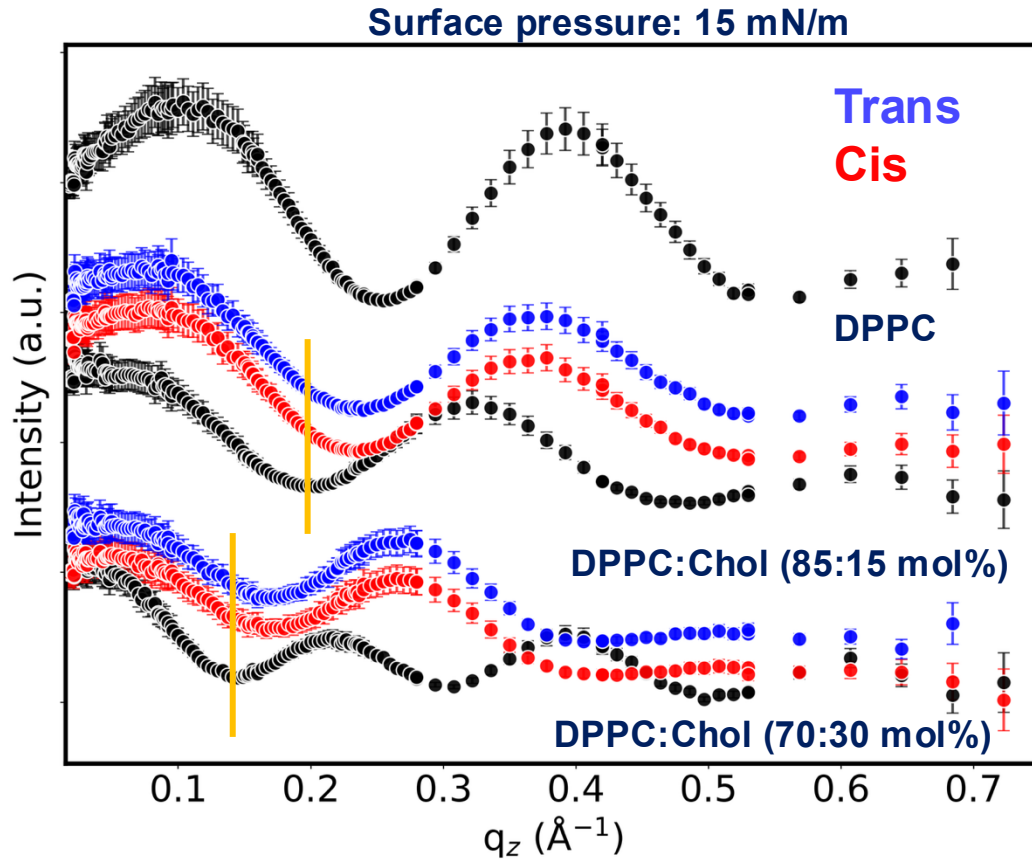


Warias et al., Scientific Reports 13, 11480 (2023)



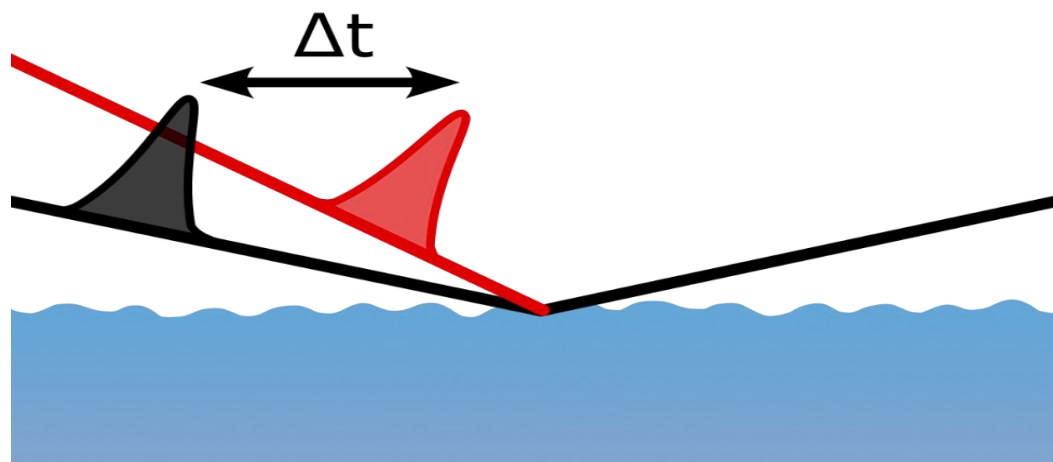
Hövelmann et al. J. Appl. Cryst. 58 (2025)

X-Ray reflectivity from a monolayer at air-water interface



AZGL-C16 (10 Mol%)

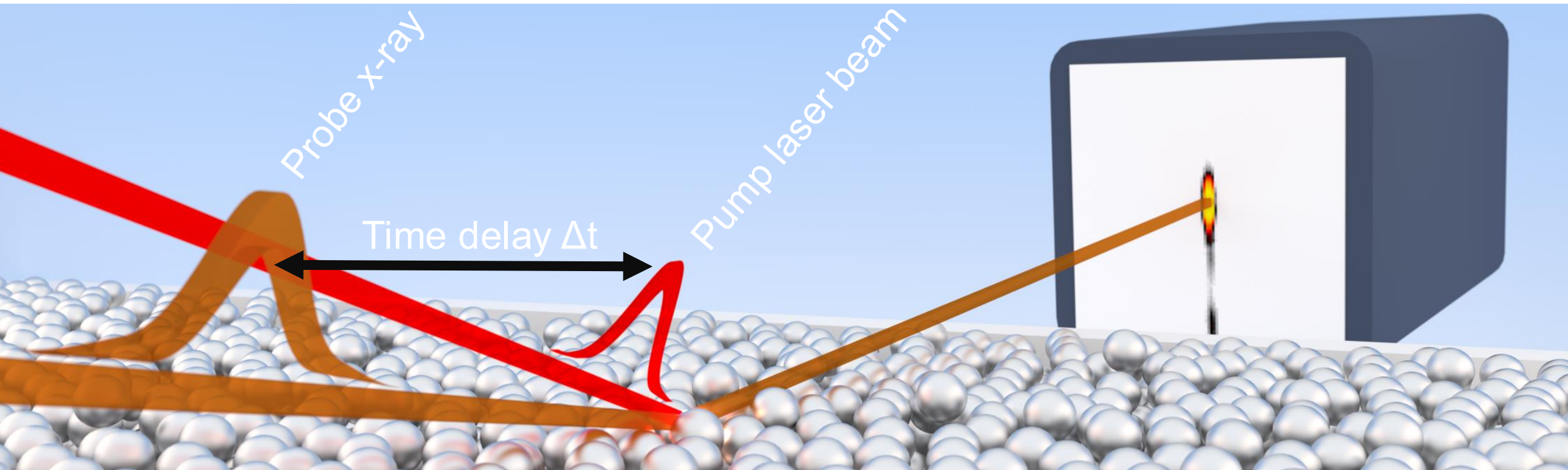
Light-induced dynamics at liquid interfaces



Laser pump – X-ray probe dynamics

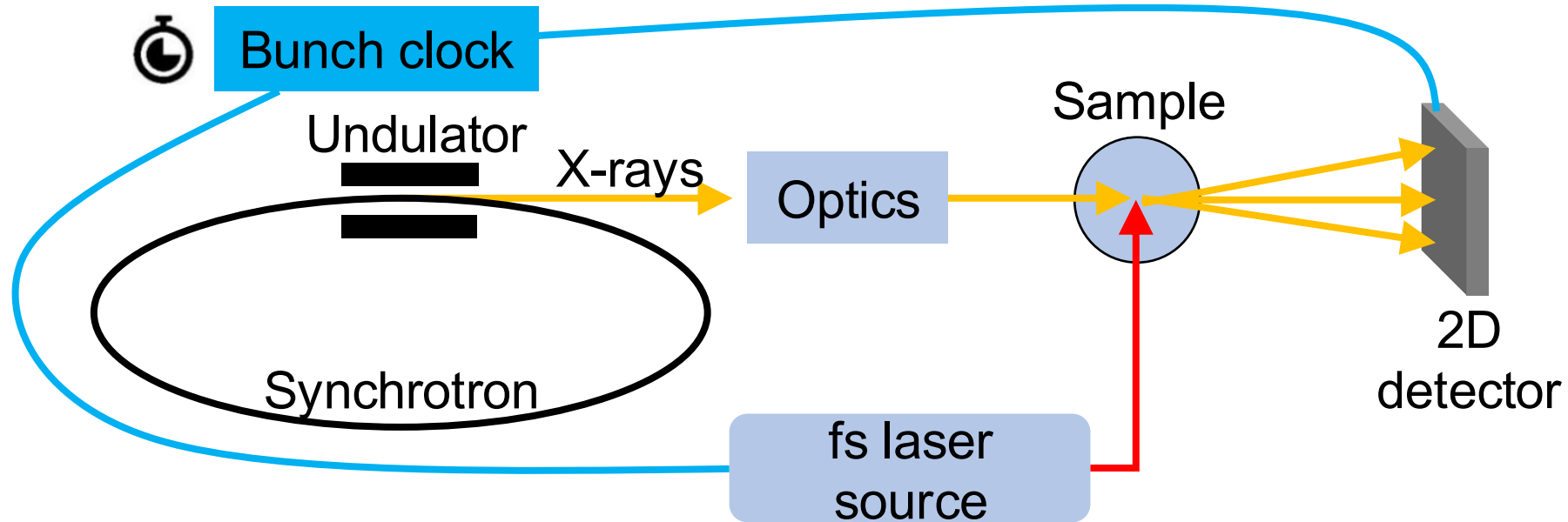
- Structure at liquid interfaces
- Ions at the interface
 - Enrichment?
 - Depletion?
- Ions in solution
 - Hydration effects
- Reaction to illumination

Investigating dynamics: Pump – Probe Principle



- Varying the time delays to get the temporal evolution
- Resolution influenced by length of pump and probe event, jitter, resolution of mechanical components

Laser pump – X-ray probe setup @ LISA, P08



Timing mode PETRA III:

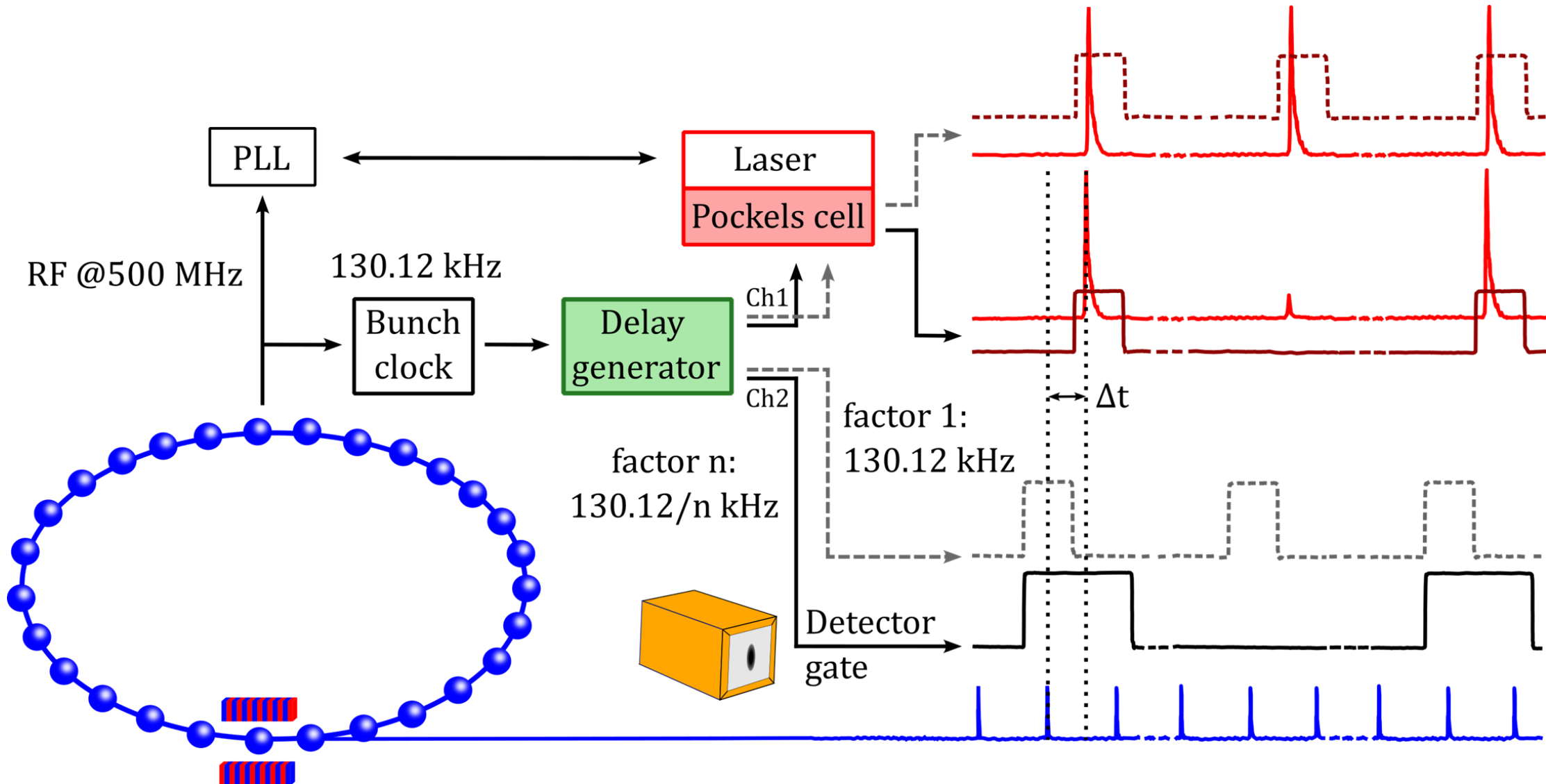
Bunch number: 40

Bunch length: ~ 100 ps

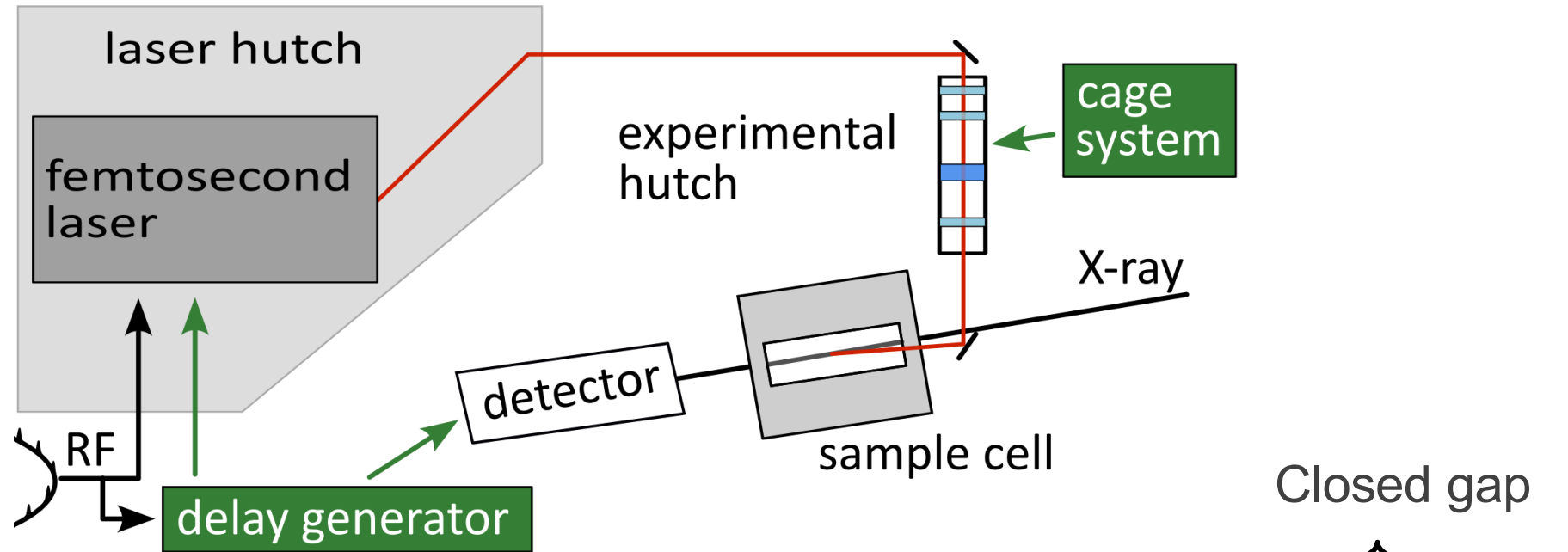
Bunch separation: 192 ns

Bunch repetition rate (one turn): 130.12 kHz

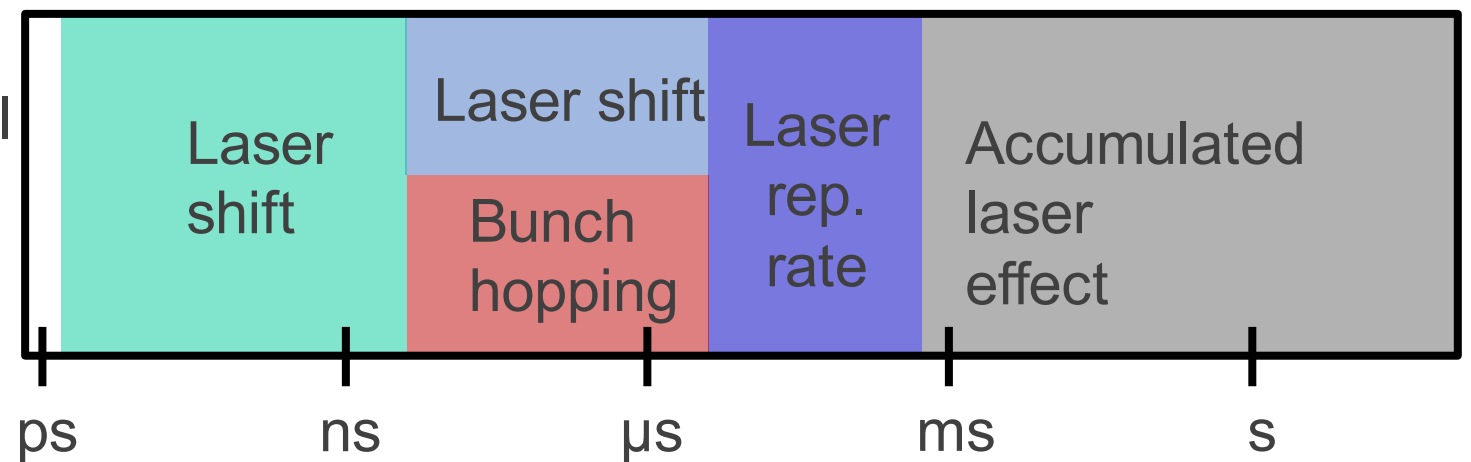
Laser and X-ray synchronisation



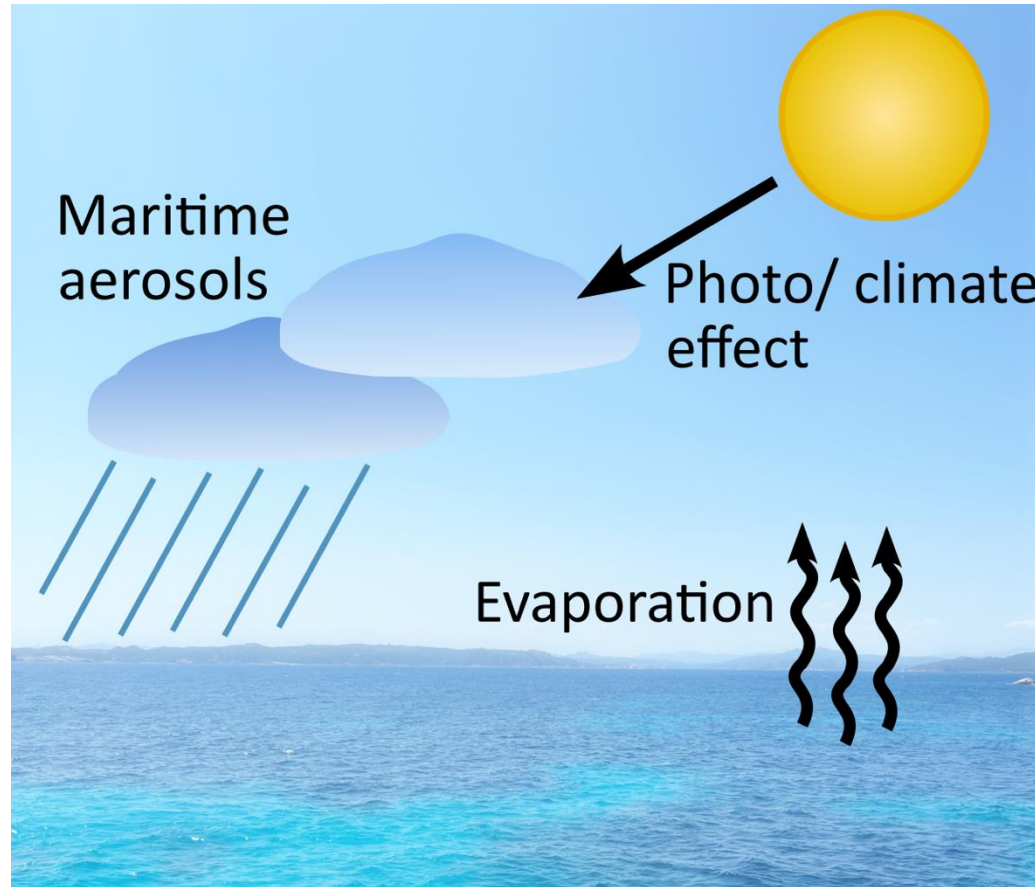
Overview of new developments on laser pump – X-ray probe setup



