Chemistry and Life Science Support (CLS)

SAD Division

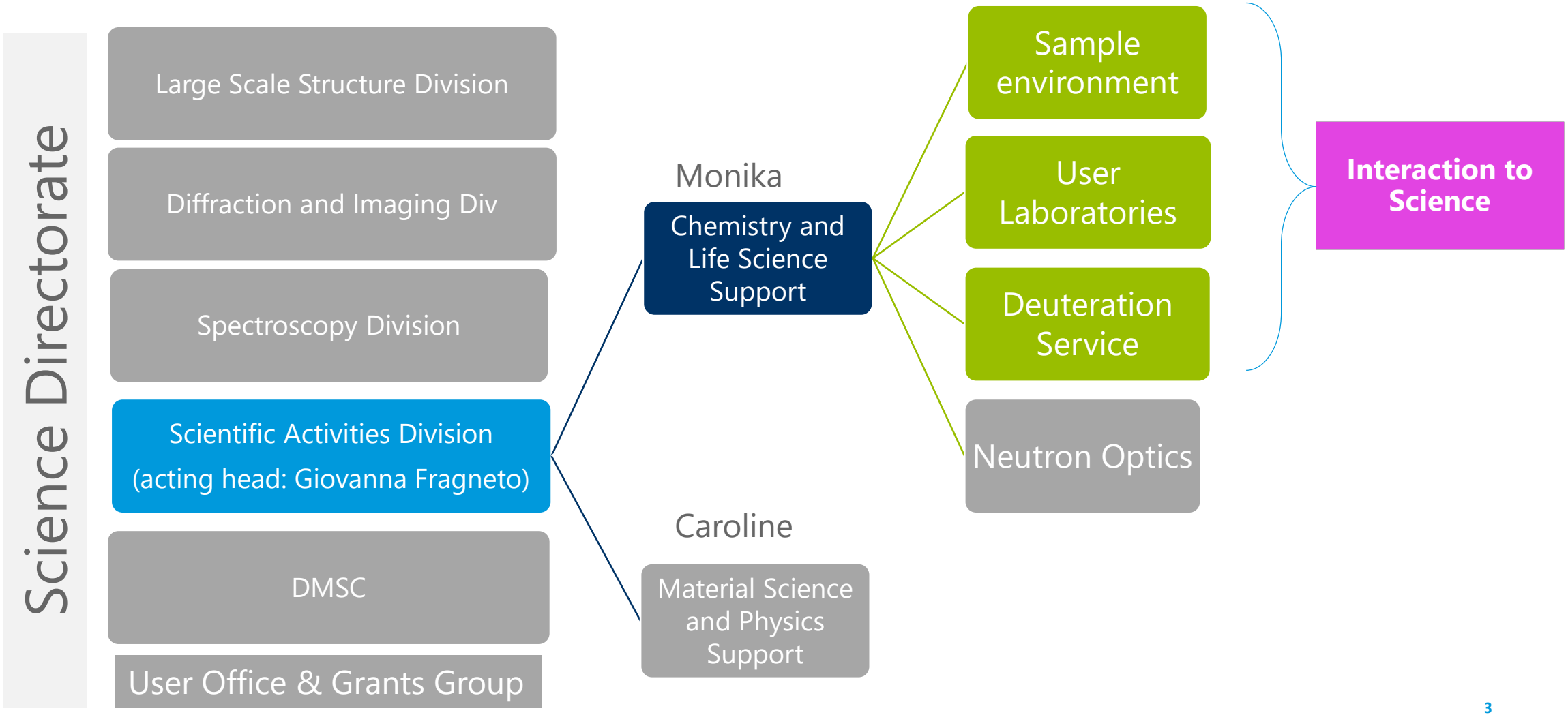
PRESENTED BY MONIKA HARTL

2024-04-21

CLS group

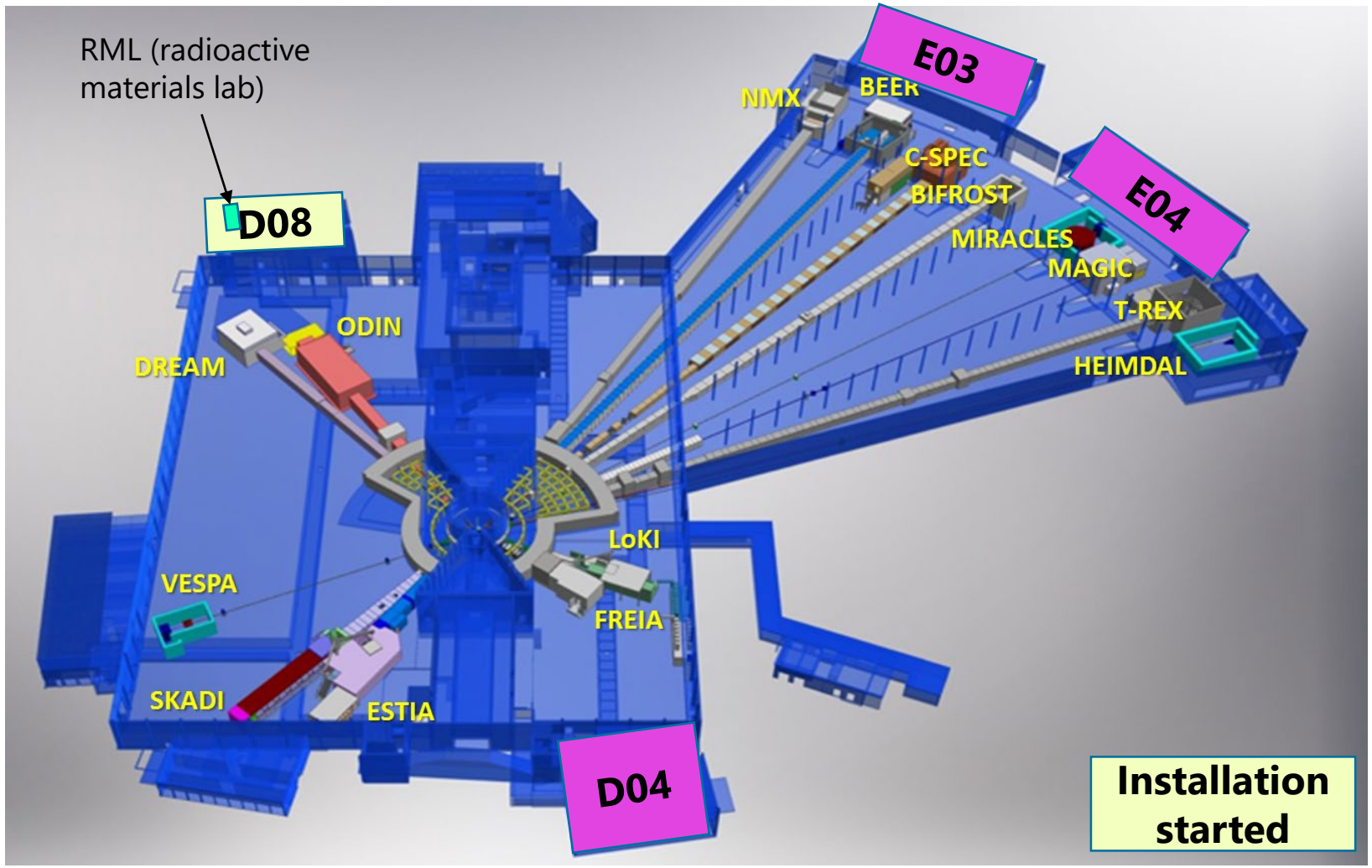
Chemistry and Life Science Support - CLS

Enable high impact science on ESS instruments in chemistry and life science



