Scientific Support Division Update

HANNA WACKLIN-KNECHT

2024-10-24

Aug 2024- Head of Scientific Support
2023-2024 Senior Scientist, I2S (CLS)
2018-2022 Life Scientist (DEMAX)
2011-2018 Instrument Scientist/ICC
Neutron Reflectometry (FREIA/GISANS)

DeuNet

EUROPEAN SPALLATION SOURCE

LUND UNIVERSITY

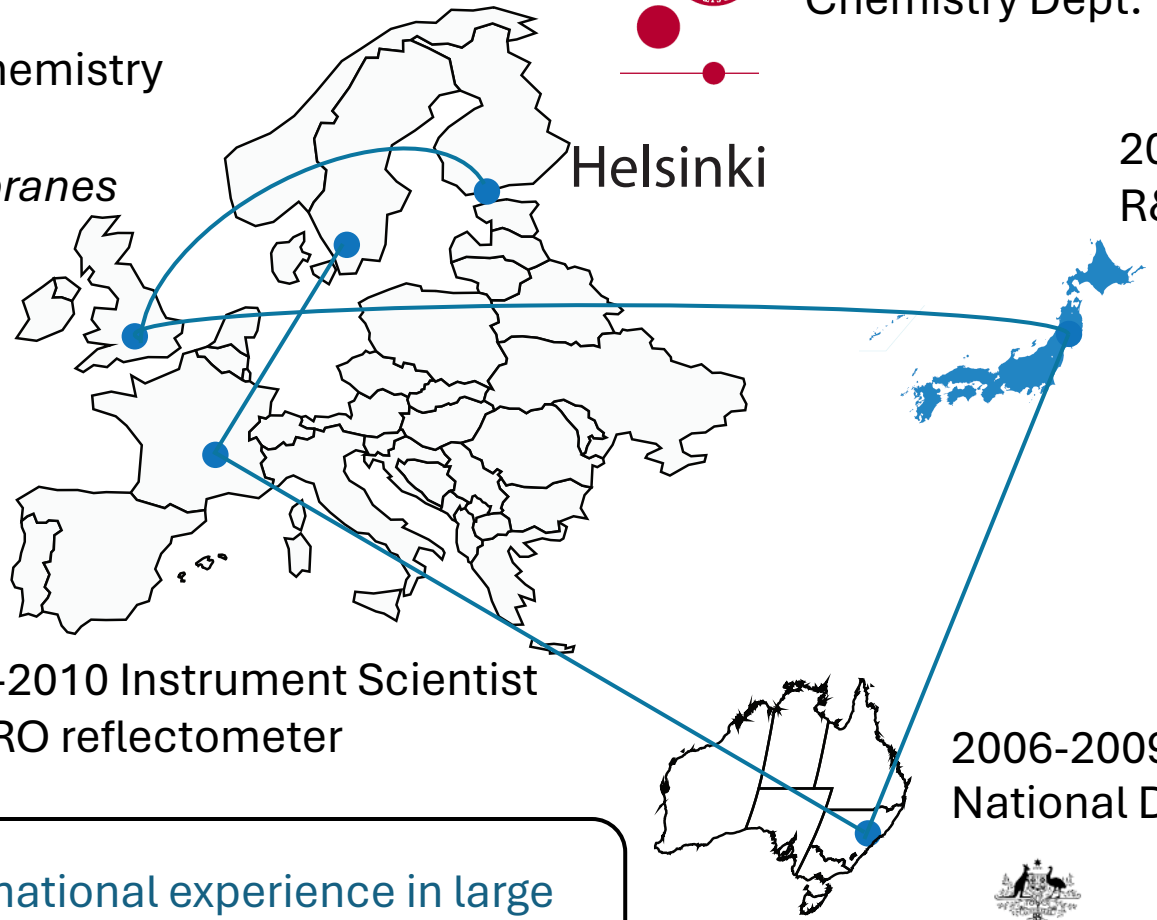
2015 - Adjunct Assoc. Professor
Physical Chemistry (docent)

2011-2016 Adjunct Assoc. Professor
Chemistry Dept. CPH

2000-2004 DPhil Physical Chemistry
2003-2005 BBSRC Postdoc
Neutron reflection/biomembranes