Experimental
resolution
at ~ 40 ps

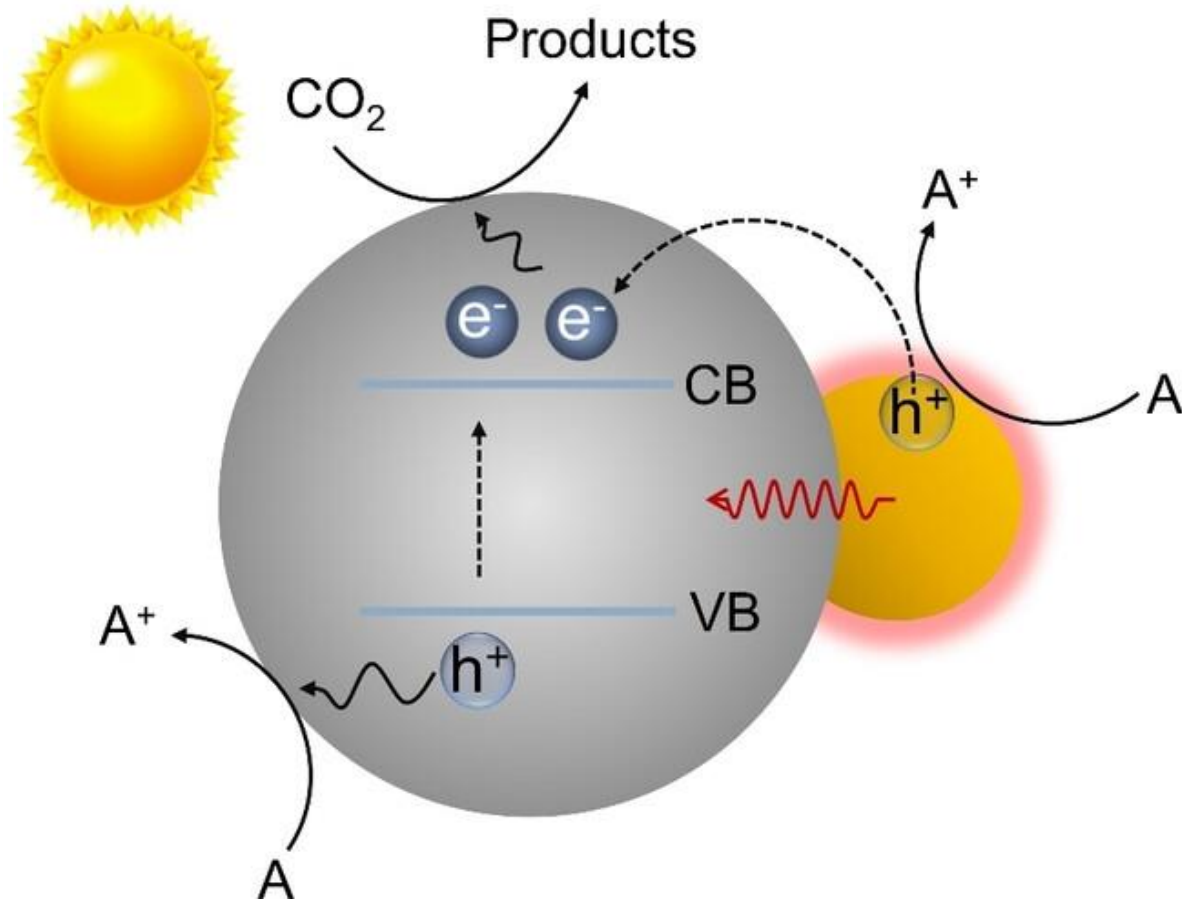


Hydrological cycle and liquid interfaces



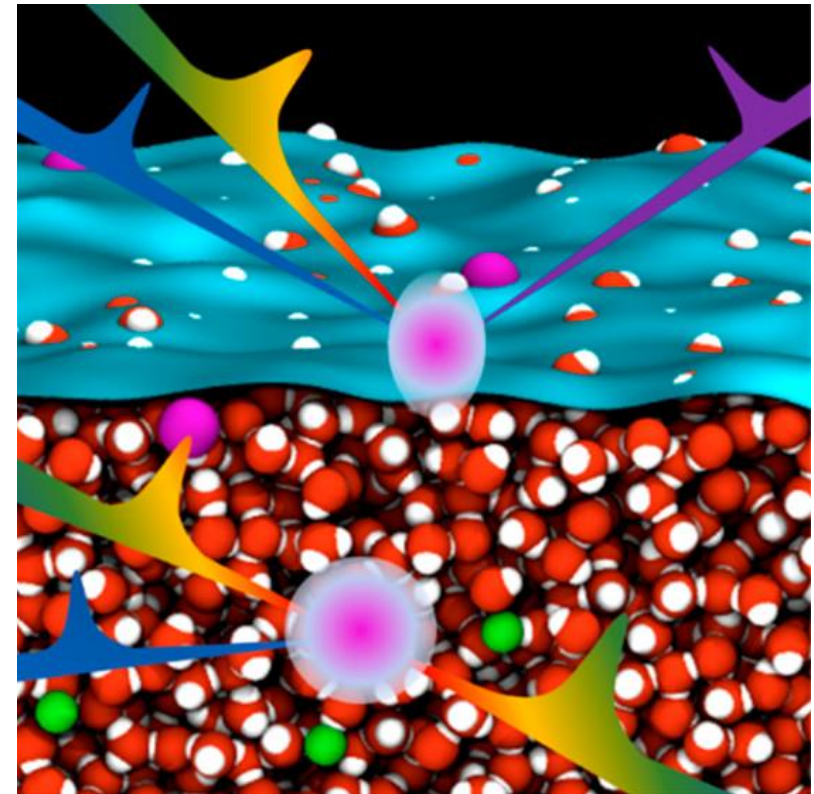
based on:
Yang et al., *Geogr. Sustain.*, **2** (2021).

Photocatalysis



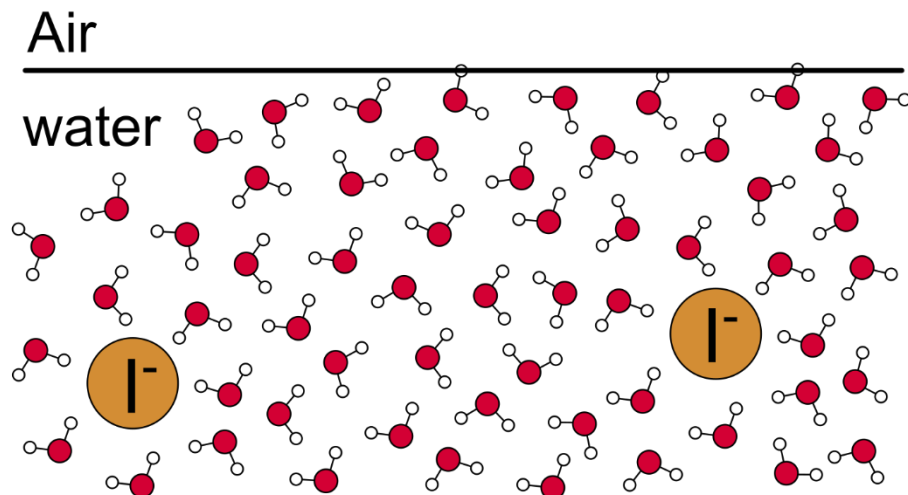
Wang et al., *Chem. Eur. J.*, **29** (2023).

Charge-transfer-to-solvent states



Bhattacharyya et al., *J. Phys. Chem. Lett.*, **11** (2020).

Are ions depleted or enriched at the interface?



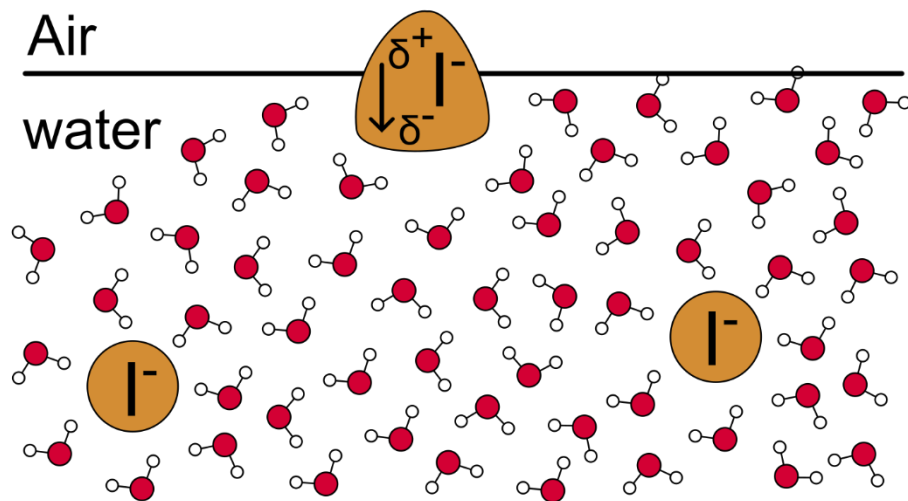
Depletion

- Classic thermodynamic
- Ion-depleted outermost surface

Harkins et al., *J. Am. Chem. Soc.*, **47** (1925).

Adamson, Gast, *Physical Chemistry of surfaces*, Wiley (1997).

Litmann et al., *Nat. Chem.*, **16** (2024).



Enrichment

- Chemical reactions
- Surface layering
- Large polarisable anions

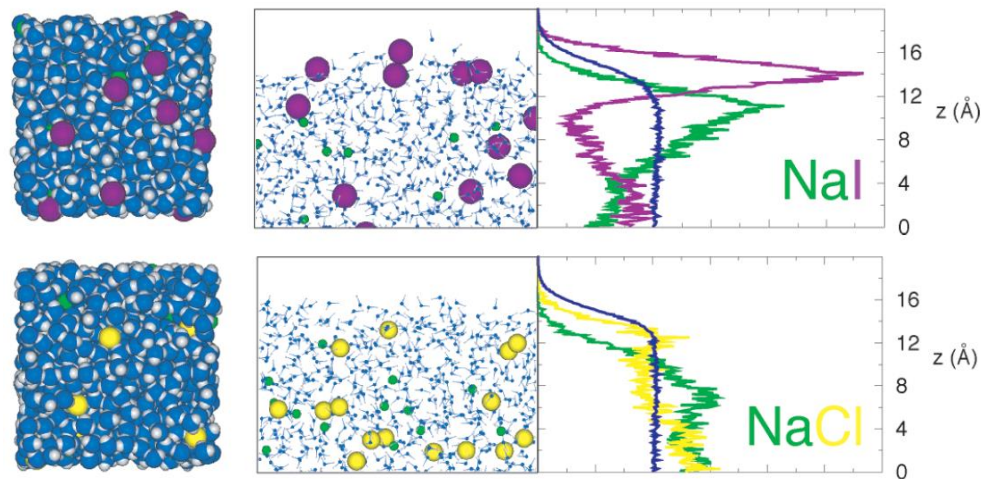
Nguyen et al., *J. Mol. Liq.*, **298** (2020).

Tobias et al., *Ann. Rev. Phys. Chem.*, **64** (2013).

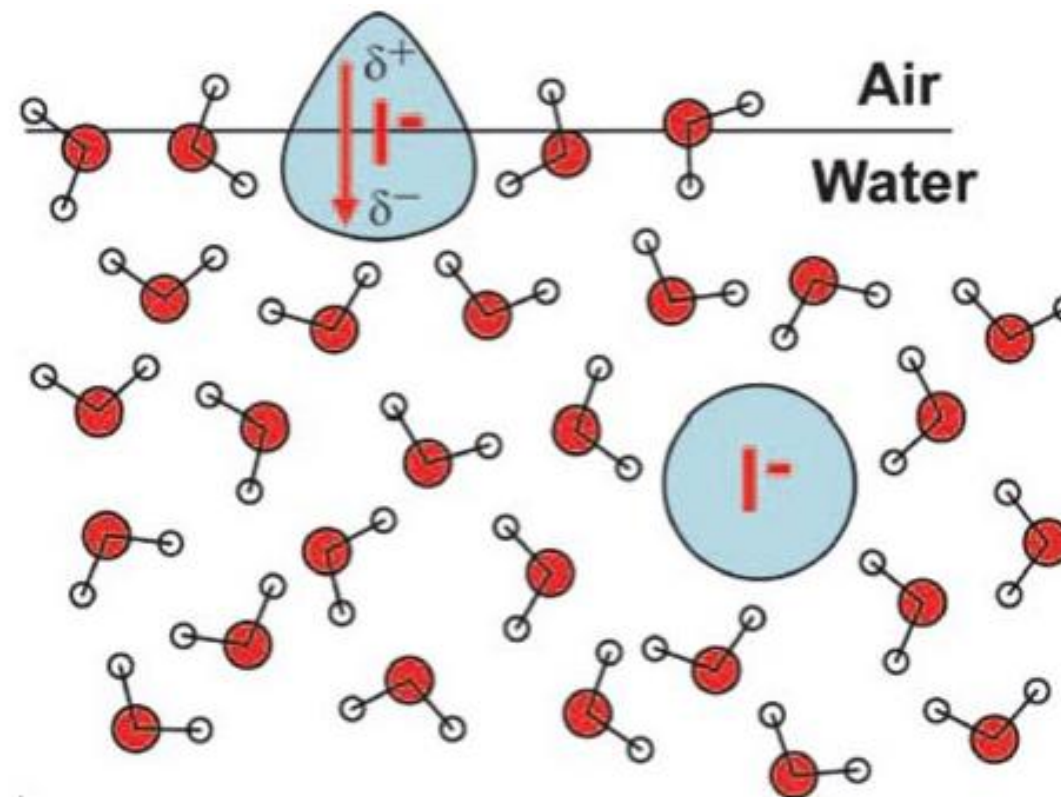
Sloutskin et al., *J. Chem. Phys.*, **126** (2007).

Ion Repulsion

- Classical model of ion depletion cannot explain the atmospheric ion repulsion
- Need molecular dynamic simulations with highly polarizable anions which are absorbed at interface (dipole)



Jungwirth, Tobias, *Chem. Rev.* **106**, 1259 (2006).