Chemistry and Life Science Support

Locations



Chemistry and Life Science Support :

- 1120 m^2, 25 rooms
- 4 buildings

Offices:
D08, E04

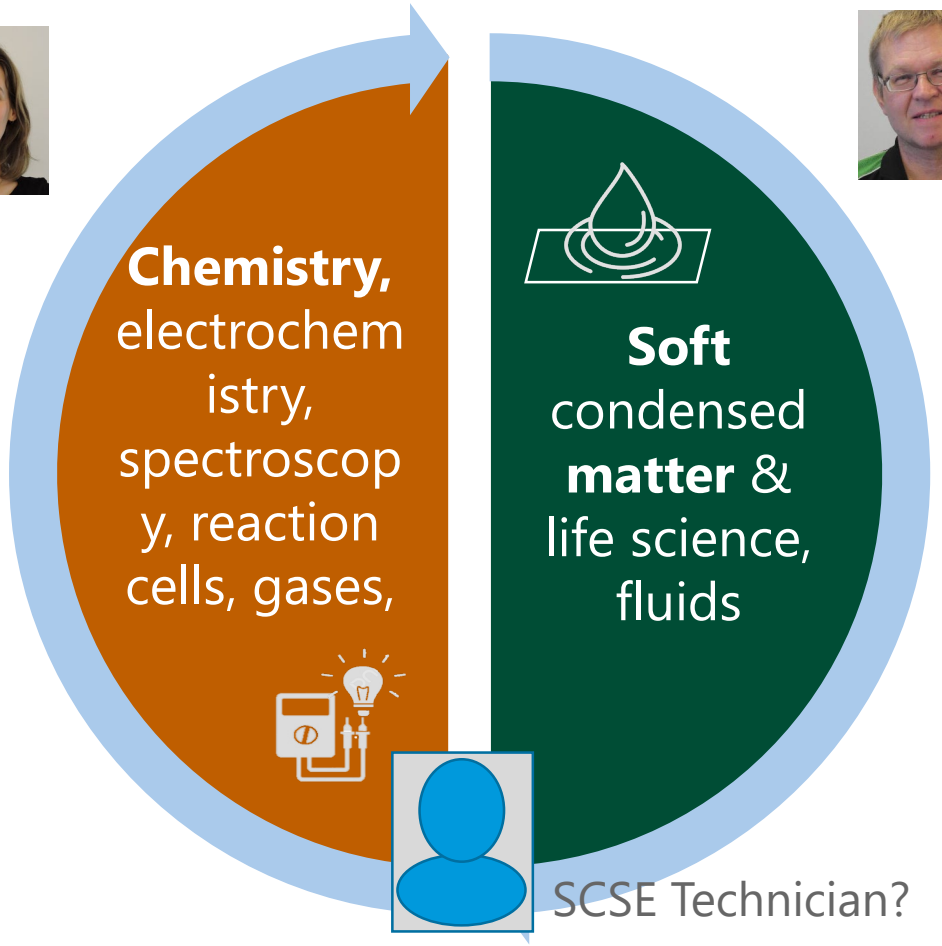
CLS - SCSE

Design, setup, maintain & operate sample environment equipment.