1995-1999 MSci Chemistry

Imperial College London



2005-2006 UK-Toshiba Fellow
R&D Centre Kawasaki

NEUTRONS FOR SCIENCE

2009-2010 Instrument Scientist
FIGARO reflectometer

2006-2009 Postdoc
National Deuteration Facility

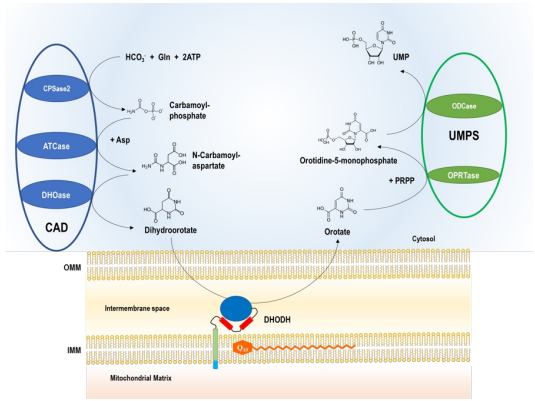
Australian Government | ANSTO

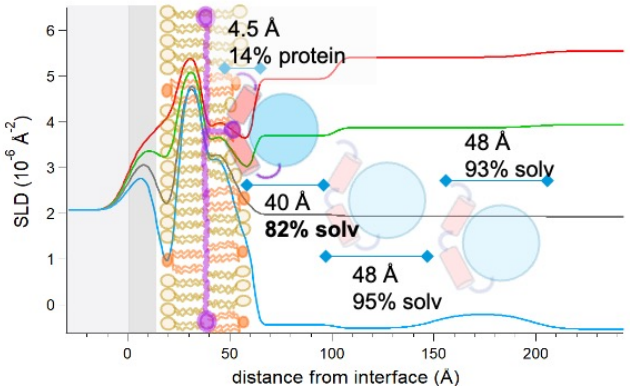
25 years of international experience in large scale infrastructures, academia and industry

My scientific interests

Membrane biophysics + surface/colloid chemistry in soft and biosystems

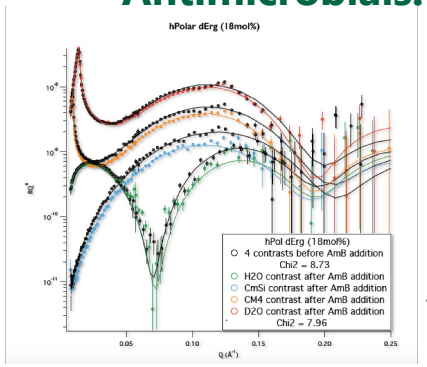
Membrane bound enzymes/proteins:

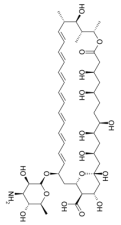




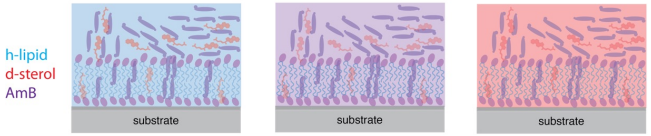
Antimicrobials:

AmB



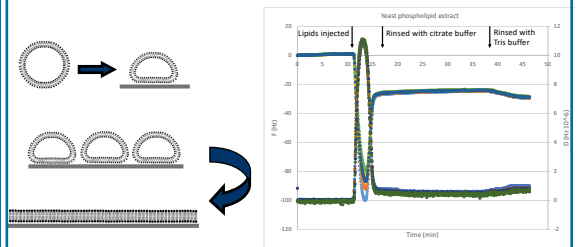


$\rho_{hlipids} < \rho_{AmB} < \rho_{dErg}$

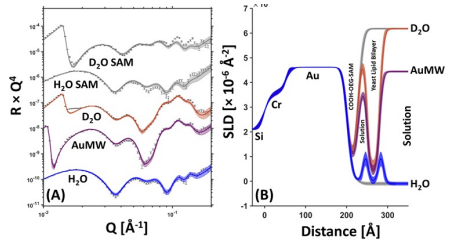


Lipid bilayers on surfaces:

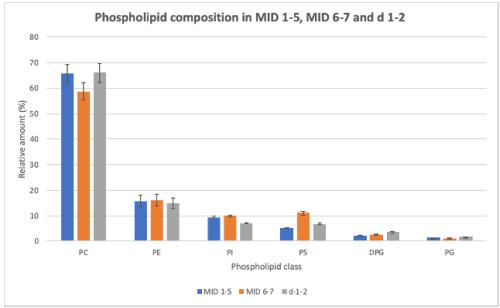
Supported bilayer (yeast lipids)



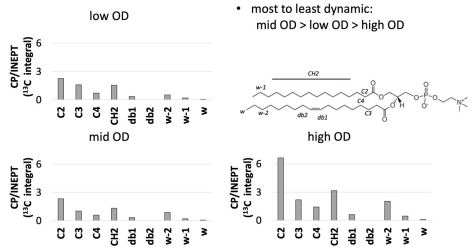
Self-assembled floating bilayer (yeast lipids)

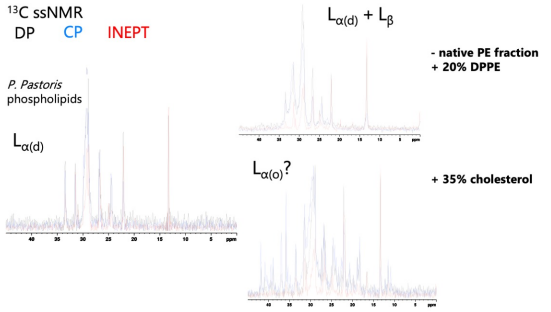


Effect of cell growth on lipid composition and dynamics:

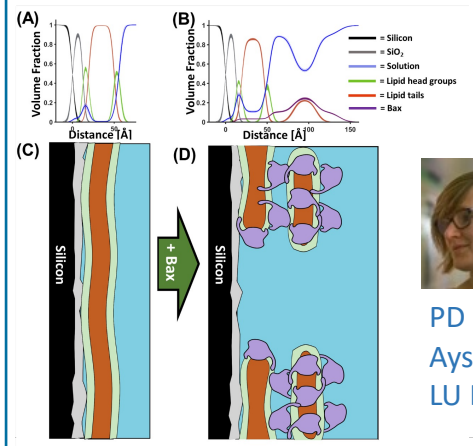


^{13}C NMR analysis: acyl chain dynamics

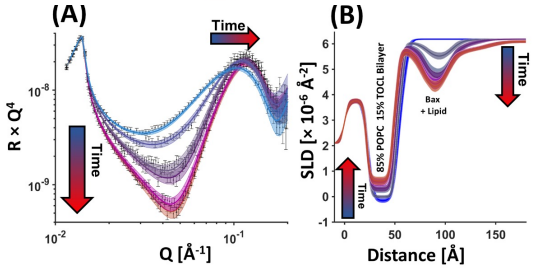


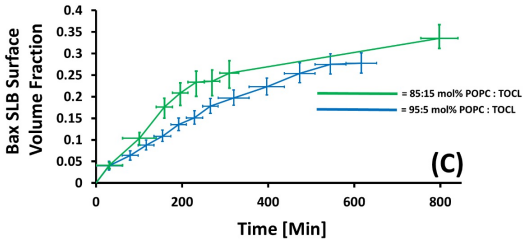


Cell-death regulating proteins MedCAN (Umeå/ISIS)



PD Sophie Ayscough LU Fkem1





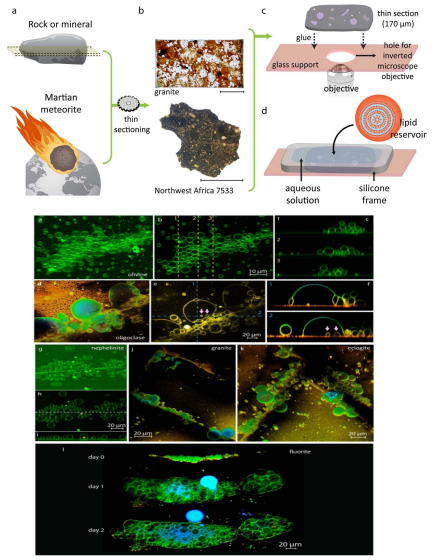
Science Advances 9, eadg7940 (2023)
Communications Biology 4, 507 (2021)