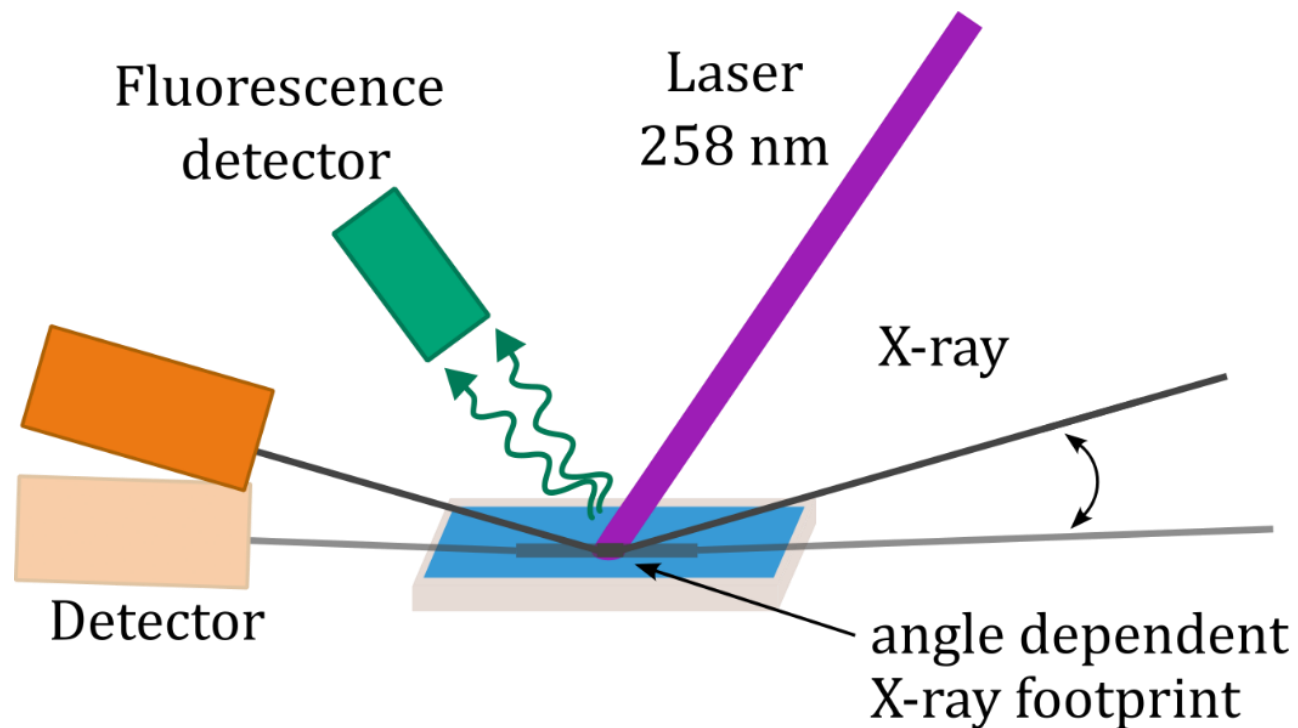


- Anions in the outermost layer, cations are repelled and present in the sublayer

Mukhopadhyay, Xantheas, Saykally, *CPL*, 700 (2018) 163.
 Petersen, Saykally, *Annu. Rev. Phys. Chem.*, 57 (2006) 333.
 Jungwirth, Tobias., *J. Phys. Chem. B* 106 (2002) 636

Laser excitation at the liquid-air interface of aqueous NaI solutions

Dr. Svenja Hövelmann

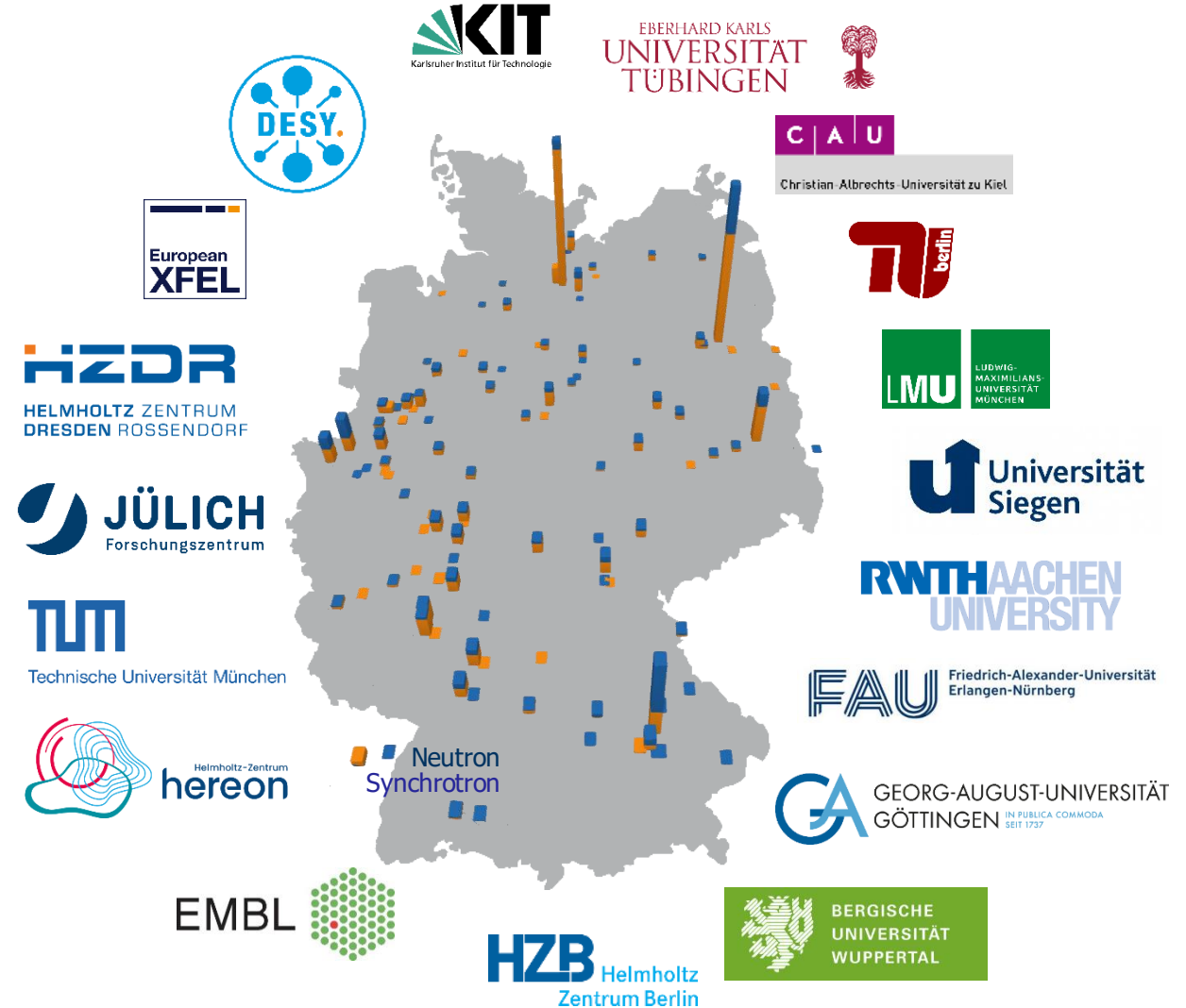
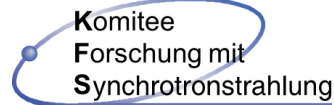
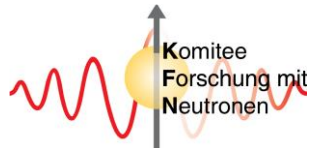


- Ion surface distribution and solvation dynamics

Probing NaI aqueous solutions to determine electron density profile and surface roughness.

Measures:

- Specification and collection of (meta)data
- Curated (meta)data repositories
- Curated repository of managed software
- **E**ducation and **t**raining in research data management
- **C**onnection to other NFDI consortia, national and international organisations