Soft Matter and Chemistry Sample Environment

Alice Corani

- Humidity
- Gas flow / gas adsorption
- Reaction Cells
- In-situ experiments (e.g. spectroscopy)



Harald Schneider

Hannah Burrall

- Liquids (liquid/solid; liquid/liquid)
- Liquid flow
- Thermalized liquid
- Shear/Rheology

SCSE Technician?

Luca Sagliano (50%)
Mech. Engineer (central)

CLS-SULF

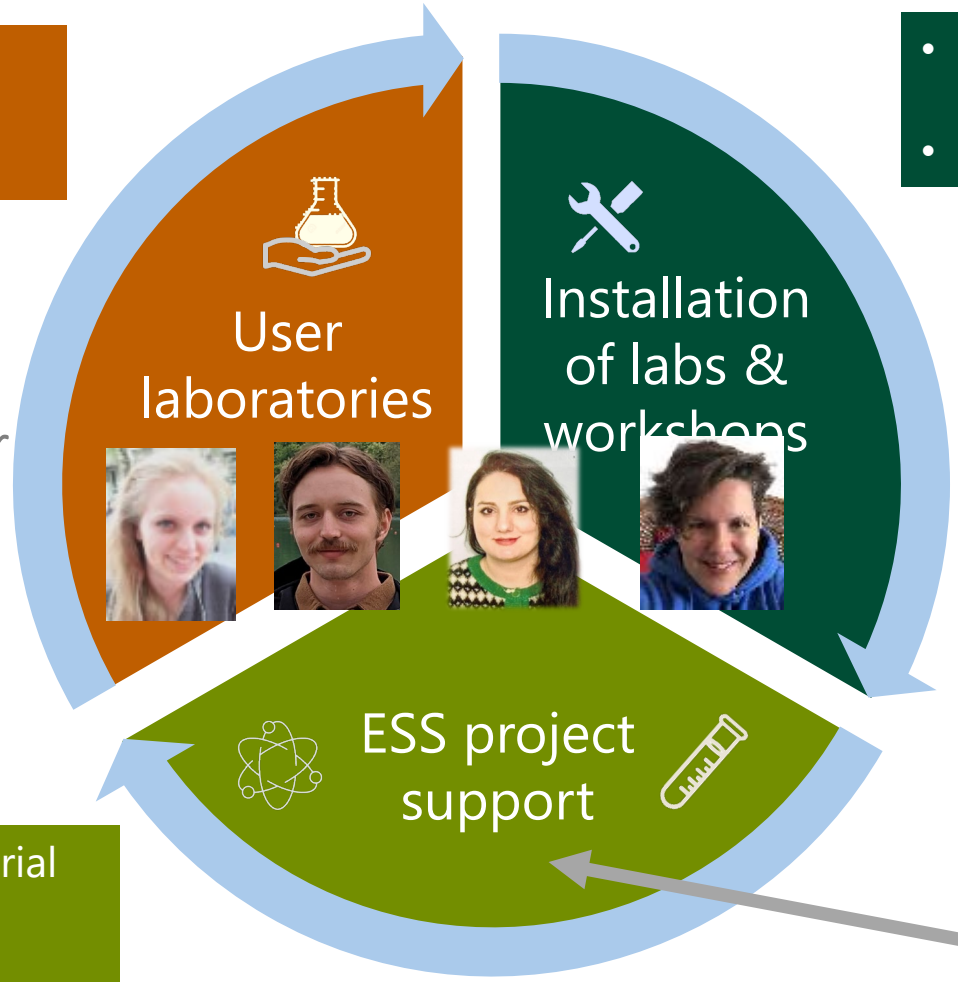
Handling, modifying & characterizing samples before, during, and after beamtime.

Sample Handling and User Laboratory Facility (extended team)

- Operate and maintain sample handling and user lab facility
- Scientific&technical support




Katrin Michel, Melissa Sharp, Nick Weisend, Christopher Mosunda (INTERN)



- Complete user lab installation and workshops in D08 for SAD
- Provide area coordination

Ghazaleh Roostaei

CLS planning, budget, EAM system, inventory

- Support ESS project with material analysis (accelerator, target, science)
- Support with radiation chemistry

Monika Hartl

Damian Martin Rodriguez

Neutron Optics

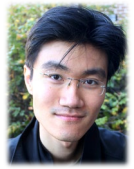
- Beam characterization for instruments (γ-spec /foil)
- Material characterization
- Neutron Guide degradation/simulation

CLS – DEMAX

Supply of deuterated samples and protein crystallization.