My scientific interests

Membrane biophysics + surface/colloid chemistry in soft and biosystems

Experiments simulating protocell formation

Spontaneous formation of protocell colonies on Hadean earth and pre-noachian Mars surfaces:



Köksal, E.S. et al., *ChemSystemsChem* **2022**, *4*, e202100040 (4 of 8)

Formation of protocell-like vesicles in a thermal diffusion column

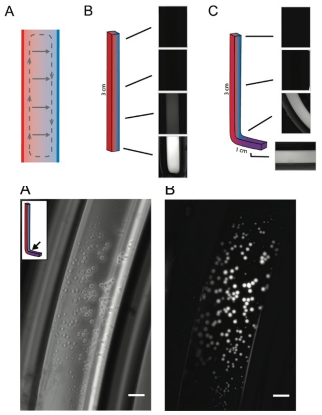


Figure 2. Locally concentrated oleate forms vesicles in bent capillaries incubated at $\Delta T = 30$ for 48 h. (A) Phase-contrast image of a bent capillary loaded with 70 μM buffered oleate and 40 μM HPTS. The oleate concentrated in the capillary and formed large vesicles. (B) Fluorescence image of the same frame. HPTS in the solution was washed away with dye-free buffer, leaving only encapsulated cargo to be visualized. Scale bars = 50 μm.

Budin i. et al., JACS. 2009, 131, 9628–9629

J.P. Dworkin et al., PNAS 2001, 98, 815–819

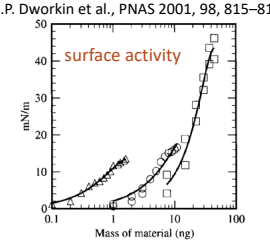
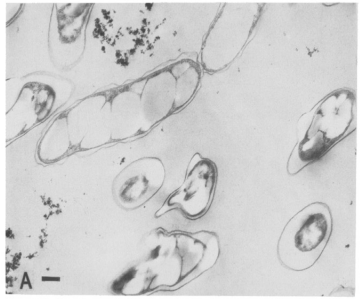


Fig. 2. Surface pressure of monolayers of the residue produced by the UV photolysis of an H_2O:CH_3OH:NH_3:CO = 100:50:1:1 ice (circle), Murchison extract (square), and decanoic acid (triangle).

Membrane structures formed by meteorite extracts:



Deamer, D.W., Pashley, R.M. Amphiphilic components of the Murchison carbonaceous chondrite: Surface properties and membrane formation. *Origins Life Evol Biosphere* 19, 21–38 (1989). https://doi.org/10.1007/BF01808285