Research Data Workflow

Establishing digital solutions for FAIR data

Collect

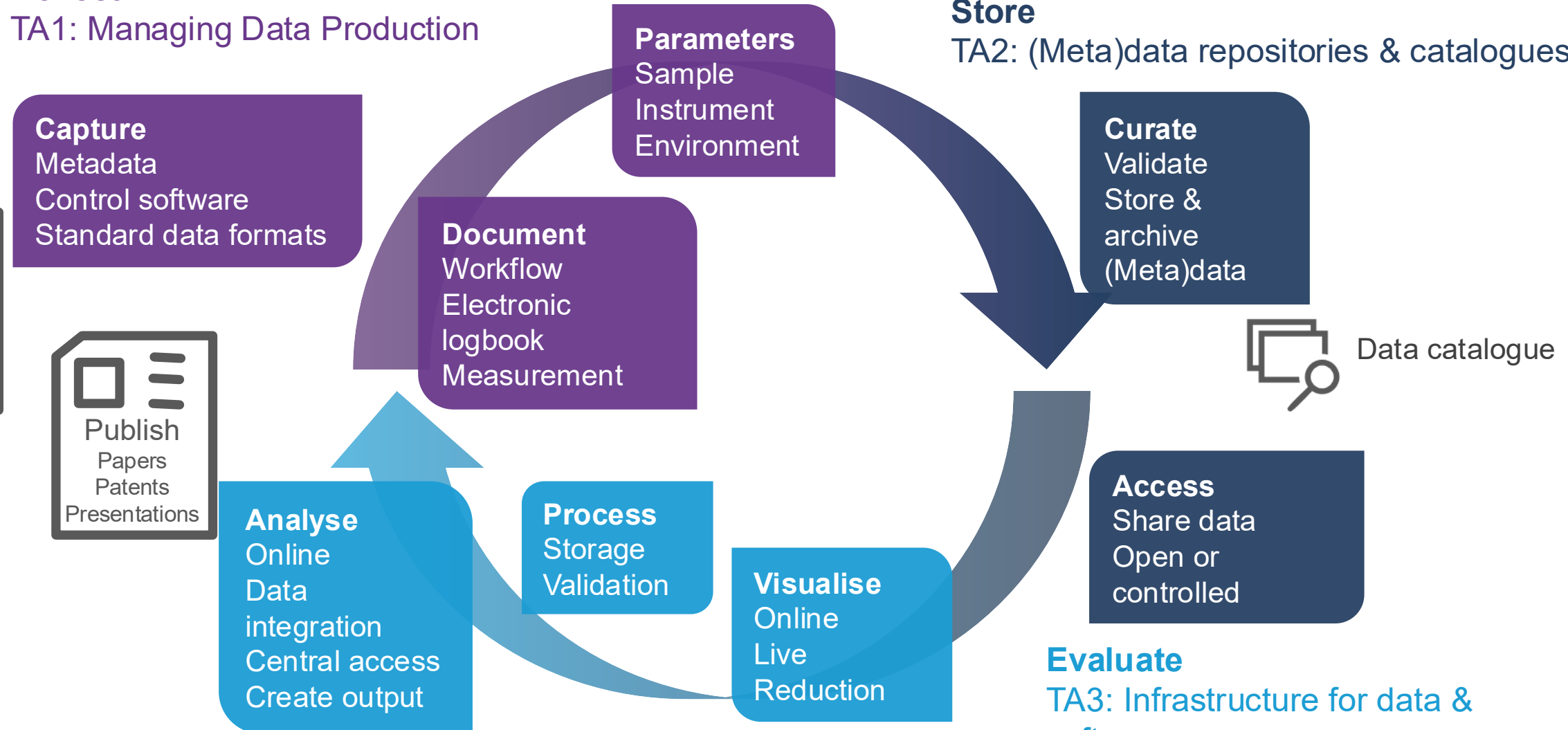
TA1: Managing Data Production

Store

TA2: (Meta)data repositories & catalogues

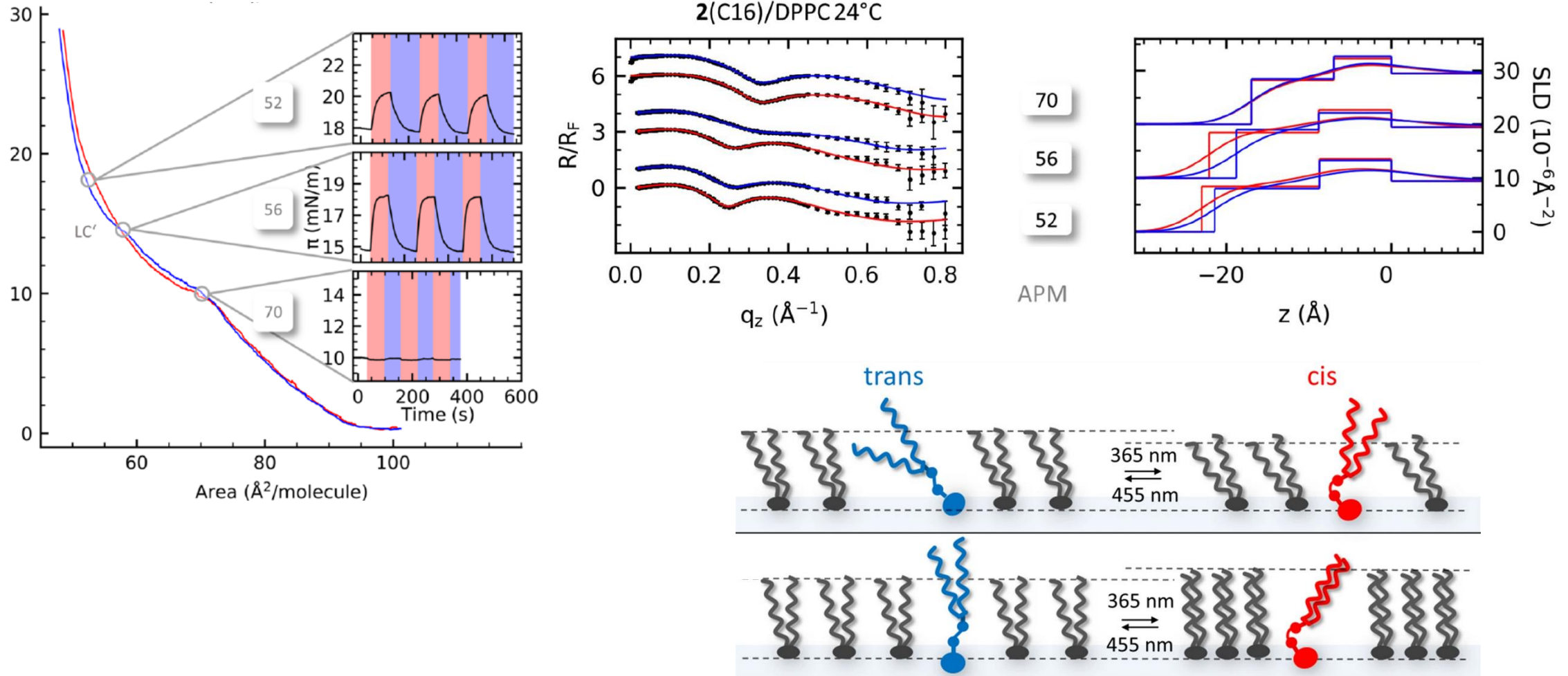
Evaluate

TA3: Infrastructure for data & software reuse



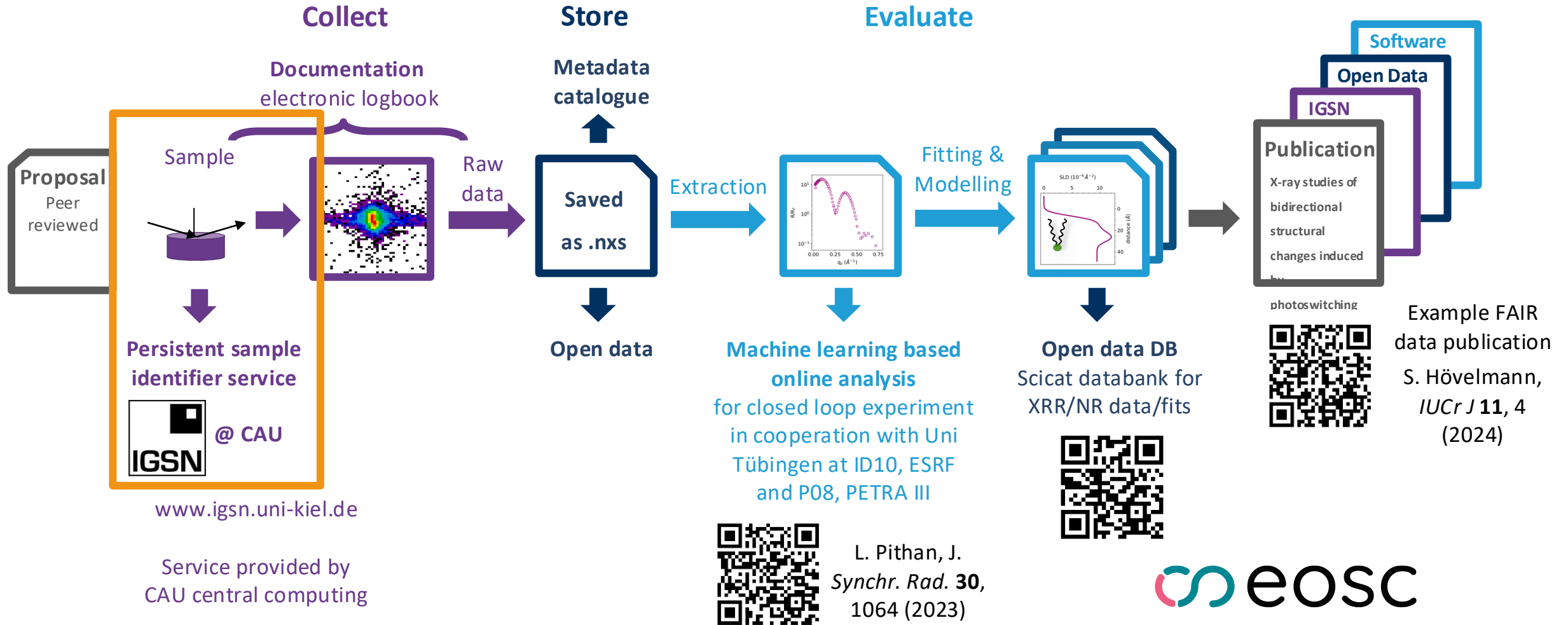
Photoinduced bidirectional switching in lipid membranes

DPPC containing 5% azobenzene glycolipid mimetics



X-ray reflectivity data pipeline

Collecting and using all the information



Sample identifier: IGSN



igsn.uni-kiel.de

Kiel University

Published

2024

Physical Object

Mixed 10% Azobenzene Amphiphile
AZOL-C16 and 90% 1,2-Dipalmitoyl-
sn-glycero-3-phosphocholine

Hövelmann, Svenja



General information

IGSN ID

[10.60578/reqz-rk9v](#)

Type

Physical Object

Publisher

Kiel University

Publication year

2024

Descriptions

Technical Info

Mixture of 10% AZOL-C16 and 90% DPPC forming lyotropic liquid crystals in water.
The AZOL-C16 can be present in its trans and cis conformation.

Contributors

Hövelmann, Svenja

Data Collector

Lindhorst, Thisbe K.

Producer

Murphy, Bridget M.

Project Leader

Related Identifiers

[10.60578/h7ys-hjbt](#)

Has part

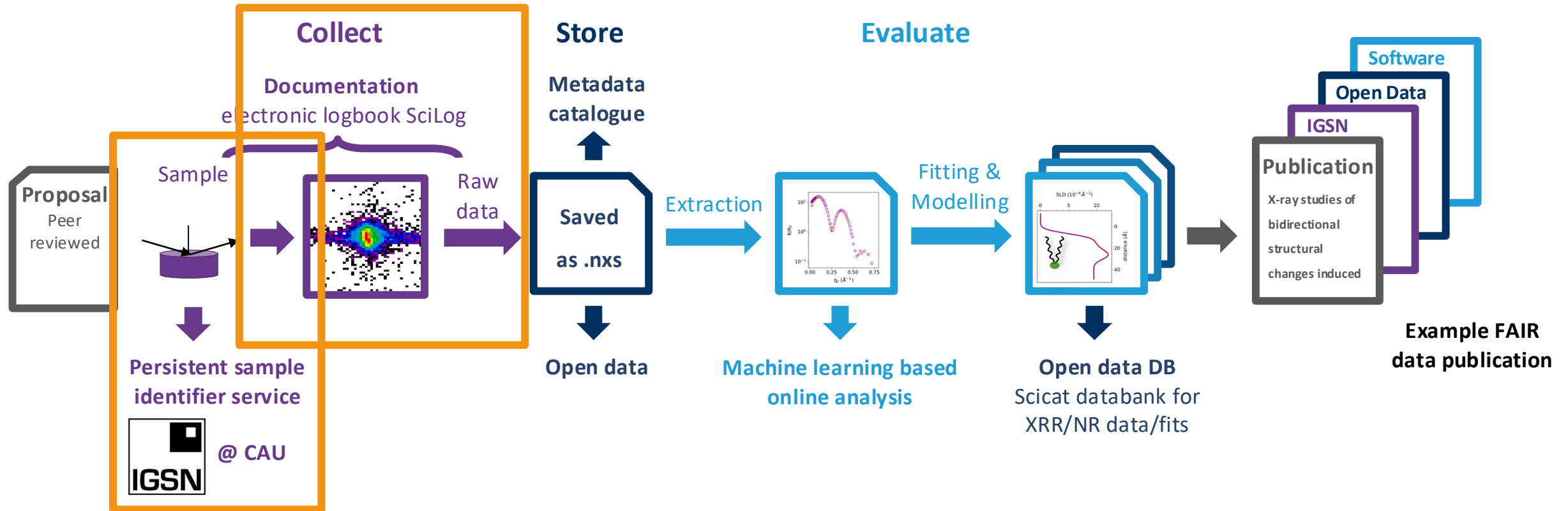
[10.60578/ceuz-rq0x](#)

Has part

[10.1107/S2052252524004032](#)