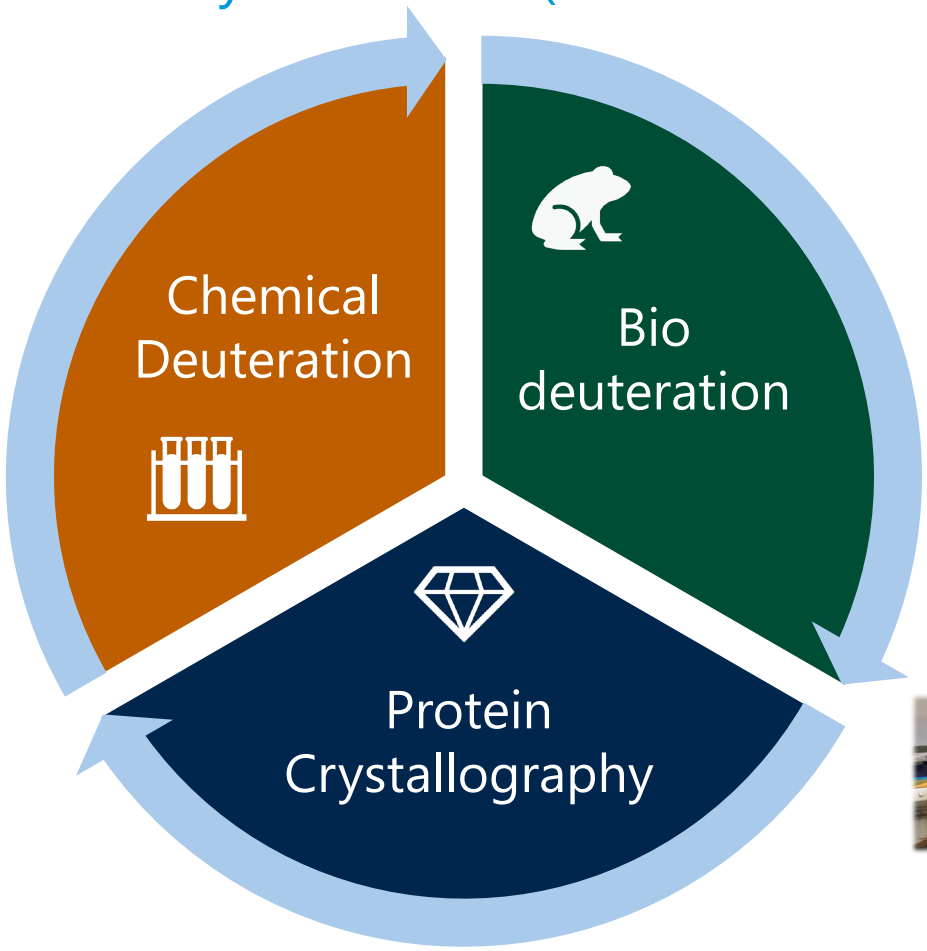
Deuteration and macromolecular crystallization (extended team)

Anna Leung



Jia-Fei Poon

- Small organic molecules,
- Lipids (e.g. POPC, SOPC, POPE)
- Surfactants (e.g. sugar-based)
- Novel molecules



Sophie Ayscough

Hanna Wacklin-Knecht

NEUTRONS FOR SOCIETY

0.2 FTE Lipids

- Deuterated biomass from algae, yeast, *E. coli*, …
- Recombinant soluble proteins, DNA
- Yeast-derived lipids

Zoë Fisher

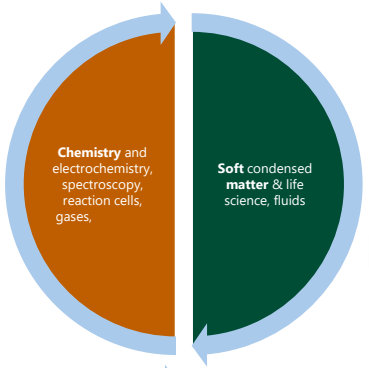
LUND UNIVERSITY

0.7 FTE LP3

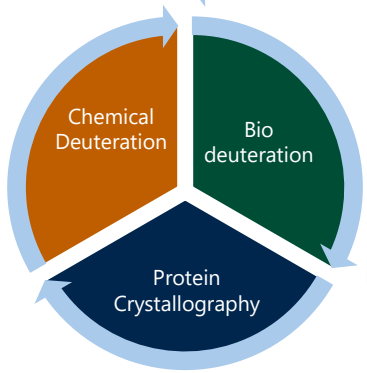
- High- and low-throughput screening,
- fine screening in large volumes
- r.t. crystal mounting & data collection, X-ray testing at MAX lab

CLS – Bringing the pieces together

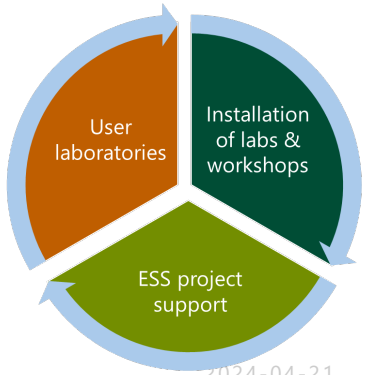
Support is starting with the sample – **unified approach throughout CLS**