The Pufendorf Institute for Advanced Studies

Lund University

På svenska

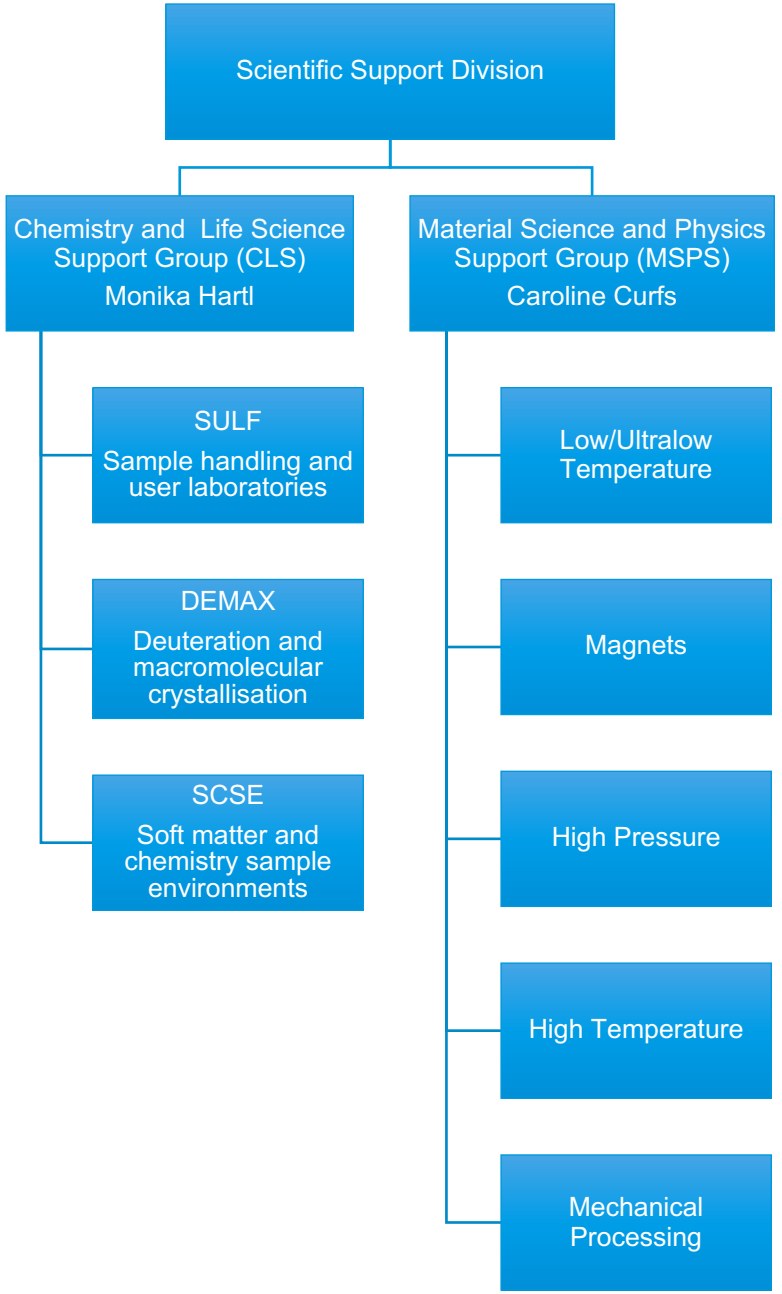
Neobiogenesis: The Inevitability of Life

ASG 2024-2025

How the earliest forms of life arose on Earth is one of the great unanswered scientific questions. The fundamental question is in what ways and under what circumstances a collection of inanimate matter can be transformed into something that can be considered alive.

Participants

Hanna Wacklin-Knecht (coordinator)
Daniel Topgaard
George Attard
Joakim Stenhammar
Peter Spégel
Anders Scherstén
Anders Johansen
Jessica Abbott
Christian Lindh
David Dunér
Erik Persson