Is described by

X-ray reflectivity data pipeline

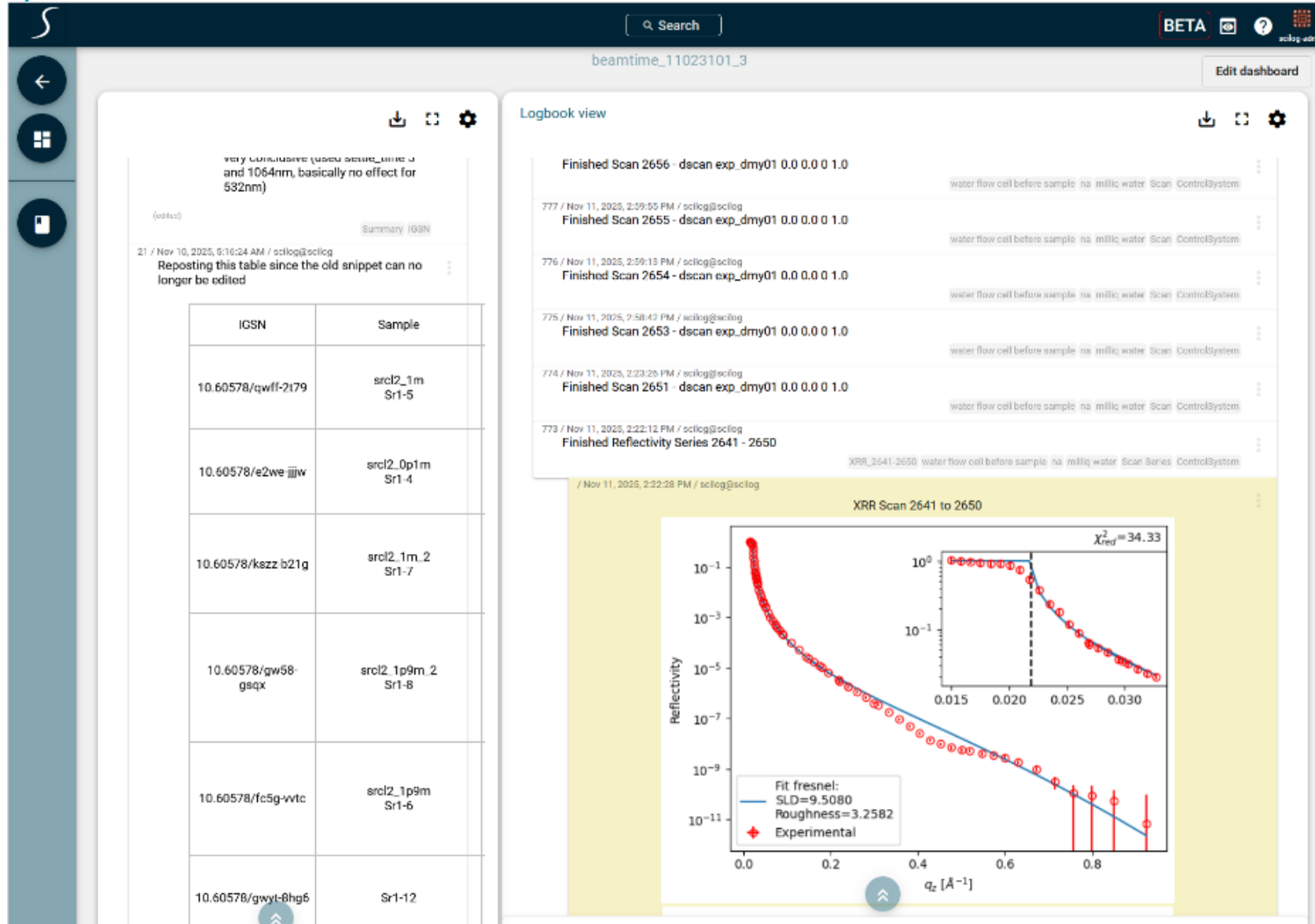


www.igsn.uni-kiel.de

Service provided by
CAU central computing

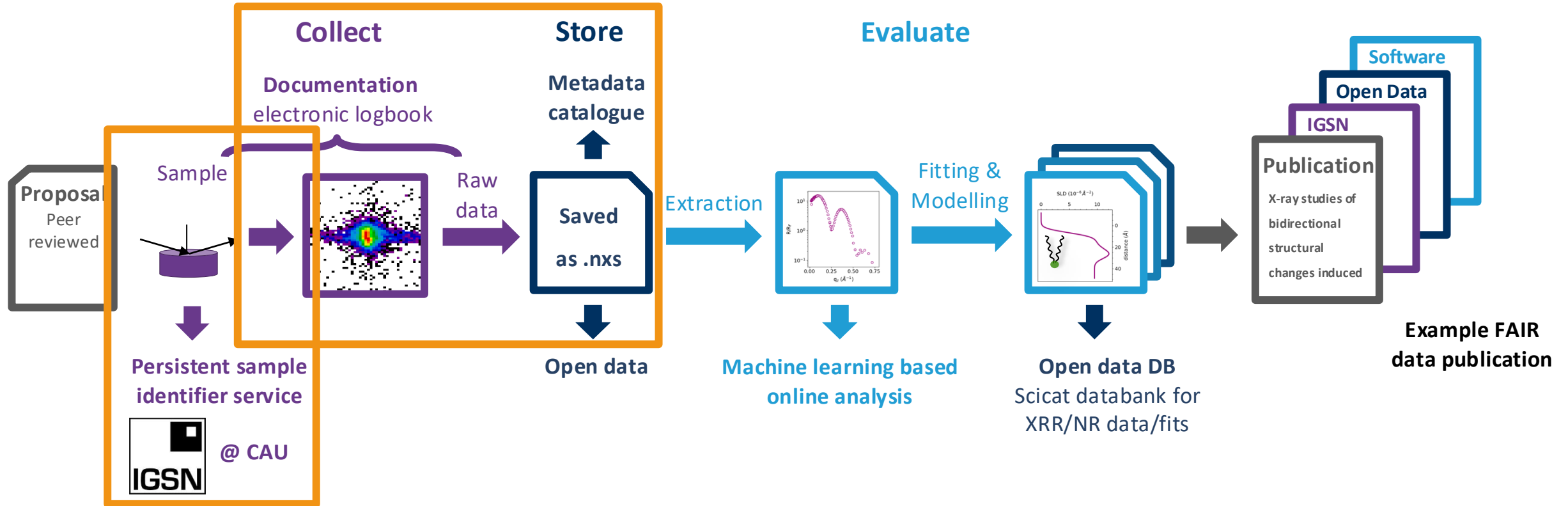
Documentation – SciLog Electronic logbook

Recording experiment and initial results via application programming interfaces (API)



X-ray reflectivity data pipeline

All experimental and planning data is valuable for use and reuse



Documentation – metadata Catalogue

Cataloguing the data and metadata in a user friendly format



SciCat - metadata catalog at DESY

Help About Nicolas Hoyer

Datasets / 11023101/ X R R dppc 80mol mr10 20mol 02675-02683 /

Details Datafiles Related Datasets Lifecycle

General Information

Dataset name XRR 02675-02683 / 10.60578/Buhs-x011

PID 11023101/XRR_dppc_80mol_mr10_20mol_02675-02683

Creation time 2025-11-11 16:56

Type derived

Keywords XRR lisa-output

Contact Information

Principal investigator Hitaishi

Contact email pkh3194@gmail.com

Files Information

Number of files 4

Size 8846

Data Overview

The Data Overview section contains two plots. The left plot shows a 2D intensity map with a color scale from 0 to 1. The right plot shows a 1D intensity profile with a color scale from 0 to 1. Both plots have axes labeled with numerical values.

Related Documents

Proposal IDs 11023101 20230678

Instrument IDs /desy/petra3/p08

Sample IDs -

Input datasets 11023101/dppc_80mol_mr10_20mol_02675 11023101/dppc_80mol_mr10_20mol_02676 11023101/dppc_80mol_mr10_20mol_02677 11023101/dppc_80mol_mr10_20mol_02678 11023101/dppc_80mol_mr10_20mol_02679 11023101/dppc_80mol_mr10_20mol_02680 11023101/dppc_80mol_mr10_20mol_02681 11023101/dppc_80mol_mr10_20mol_02682 11023101/dppc_80mol_mr10_20mol_02683

Creation location /DESY/PETRA III/POB

Scientific Metadata

Search

scanmode	measurement
sample_name	DPPC 80 mol% + MR10 20 mol%
sample_composition	80(C ₄₀ H ₈₀ NO ₈ P)+20(C ₂₈ H ₄₅ N ₄)
sample_id	10.60578/Buhs-x011
sample_description	1 Molar DPPC 80 mol% + MR10 20 mol% in chloroform

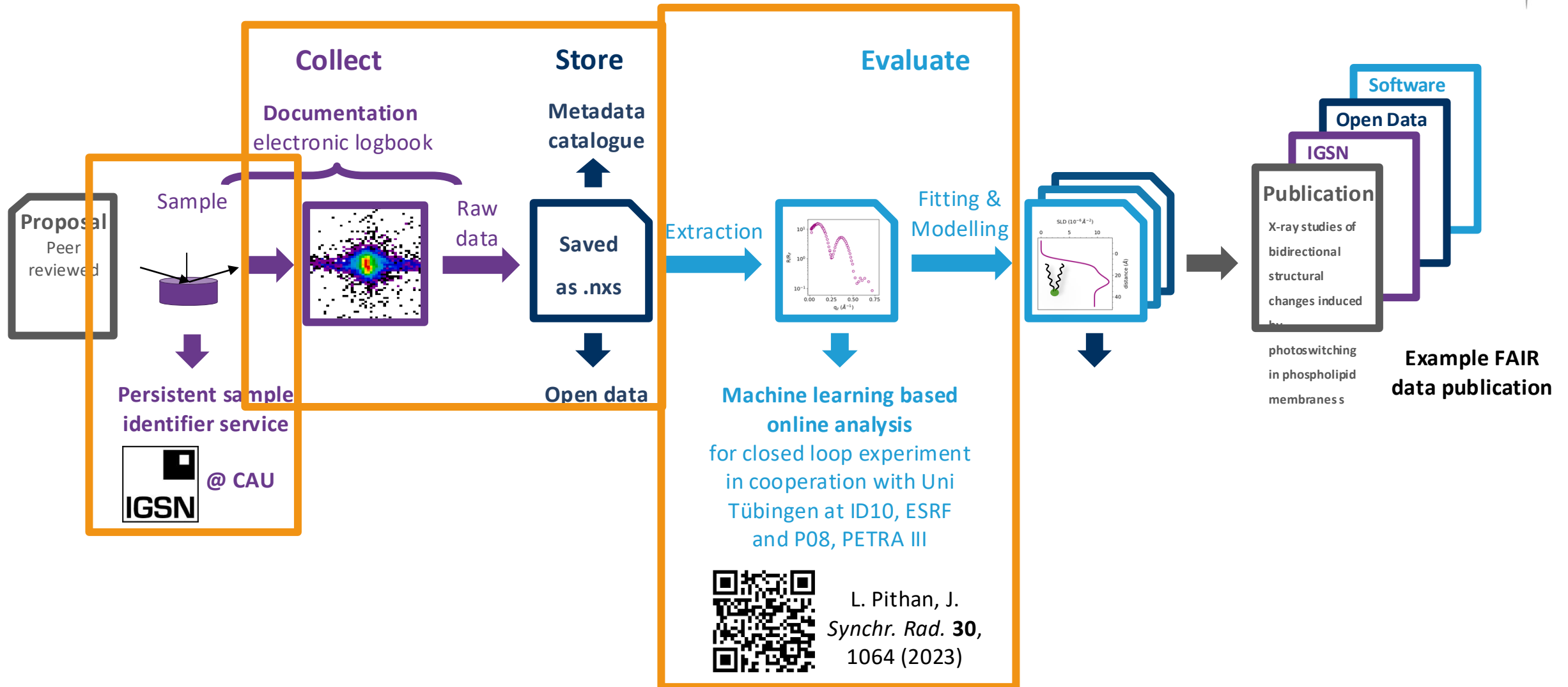
Dataset JsonView

Show JSON View

<https://www.scicatproject.org>

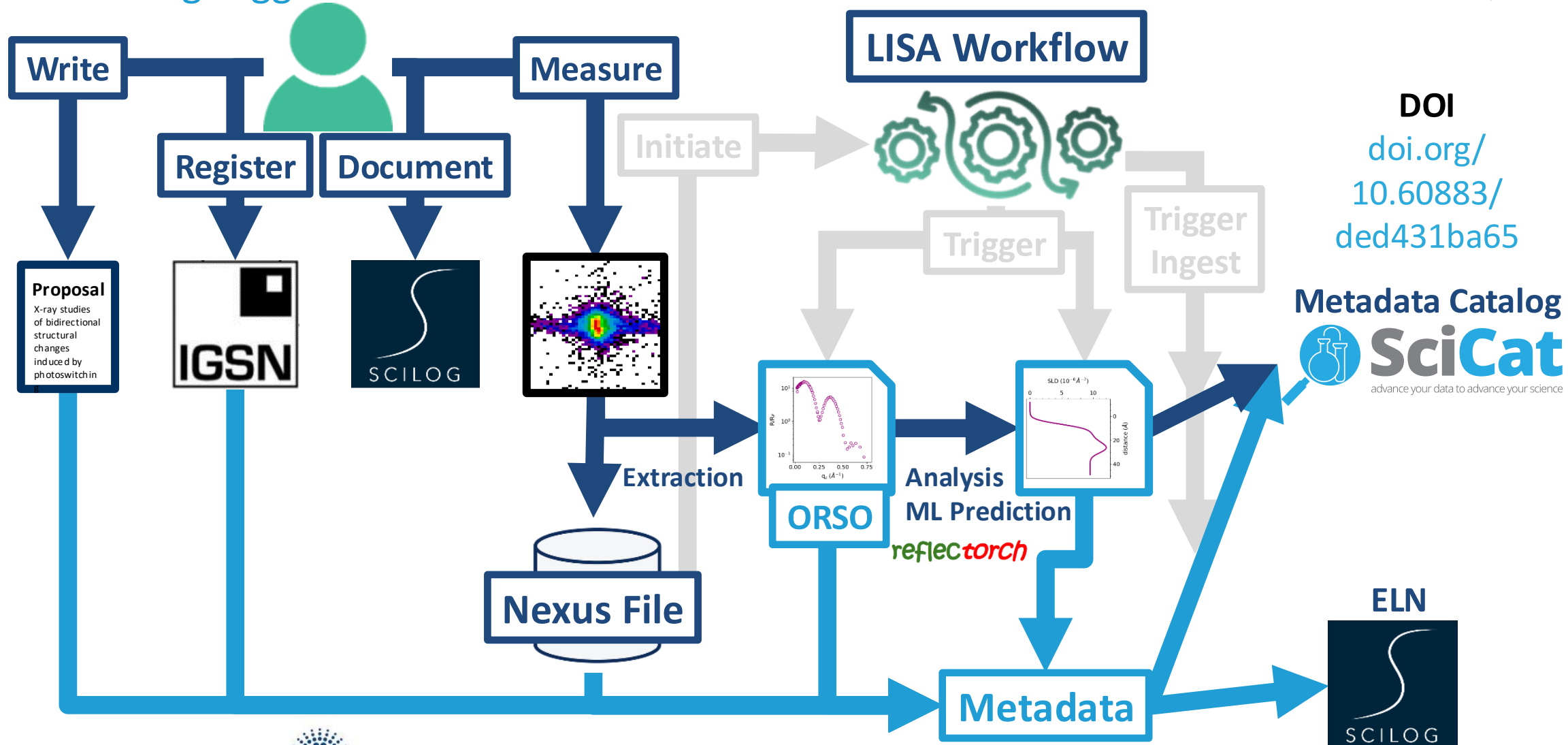


X-ray reflectivity data pipeline



Automated Workflow

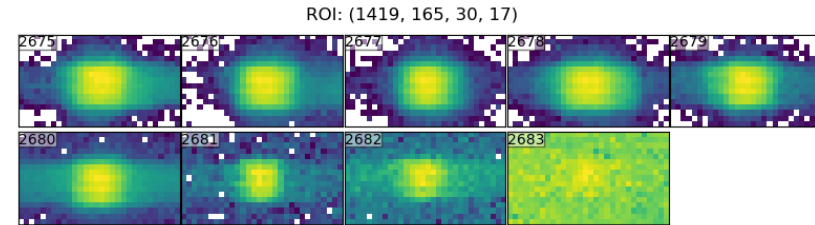
Machine learning triggered when new data set is saved