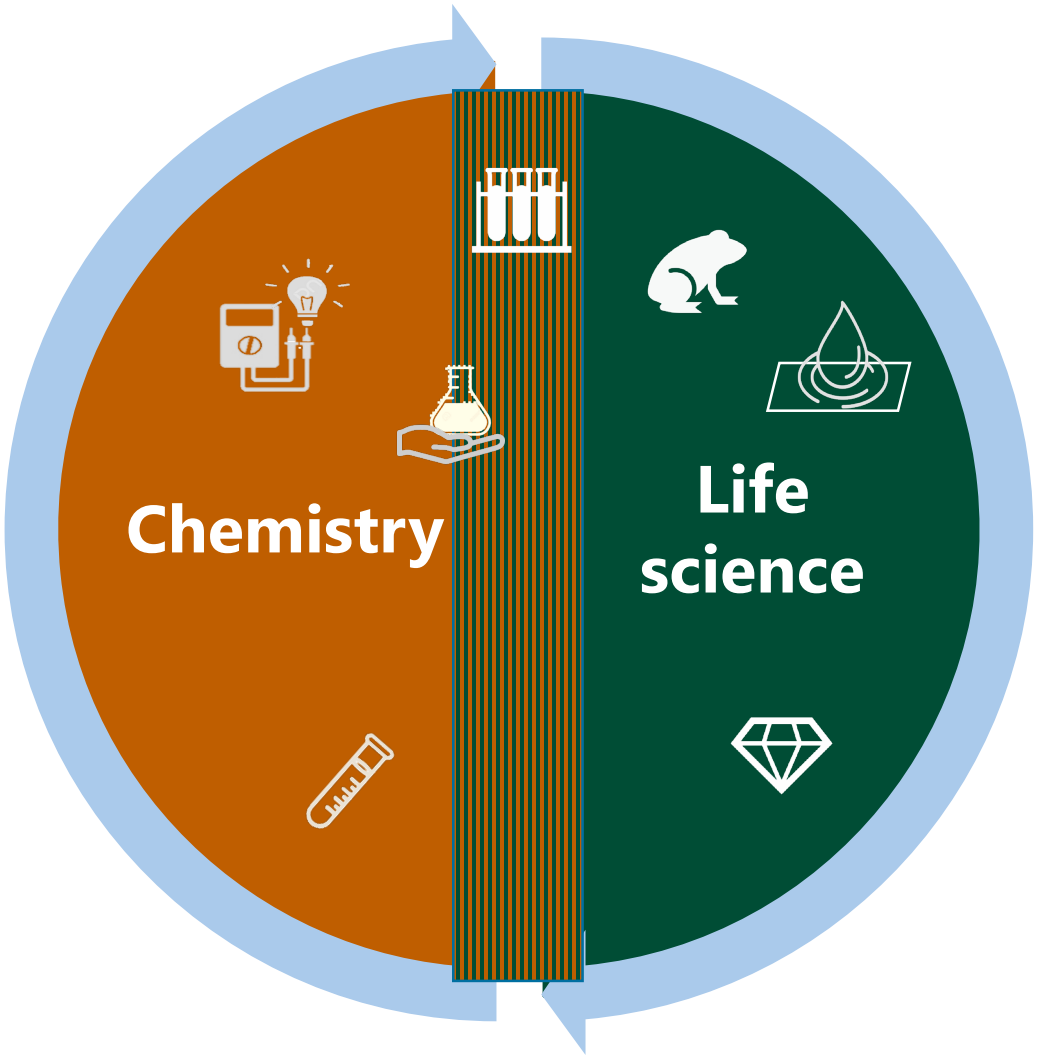
Sample environment



Deuterated samples for the experiment



User laboratories (sample preparation for the experiment)



CLS-I2S

Assure CLS has everything in place for first science at ESS.

Interfaces to Science in CLS

	Instrument Cold commissioning	Instrument hot commissioning
SCSE	❑ Test SE equipment on instrument with focus on basic equipment (sample changer and similar)	❑ Basic SE equipment ready for instrument hot commissioning; testing and completing equipment for first science
SULF	❑ Get labs/lab buildings ready for handling activated samples (sample handling procedures, radiation monitors); verify labs are ready for hot commissioning experiments.	❑ Get labs ready for specific first science experiments (consumables, chemicals & equipment); HC sample handling ongoing;
DEMAX	❑ Get ready for specific hot commissioning experiments, i.e. determine if/what deuterated standards are needed.	❑ Have necessary compounds for HC available; start developing synthesis methods for FS experiments

CC

HC

Soft matter/life science

Hanna

Melissa

First science

Alice

Monika

Chemistry

Sorting by instruments (not complete yet)

Check by instrument and instrument class to fill the gaps (one example)