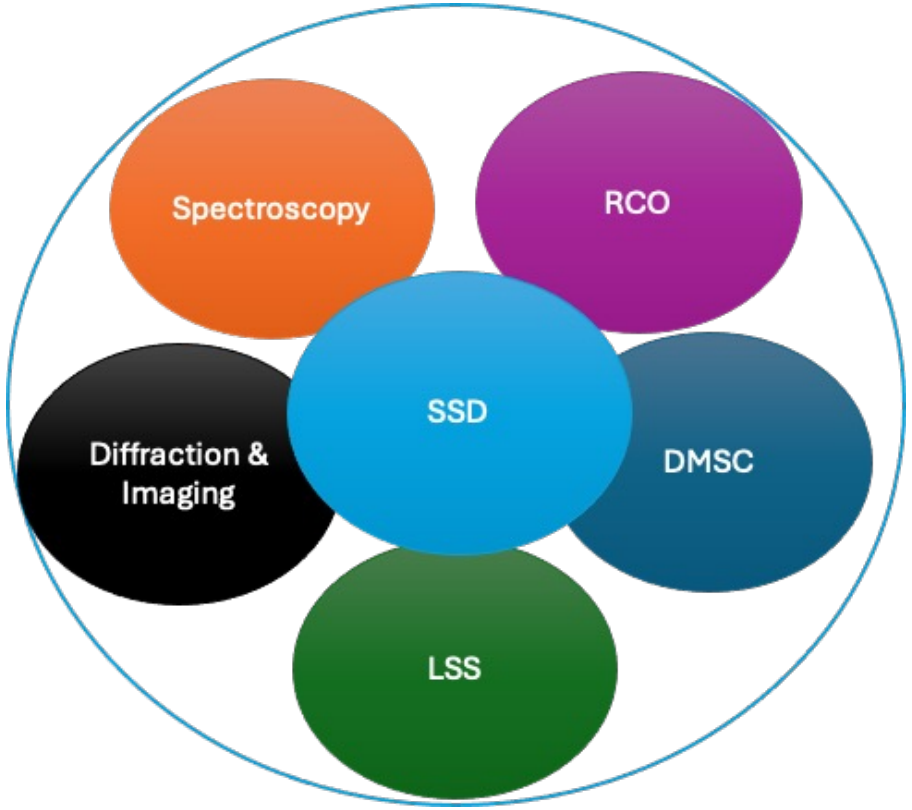

Scientific Support Division
Chemistry and Life Science Support Group (CLS)
Monika Hartl
Material Science and Physics Support Group (MSPS)
Caroline Curfs
SULF
Sample handling and user laboratories
DEMAX
Deuteration and macromolecular crystallisation
SCSE
Soft matter and chemistry sample environments
Low/Ultralow Temperature
Magnets
High Pressure
High Temperature
Mechanical Processing

Scientific Support Division (SSD)

Provides sample environment and laboratory services required **for user science on ESS instruments**

Supports science directorate scientifically and technically in **delivering the user programme**

Provides a platform for carrying out in-house science, method development and project support



The instruments are the scientific gateway of ESS

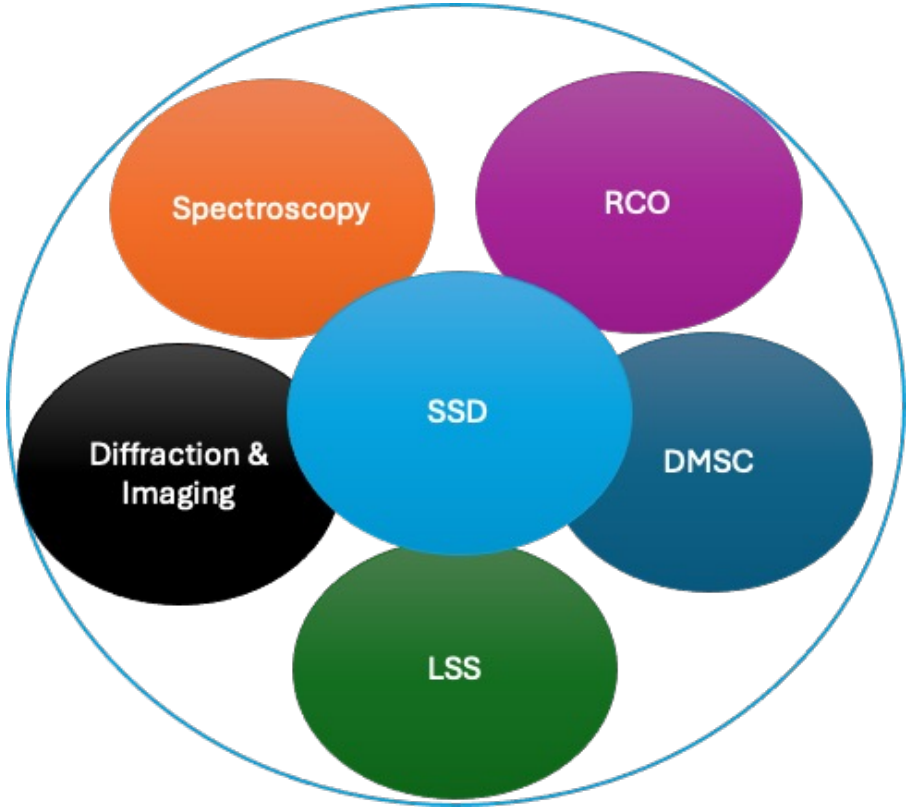
Scientific Support Division (SSD)

The services provided are **stakeholder-driven**

The model for scientific support is collaborative and utilizes all expertise at ESS

Outside the user program, access is provided to facilities for in-house R&D driven by instrument staff

Other support activities should be driven by project priorities and typically resourced by the stakeholder



The instruments and their users are the primary stakeholders of SSD

Support for instruments and users:

Sample environment:

- Development and design of SE
- Support and maintenance of SE
- Installation and operation support for all SE
- Provision of spares
- Mechanical/control integration & electronics for all SE
- Provision of a mechanical workshop
- Liquid helium management
- Operation of mechanical processing workshop