LISA Pipeline for Reflectivity Extraction and Analysis



Extraction



ML-based
Analysis

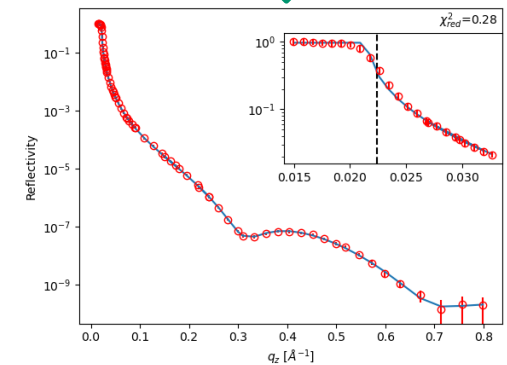
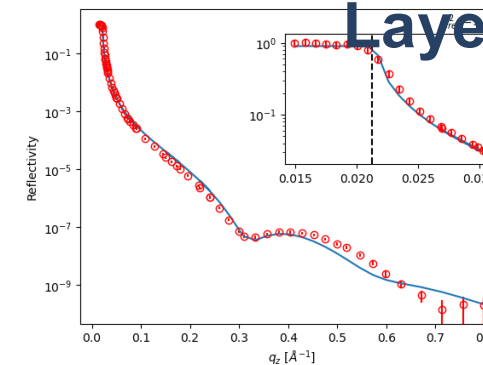
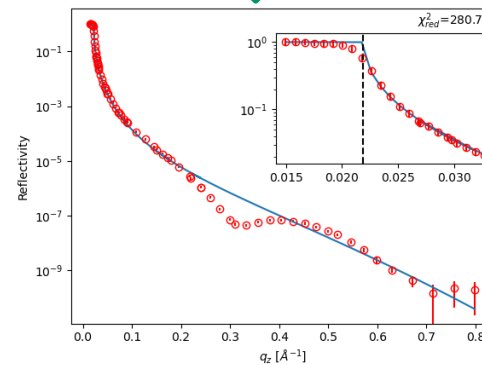
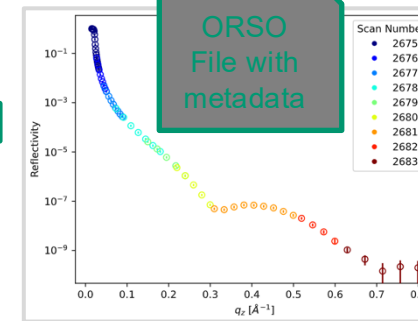
reflectorch^{1,2}



0
Layer

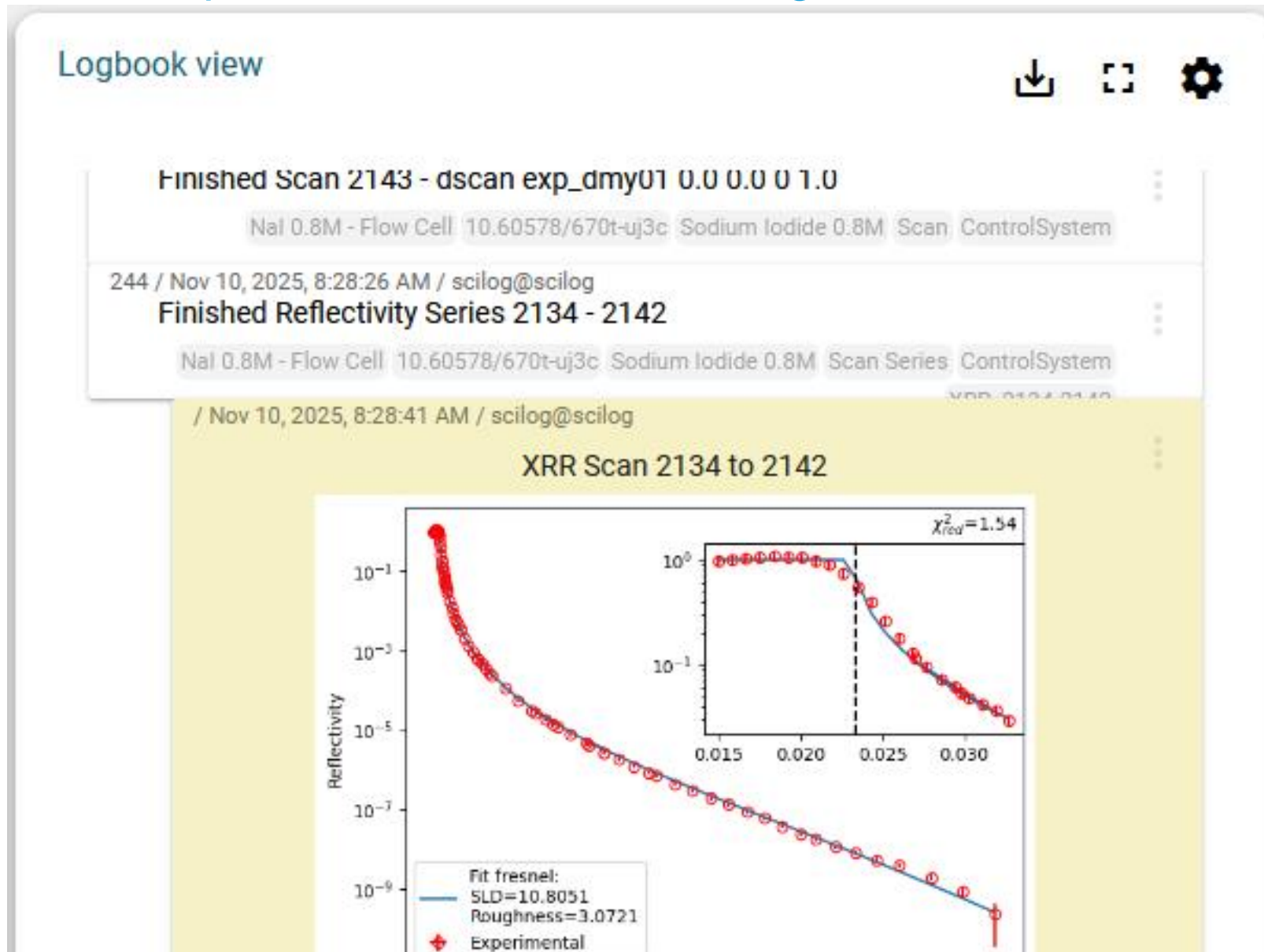
1
Layer

2
Layer

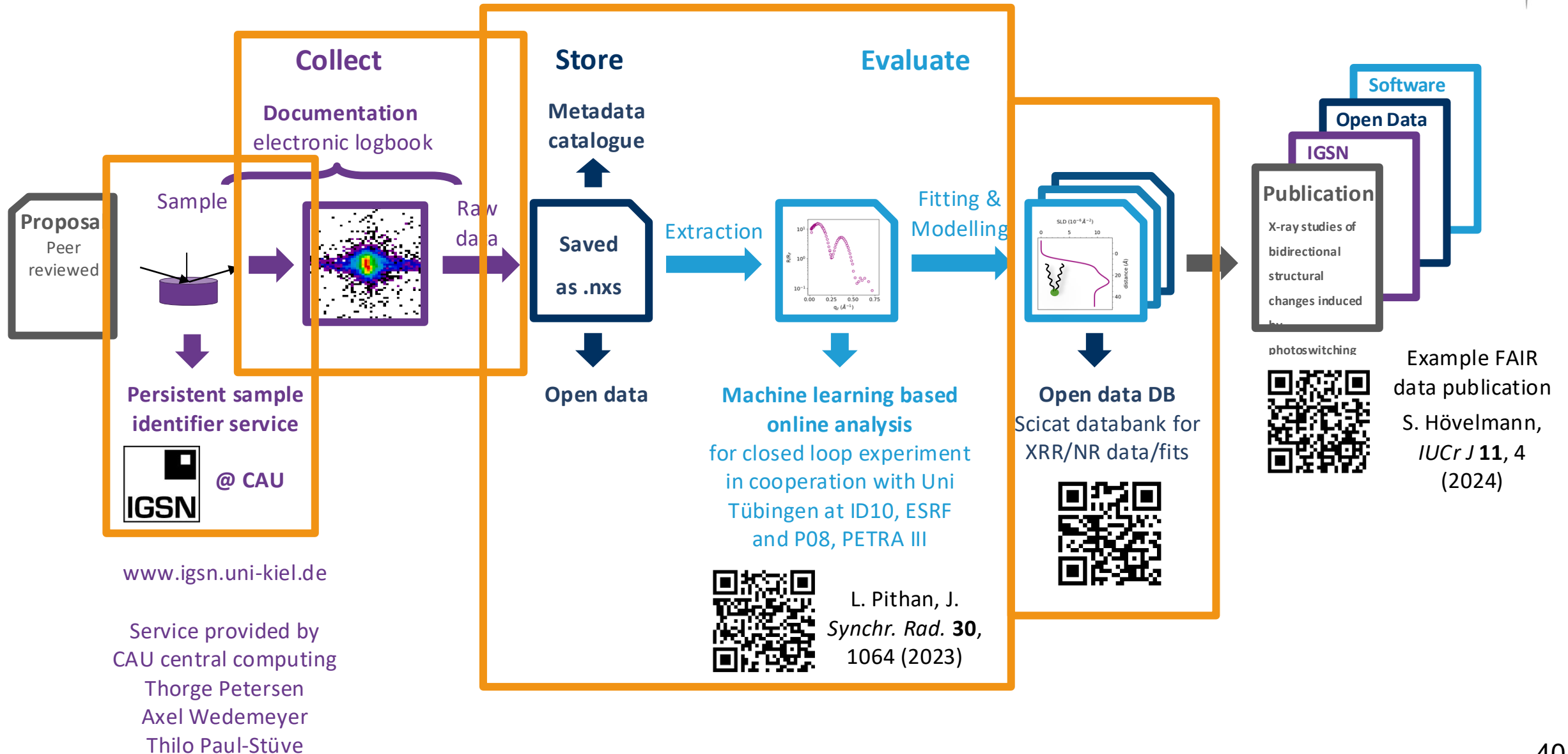


Analysed Data Auto-Ingestion Electronic Log Notebook

Facilitate better experimental decision making



X-ray reflectivity data pipeline



Open Databank for data



Datasets /

Datasets / [public-data/b77dfdb1-7271-4858-a128-7f4de1dfea28](#) /

Details

Datafiles

Related Datasets

Lifecycle

Jupyter Hub

General Information

Name	GIXOS-derived pseudo reflectivity of the surface of water and 10vol% ethanol at 293K, circular Qxy resolution
Description	pseudo reflectivity derived from grazing incidence off-specular scattering data from the surface of water and 10vol% ethanol at 293K
PID	public-data/b77dfdb1-7271-4858-a128-7f4de1dfea28
Type	raw
Creation Time	2024-10-16 16:55
Keywords	

Creator Information

Owner	Chen Shen
Principal Investigator	Chen Shen
Contact Email	chen.shen@desy.de
Owner Group	ingestor
Access Groups	

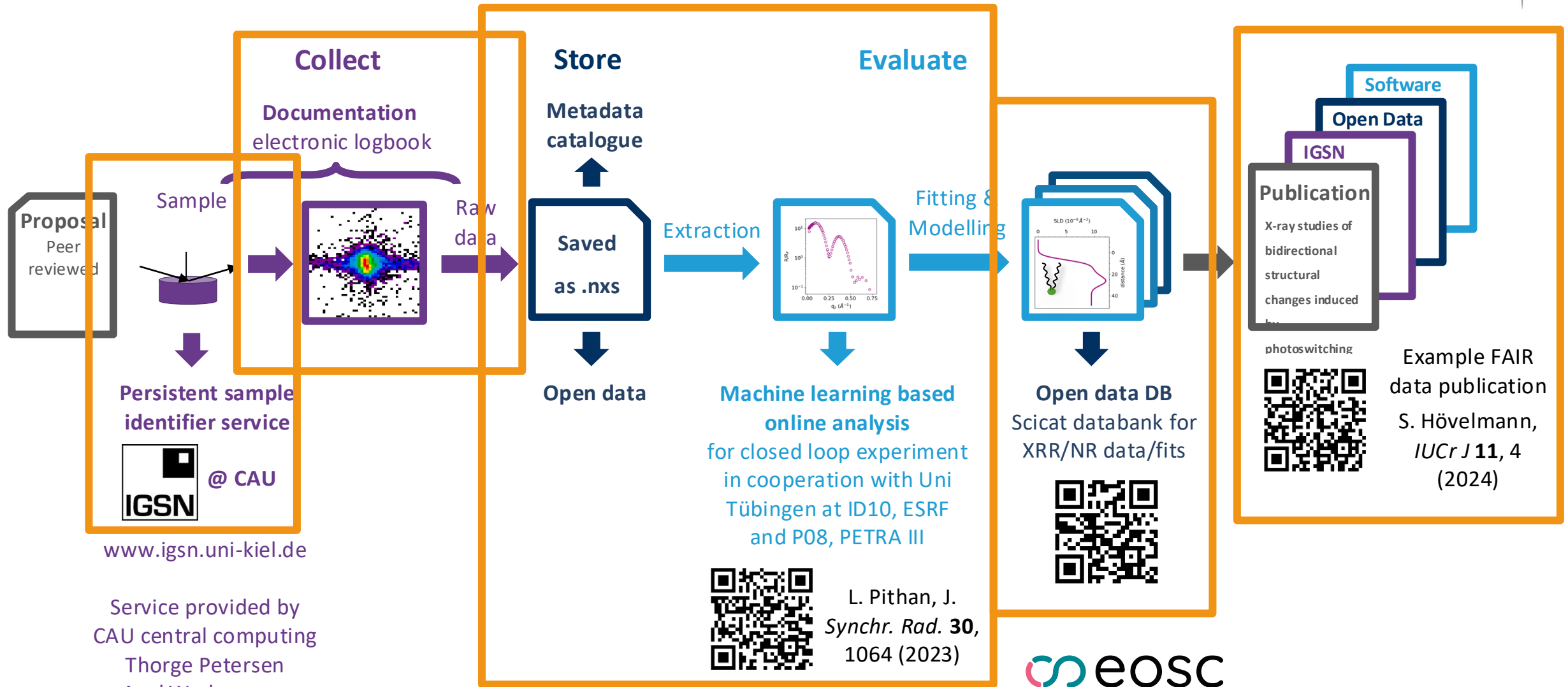
Search	Clear
PID	
Text Search	
Location	
Group	
Type	
Keywords	
Start Date – End Date	
+ Add Condition	