	LOKI	DREAM	ESTIA	BIFROST	BEER	CSPEC
SCSE	• **SAMPLE ENVIRONMENT** • Rheometer • Liquid/gas mixing supercritical • EC cell (impedance, battery menbrane, humidity …) • UV pump, photo excitation • Humidity cells extreme condition, D2O/H2O • Vapor sporption (liquids) • Insitu reaction (stopped flow for corrosive mat.) …	• **SAMPLE ENVIRONMENT** • Gas handling system (<1 bar up to 200 bar) • H_2 / CO_2 Adsorption • EC cell (batteries/ coin cell/ cylindrical) + potentiostat • Reaction cells with injection system • In-situ thermogravimetric analysis…..	• **SAMPLE ENVIRONMENT** • Solid-Liquid cells, • Liquid-liquid cells/troughs • EC cell (batteries, potentiostat) • In-situ light scattering (seen but not common) •	• Furnace, cryostat, electric field, magnetic field 7 tesla • Sample changer is foreseen 4 samples, 3D print sample holder for the cryostat.	• Full battery set • H2 embrittlement • Structural changes • Gas adsorption ? • Laser for heating, no light insitu devices	• Gas handling (medium to low pressure, < 10 bar) • Electrochemistry (decide if installed in table or in cryostat depending on measurement temperature) • Humidity cell • Pump-probe • Sample changer (also for powders), e.g. a small LOKI sample changer, 4-5 samples
SULF	• **USER LABORATORIES** • Rheometer test stand • Dynamic light scattering • potentiostat • pipettes, balances, sonicator,…..	• **USER LABORATORIES** • gas handling system • EC setup (potentiostat, glove box, press etc.) • DSC/DTA…	• **USER LABORATORIES** • Coin cell crimper • Drying equipment (ampoule that can be pump and warm and trnafer to the glovebox name??) • Spin coater, silicon wafer	• **USER LABORATORIES** • Laue diffractometer (neutron diffractometer like in PSI) Squid, heat capacity measurement	• **USER LABORATORIES** • SLIME (MSPS) • Hydrogen lab	• **USER LABORATORIES** • Laue diffractometer for alignment
DEMAX	• **DEUTERATION** • Constrast matching ! • chemical deuteration (small(er) organic molecules, surfactants,…) • biodeuteration (proteins, yeast lipids …)	• **DEUTERATION** • Reduction of inelastic background • Chemical deuteration (small organic molecules/MOFs,	• **DEUTERATION** • Constrast matching ! • chemical deuteration (small(er) organic molecules, surfactants,…) • biodeuteration (proteins, yeast lipids …)	• **DEUTERATION** • No requests	• **DEUTERATION** • No requests	• **DEUTERATION** • No requests

NEXT STEPS

- continue to get everything in place to cover the basics and for first science
– planning is now connected to milestones for the instruments (HC,CC,FS)
- prioritize list together with the instruments (already started)
- **provide COMPLETE SCIENCE SUPPORT: check that we have user labs and deuteration support that fits with SCSE equipment & first science -> discussion in I2S session**
- check that we did not miss scientific areas (exchange with other facilities, conferences).

Installation for SAD:

continue to install labs & workshops in D08 in 2024 to have best support available for D01 hall (DREAM/ ODIN) –**installation started in Feb. '24**

Steady-State Operations

Steady-State-Operations Review

SSO

- ESS is in initial operations until end of 2027.
- CLS has a defined budget until end of 2027, which includes currently:

  - SULF: 2 scientist, 3 technicians
  - DEMAX: 4 scientists
  - SCSE: 3 engineers, +???

We have:

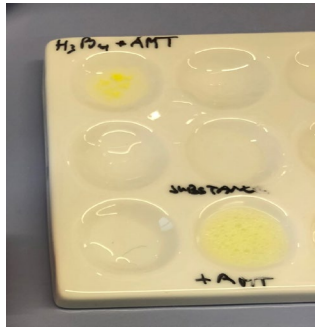
2 scientists (1 group leader, 1 long term sick leave), 2 lab technician + 1 technician/admin limited term

4 scientists (technician planned for 2025 moved due to BOT moving, but need (permanent) bio-deuteration support

Planned 4 scientists/engineers; cannot currently replace 3rd engineer until SSO is sorted out.

Your input is very welcome as we are currently waiting to convert the SULF limited term to permanent, waiting to be able to hire for bio-deuteration and replace the SCSE engineer that left with a technician.

Scope during operations (ESS.120.06.03.01)

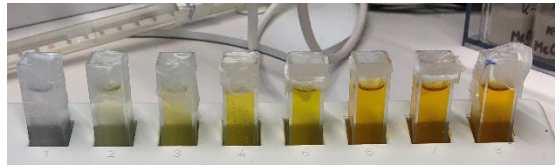


SULF sample handling and user laboratory facilities

Scientific user support, e.g. user education on lab instrumentation, support with sample preparation and characterization to optimize user beamtime on the neutron scattering instruments and to facilitate high impact publications by the users.

Operation, maintenance and upgrades of the user labs (1120 m^2, 25 rooms) year-round:

- **during the run cycle, we will focus on user support** (incl. 1 person on call), during down times, we will restock, refurbish, repair and support internal science and maintenance projects
- **provision of PPE, consumables**, chemicals, gases, chemical waste removal.
- **maintenance of lab instrumentation, safety-related equipment/furniture** (fume hoods, ventilated cabinets, specialized fire extinguishers..)
- **Cradle-to-grave sample handling** together with ESS instruments, ESH and Logistics.
  - participation in experimental safety reviews for user proposals prior to beam time
  - ability to register, tag, temporarily store samples
  - user safety orientation in labs, user support in safe handling of samples, safety walk downs
- **Radiological Materials Laboratory** (RML) in the controlled zone: SULF personnel needs to be present when users are



Projected resources (ESS.120.06.03.01)

SULF sample handling and user laboratory facilities

12 FTE (includes 1 group leader for CLS):

- 5 scientists (1 chemistry, 1 life science, 1 physical chemistry, 1 materials chemistry, 1 radiation chemistry)
- 6 technicians (4 chemistry, 2 life science)
- Justification: 1 scientist and 2 technicians per lab building (E04: chemistry/materials chemistry, D04: soft matter/life science, D08: physical chemistry) & 2 scientists for the Radiological Materials Laboratory

Scope during operations (ESS.120.06.03.02)

DEMAX - Deuteration and Crystallization

DEMAX will support ESS neutron scattering users with deuterated materials for their beamtime at ESS as part of the ESS proposal system.