Responsibility for all SE being available, maintained, correctly installed and functional

User Laboratories:

- Sample preparation and characterization facilities for users
- User training and access
- Maintenance of laboratories and equipment
- Provision of consumables
- Sample handling and storage
- Chemical waste management
- Support for instruments
- Scientific user support by local contacts
- Instrument scientists can be responsible for some equipment

Responsible for laboratory safety, training, maintenance and sample/waste handling

Deuteration:

- Provision of deuterated samples for user program
- Chemical synthesis on-site (D04)
- Biological deuteration at Lund University (LP3)
- Macromolecular crystallisation for NMX
- Analysis certificate and DOI for all samples provided

Responsible for operating deuteration user service

Service model:

Sample environment:

- Has overall responsibility for SE but works in close collaboration with instrument staff to:
- Develop and design SE according to needs of instrument
- Carry out installation and testing (incl. user supplied SE)
- Train instrument staff on installation and operation
- Support each experiment with dedicated SE contact

User Laboratories:

- Has overall responsibility but collaborates with instruments on:
- Optimization of laboratories to the instruments/users needs
- Prioritization of equipment
- Providing user training and technical support
- Provision of scientific support in laboratories
- Responsibility for advanced instrumentation
- Maintaining instrument sample preparation areas

Deuteration:

- Provision of deuterated samples and crystals
- Non-commercially available materials for neutron scattering
- Access via user proposals for beamtime
- Primarily full-service mode
- Hosting experienced users possible depending on expertise
- Longer term collaborations for method development desirable

Adjusted and optimized support according to type of SE and instrument expertise

Technical support and maintenance to enable scientific support by scientists

Deuteration aimed at enhancing experimental capabilities on instruments

The way to First Science and user operations

Strategy for supporting science on ESS instruments

3. Develop a long term strategy for scientific support for SSO

2. Utilise all expertise and resources in CLS, MPS, instruments and external projects

1. Review & prioritise scope for first science

2025->

First science

24/7 essentials for common types of experiments

2027->

First user proposal call

Support first instruments:

- more specialised SE and lab equipment
- automation if critical to early exp

2028 ->

Towards steady state ops

- Advanced SE + characterisation and sample prep facilities
- in-situ techniques
- automation

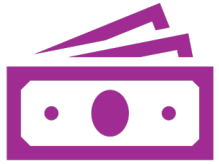
Support for:
World leading science
Partnerships
Science Village
Industry

Challenges

Building a strong user support team together with instruments

Shifting focus to first science and user program while completing project

Recruiting and training staff to build competence and experience for operations



Funding and prioritisation SE and lab equipment

Ensuring readiness of for first science:

Establish a clear path to completing project and build a service-oriented team

Establish a clear path for completing SE and laboratories: (both were heavily descoped)

- Perform a capability gap analysis (equipment, services, modes of operation) by reviewing current status and plans
- Work with instrument divisions, STAPs and first science workshops to *define an up-to-date, stakeholder driven scope and model for service provision*
- Develop a clear set of goals to meet for first science, start of user operations and steady state respectively
- Develop a clear process for reaching the identified goals

Build a strong service-oriented division:

- Streamline common in-house support tasks to optimize the quality of support provided
- Develop a shared user service model with the instruments and inclusive working culture
- Work on the interfaces to the rest of ESS to obtain optimal support for the division
- Develop an optimal division structure with clear roles/responsibilities
- Establish/implement a clear plan for competence development

Three main activities Q4/24 – Q2/25:

1. **"Road to operations" workshops** at montly SSD meetings to discuss use case scenarios and roles/responsibilities and communication/interfaces during operations.
2. **Internal review of sampe environment and lab equipment needs** for first science an beyond
3. **Preparation of a user community and facility usage survey** to aid prioritisation of scientific support capabilities at ESS

Contributing to the overall scientific strategy of ESS

Strengthening collaboration with instrument divisions and DMSC

Actively working together on scientific requirements, priorities and use cases

Examples:

- Discussing/developing different roles contributing to scientific support *(e.g. IOE/SE)*
- Solving common needs/problems (out-of hours user support)
- Facilitating joint development of labs/SE
- Creating a strategy together for the overall scientific support for users
- Involving eachother in collaborations/ projects/grants whenever possible
- Involving IS/IDS in SSD as technique specialists