Name	Source Fo
GIXOS-derived pseudo reflectivity of DPPG monolayer on tris-EDTA buffer surface (pH7.3) at pi = 45mN/m, 295K	...40497
GIXOS-derived pseudo reflectivity of DPPG monolayer on tris-EDTA buffer surface (pH7.3) at pi = 35mN/m, 295K	...38649
GIXOS-derived pseudo reflectivity of DPPC monolayer on water at pi = 35mN/m, 295K	...74735
GIXOS-derived pseudo reflectivity of the surface of water and 10vol% ethanol at 293K, circular Qxy resolution	...26393
GIXOS-derived pseudo reflectivity of water surface at 295K, circular Qxy resolution	...45823
GIXOS-derived pseudo reflectivity of water surface at 293K, rectangular slit resolution	...57053
GIXOS-derived pseudo reflectivity of DSPC monolayer on water at 45mN/m at 293K	...95278
reflectivity of DSPC monolayer on water at 45mN/m at 293K measured by specular reflectometry	...60197 Wed 15:08
water reflectivity at 293K measured by specular reflectometry	...5850078741 2024-10-16 Wed 14:42

<https://public-data.desy.de/>



X-ray reflectivity data pipeline



research letters

IUCr

ISSN 2052-2525

PHYSICS | FELS

Received 6 March 2024
Accepted 2 May 2024

Edited by F. Maia, Uppsala University, Sweden

This article is part of a collection of articles from the IUCr 2023 Congress in Melbourne, Australia, and commemorates the 75th anniversary of the IUCr.

† Present address: Department of Physics, Indian Institute of Technology (ISM) Dhanbad, Jharkhand 826004, India.

Keywords: lipid mesophase; photoswitches; azobenzene; vesicles; small-angle X-ray scattering; light-induced mesophase transformations; temperature-induced mesophase changes; structure determination;

Photoinduced bidirectional mesophase transition in vesicles containing azobenzene amphiphiles

Svenja C. Hövelmann,^{a,b,c} Ella Dieball,^a Jule Kuhn,^a Michelle Dargasz,^d Rajendra P. Giri,^{a,†} Franziska Reise,^e Michael Paulus,^f Thisbe K. Lindhorst^e and Bridget M. Murphy^{a,c,*}

^aInstitute of Experimental and Applied Physics, Kiel University, Leibnizstraße 19, 24118 Kiel, Germany, ^bDeutsche Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany, ^cRuprecht Haensel Laboratory, Olshausenstraße 40, 24098 Kiel, Germany, ^dDepartment Physik, Universität Siegen, Walter-Flex-Strasse 3, 57072 Siegen, Germany, ^eOtto Diels Institute of Organic Chemistry, Kiel University, Otto-Hahn-Platz 3-4, 24118 Kiel, Germany, and ^fFakultät Physik/DELTA, TU Dortmund, 44221 Dortmund, Germany. *Correspondence e-mail: murphy@physik.uni-kiel.de

The functionality and efficiency of proteins within a biological membrane are highly dependent on both the membrane lipid composition and the physicochemical properties of the solution. Lipid mesophases are directly influenced by changes in temperature, pH, water content or due to individual properties of single lipids such as photoswitchability. In this work, we were able to induce light- and temperature-driven mesophase transitions in a model membrane system containing a mixture of 1,2-dipalmitoyl-phosphatidylcholine phospholipids and azobenzene amphiphiles. We observed reversible and reproducible transitions between the lamellar and *Pn3m* cubic phase after illuminating the sample for 5 min with light of 365 and 455 nm wavelengths, respectively, to

5. Data availability

Raw data, fit parameters and analysis scripts are available under: <https://doi.org/10.57892/100-49> International Generic Sample Numbers (IGSNs): DPPC:1 100:0 (<https://doi.org/10.60578/gucn-en2h>); DPPC:1 97.5:2.5 (<https://doi.org/10.60578/kw2n-ouv5>); DPPC:1 95:5 (<https://doi.org/10.60578/dg1l-5gebr>); DPPC:1 90:10 (<https://doi.org/10.60578/reqz-rk9v>); DPPC:1 80:20 (<https://doi.org/10.60578/r2j8-grzb>); DPPC:1 70:30 (<https://doi.org/10.60578/l7hw-iao2>); DPPC:1 50:50 (<https://doi.org/10.60578/p1fg-n3tw>); DPPC:1 37:63 (<https://doi.org/10.60578/g7n3-wkj3>); DPPC:1 30:70 (<https://doi.org/10.60578/q7j3-sid5>); DPPC:1 0:100 (<https://doi.org/10.60578/xke5-nz1u>).



igsn.uni-kiel.de

Kiel University Published 2024 Physical Object

Mixed 10% Azobenzene Amphiphile AZOL-C16 and 90% 1,2-Dipalmitoyl-sn-glycero-3-phosphocholine

Hövelmann, Svenja



opendata@uni-kiel
Kiel University Research Data Repository

General information

IGSN ID

10.60578/re

Type

Physical Object

Publisher

Kiel University

Publication year

2024

Search Browse Submit Document Guide 0

Research Data / SAXS and DSC data and scripts for publication: Photoinduced bidirectional...

Research Data Sat May 18 2024 CC BY 4.0 Published

SAXS and DSC data and scripts for publication: Photoinduced bidirectional mesophase transition in vesicles containing azobenzene amphiphiles

Hövelmann, Svenja Carolin; Murphy, Bridget Mary

The small angle X-ray scattering (SAXS) and differential scanning calorimetry (DSC) data, analysis results and analysis scripts are accessible for the publication "Photoinduced bidirectional mesophase transition in vesicles containing azobenzene amphiphiles".

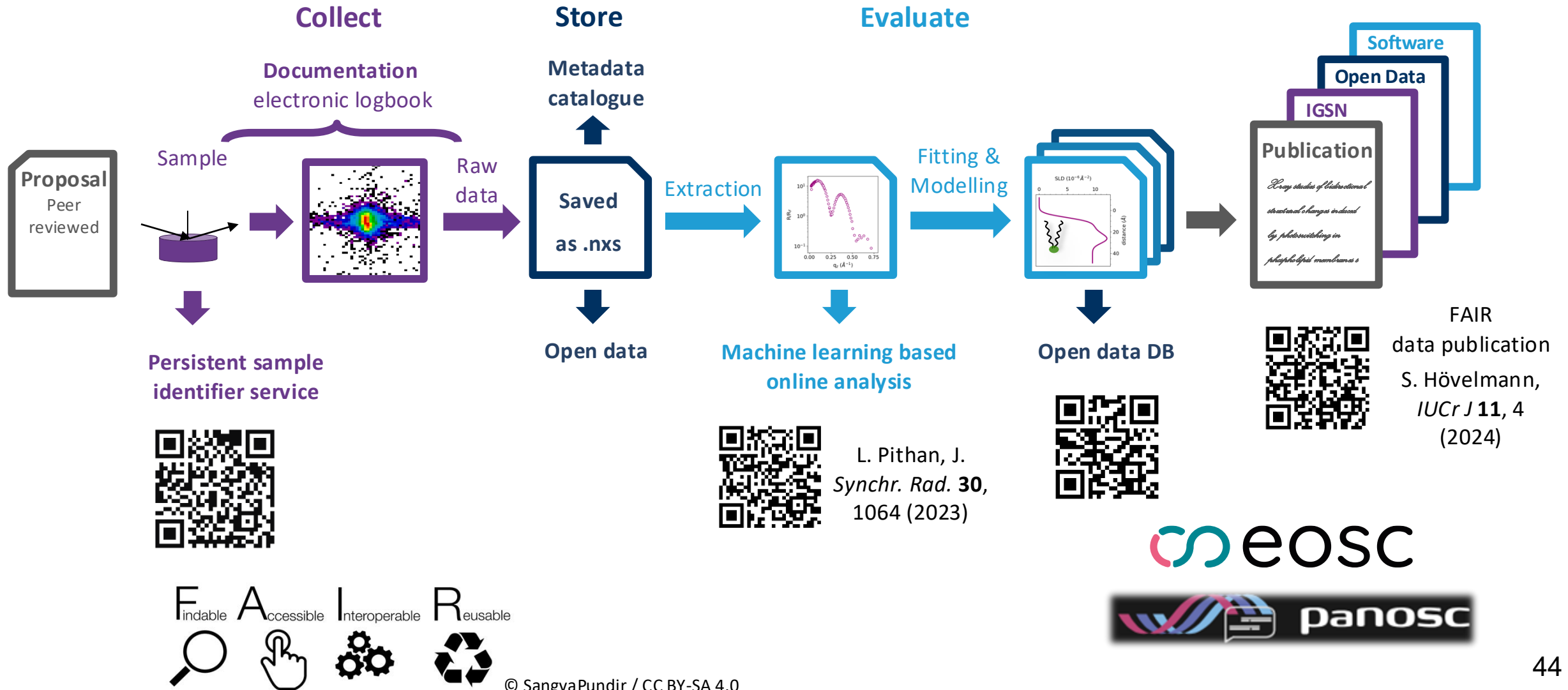
Data is made accessible under DAPHNE4NFDI.

Actions

DSC data.zip	2024-05-16	784.03 kB
Python scripts.zip	2024-05-16	4.83 kB
README.md	2024-05-16	1.48 kB

Research data management can improve science

From sample preparation to publication



Acknowledgement

Svenja Hövelmann
 Prashant Hitaishi
 Jonas Warias
 Ali Ashtiani
 Nicolas Hayen
 Julia Kobus
 Philipp Jordt
 Andrea Sartori
 Jule Kuhn
 Karin Hansen
 Ella Dieball
 Rajendra Giri
 Lukas Petersdorf
 Rabia Quamar
 Priya Derangula
 Ajit Seth
 Sunil
 Olaf Magnussen
 Ajay
 Matthias Greve
 Karsten Tarhouni
Thisbe Lindhorst
 Franziska Reise
 Michael Röhl



My Group at DESY

Zeynep Isik Dursun
 Regina Hinzmann
 Partha Tirumalai
 Anjali Aggarwal
 Otto Lippman

IT

Linus Pithen
 Tim Wetzel
 Jan Kotanski
 Noel Barth
 Anton Barty
 Patrick Furhman

Beamtime support

P08/Petra III

Florian Bertram
 Chen Shen
 René Kirchhof
 Milena Lippmann



Tom Arnold

Peter Gaal

Daniel Schmidt

Frank Schreiber
 and group

FASTER

Christan Gutt, Siegen
 Roman Obersmaisser, Siegen
 Frank Schreiber, Tübingen
 Sebastian Busch, MLZ
 Erik Brundermann, KIT
 Anke Susanne Müller, KIT
 Linus Pithan, DESY
 Fabian Westermeier, DESY
 Peter Gaal TX products

Photonic

Patrick Fuhrmann DESY
 Tim Wetzel, DESY
 Paul Miller, DESY
 Christan Gutt, Siegen
 Luca Gelisio EU-XFEL
 Will Smith HZB