Synthesis of deuterated compounds necessary for experiments at ESS year-round

- Chemical Deuteration (soft matter chemistry, organic chemistry, hybrid materials?, energy materials?), Bio- Deuteration (biomass, protein expression, yeast-derived lipids, DNA), Macromolecular crystallization facilities (protein crystal growth)
- **full service mode**: including supporting characterization data ready for user publication, deuterated pre-cursors
- **cultivating host organisms** in heavy water to achieve deuterated protein and yeasts as source for biodeuterated molecules (proteins, lipids)
- **develop new synthesis strategies** according to the change in research interests of the ESS neutron scattering user community.
- **operation** of owned or rented chemistry laboratory.

Projected resources (ESS.120.06.03.02)

DEMAX - Deuteration and Crystallization

6 FTE:

- 4 scientists (2 chemistry, 1 life science, 1 crystallography)
- 2 technicians (1 chemistry,1 life science)
- Justification: Chemical deuteration: 2 scientists & 1 technician, biodeuteration: 1 scientist & 1 technician needed to extract & purify lipids and proteins from deuterated host organisms, macromolecular crystallization: 1 scientist (crystallography) needed for crystal growth.

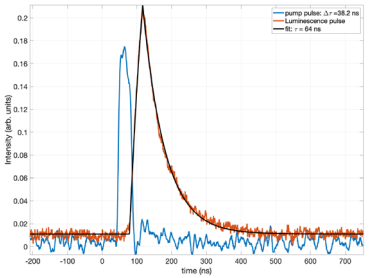
Mission for reliable operation (ESS.120.06.03.03)

SCSE – Soft matter and Chemistry Sample Environment

SCSE will support ESS neutron scattering users with setting up/removing of sample environment systems at the beamlines and assist with repair and replacement in case of issues.

SCSE provides sample environment equipment for the instruments in the areas of chemistry and soft matter/life science.

- **during the run cycle,** we will focus on user support (on call?!), during down-times, maintain/upgrade existing sample environment and develop new sample environment equipment
- **operation, maintenance and upgrade** of the equipment on the instrument and in the workshop.
- Perform **feasibility reviews and scheduling** of the SCSE equipment for approved experiments
- **Install the SCSE equipment on the neutron scattering** instrument in collaboration with the instrument teams. Train the users/instrument teams in the handling of the SCSE pool equipment.
- **Support rapid and reproducible equipment change-over at the beamline.**
- Assure **reliability of SCSE equipment and validate** the calibration.
- Assure mechanical and software integration of SCSE equipment.
- **Develop new** state-of-the-art SCSE equipment



Projected resources (ESS.120.06.03.03)

SCSE – Soft matter and Chemistry Sample Environment

5 FTE:

- 3 scientists/engineers
- 2 technicians
- Justification: 1 scientist/engineer with focus on chemistry/spectroscopy, 1 sci/eng with focus on soft matter/fluids, 1 sci/eng with focus on chemistry/gases/adsorption/reaction cells, 2 technicians for equipment change-over, workshop support, repair and assembly

Summary - WBS 120.06.03

Chemistry and Life Science Support

- **ESS.120.06.03.01 Sample Handling and General User Lab Facilities (SULF):**
  - 12 FTE: 1 group leader (CLS) + 5 scientists + 6 technicians
- **ESS.120.06.03.02 Deuteration and Crystallisation (DEMAX)**
  - 6 FTE: 4 scientists + 2 technicians
- **ESS.120.06.03.03 Soft matter and Chemistry Sample Environment (SCSE)**
  - 5 FTE: 3 scientists/engineers + 2 technicians

- ***TOTAL cost:*** ***4,720 k€***

- *Labor (23 FTE):* *2,300 k€*
- *Operations:* *1,200 k€*
- *Capital* *1,100 k€*

SSO review comments

Summary (biased …)

"ESS should consider a single sample environment group. A review of SE requests and publications in other facilities will expose the complexity of SE provision in an era when researchers want to replicate their home laboratory on the instrument. "

Not sure if the split is so complicated? Additional cost do occur…

".. the inclusion of optics support here was not well justified, especially because the assigned tasks are more related to materials characterization than optics. " this is currently under investigation, therefor not part of CLS STAP

"The user labs need support technicians to keep the labs running but the activities of the associated laboratory support scientists are not clear. Two laboratory support scientists for handling safety, and more sophisticated exploitation of the equipment as well as ensuring resilience would seem to be sufficient as opposed to the 5 FTEs suggested. " Depends on the type of support given (see ISIS, SNS…).

"Rent on the DEMAX facility seems odd since no other ESS-site based group has listed rent, or separate charges for waste disposal in their operations budgets. … Rent should only be needed if DEMAX is located offsite. "

Rent is the wrong term, but SULF/DEMAX spends time/budget to take care of facility issues (not a full service lab building).

Thank you


Deuteration and Macromolecular Crystallisation Platform

Product List

February 2023

Biological: proteins, biomass, nucleic acids 2
Biological: purified lipid mixtures ....
Chemical: carboxylic acids, aldehydes, alcohols, alkyl halides ....
Chemical: surfactants ....
Chemical: phospholipids ....
Chemical: aromatic & heterocyclic aromatic molecules ....
Chemical: miscellaneous ....
Crystallisation support: ....

Sorting by instruments

What needs to be in place from CLS – example DREAM (preliminary!)

CLS area	DREAM Hot Commissioning	DREAM First Science
Sample environment	• Gas handling system (p<1 bar and 1-200 bar) for hydrogen (D_2), e.g. H_2 / CO_2 Adsorption	• EC cell (batteries/ coin cell/ cylindrical) + potentiostat • Reaction cells with injection system • in-situ thermogravimetric analysis…..
Laboratories	• gas handling possibilities in lab (including H_2/D_2) • glove boxes for sample loading • two labs in D08 ready	• EC setup (potentiostat, glove box, press etc.) • DSC/DTA • Powder XRD
Deuteration	• possibly test samples	• Chemical deuteration (small organic molecules/MOFs, energy materials?…)

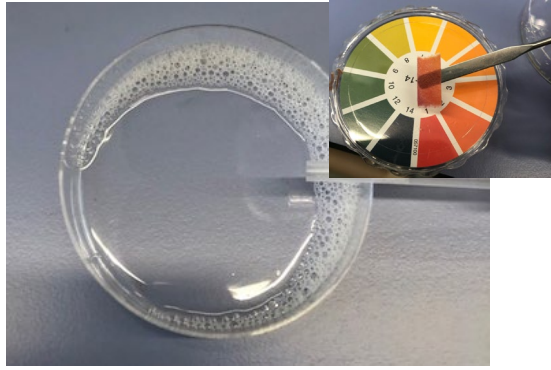
Sorting by instruments

What needs to be in place from CLS – example LOKI (preliminary!)

CLS area	LOKI (CC)	LOKI (HC)	LOKI (FS)
Sample environment	• Sample changer/tumbler	• Flow cells (HPLC pumps ready) • Preparation for first science: rheometer, stopped-flow cell;	• Rheometer • Liquid/gas mixing • Electrochem. Cell • Laser pump probe system • Humidity cell • Insitu reaction (stopped flow for corrosive mat.) …
Laboratories	• D04 labs ready	• Rheometer test stand; Dynamic light scattering • pipettes, balances	• Potentiostat, • Sonicator, UV/VIS, • ….
Deuteration	• N/A	• possibly protonated/deuterated Ag-behenate as standard	• Chemical deuteration • Biodeuteration

Benchmarking (ESS.120.06.03.01)

SULF sample handling and user laboratory facilities



User labs are strongly impacting the quality of the scientific publications resulting from beamtime at the neutron sources. This unit best compares to the ISIS and SNS user laboratories.

- ISIS (8 FTE): 1 group leader, 4 (2 chemistry, 1 bio/life science, 1 material), 3 technicians (1 materials, 2 chemistry); in addition 2 junior scientists (placement students). **No sample tracking** but safety reviews, lab areas similar (1100 m^2) but **more users/ more in operando at ESS.**
- SNS (7 FTE): 1 group leader, 1 technician sample handling& shipping, 2 technicians for receiving/ bar coding/delivering samples, general user support, 2 technicians for bio lab, 1 scientist for X-ray lab; **Approx. 300 m^2 = 1/3rd of the ESS space**; other specialized support labs available (X-ray lab, bio X-ray lab, bio crystallization/protein lab, Raman lab, thin film lab, soft matter lab, synthesis lab, hot lab (no users!)) provided by (instrument) scientists from SNS …
- ILL (4 FTE) provides chemistry and soft matter **support primarily in partnerships** and **sample handling is not included** (performed by ESH).

Benchmarking (ESS.120.06.03.02)

DEMAX - Deuteration and Crystallization

This unit is difficult to compare to the three large existing deuteration services at ILL, ISIS and ANSTO as these three facilities are deviating a bit in what they offer. ESS is splitting into half chemical deuteration and half biodeuteration/macromolecular crystallization.

- ILL D-LAB (6 FTE) for biological deuteration and crystallisation platform joint with ESRF PSB (4 FTE). 1FTE for lipid activities. No chemistry.
- ISIS (5 FTE) for chemical deuteration, no biological deuteration nor lipids.
- ANSTO (10 FTE) for chemical and biological deuteration. No lipids.

ESS is presenting 6 FTE and will rely on collaborations between the facilities e.g. through Deunet for special deuterated compounds. This effort scales with amount of instruments in operation and amount of science areas evolving.

Benchmarking (ESS.120.06.03.03)

SCSE – Soft matter and Chemistry Sample Environment

SCSE is setup very similar to ISIS except that **we also cover chemistry**. Some support is expected from the ESS scientific associates from the instruments.

- ISIS (5 FTE): soft matter sample environment (does not contain gas adsorption, reaction cells), e.g. catalysis hub is run by instrument scientists/collaborators
- SNS / HFIR (5 FTE) but 6 FTE Technical and R&D support not included in this number
- ILL LSS (3 FTE): resources provided as part of the LSS group not sample environment. Does not include sample environment for chemistry (gas adsorption, reaction cells, …).