Support collaborations with other laboratories, participate in networks and and funding programs to enhance the scientific scope and user support at ESS

Participate in facility collaborations and networks

Engage with local partners

Learn from other partnerships

Identify& engage in relevant consortia

Network with university centres and programs

Collaborate with instrument staff to:

- identify funding opportunities that could contribute to neutron science at ESS
- work with RCO on an ESS model for COFUNDs and PhD schools
- Work with key partners on relevant grant initiatives
- Idendify and seek relevant in-kind and funding opportunities for SSD together with instruments and DMSC

Material Science and Physics Support

Systems to be delivered before end of 2027

Low Temperature

6 cryofurnaces
10 cryostats (7 wet/3 dry) – tender awarded AS
3 dilution fridges (HZB 27mK tested) and 1 ^{3}He insert
Automatic pumping cards (6 in production)

Magnets

8 magnets from 2.5 T to 15 T (+ LU 17T)
- in different stages on-going/on-track

High Pressure

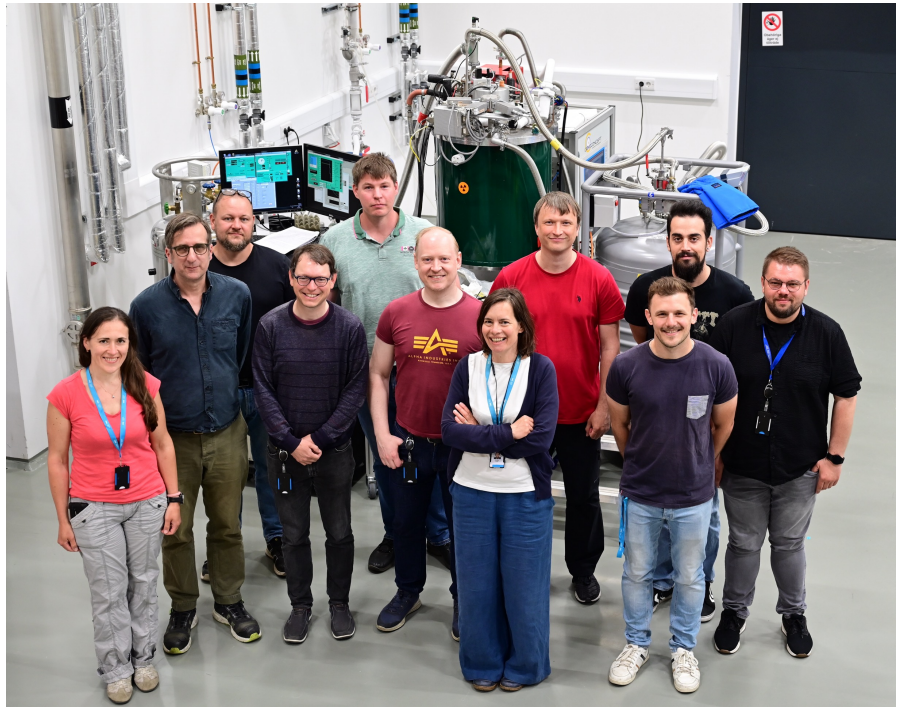
10 HP cells (5 gas, 4 liquid and 1 clamp) at ESS
2/5 compressors at ESS (4 automatic and 1 manual)
3/5 Paris Edinburgh presses with gas loader at ESS
1 DAC for lab XRD

High Temperature

3 ILL-type furnaces (2 Niobium/1 Vanadium),
1 induction/1 lamp, and 1 hot air/cryostream (DREAM/HEIMDAL)

Mechanical Processing

2 stress rigs (uniaxial and torsion at ESS/rotation in construction)
1 thermo-mechanical instrument (dilatometer) – specifications on-going



Caroline Curfs, Niklas Ekström, Andreas Hagelberg, Alex Holmes, Damian Paliwoda, Yulia Pedersen, Luca Sagliano, Lauritz Saxtrup and Oleksiy Zadorozhko; Richard Ammer (-> ODIN IOE)

MSPS cont.

Priorities for HC and CC

Instrument		Cold Commissioning		Hot Commissioning	
		SES	Timeline	SES	Timeline
TRANCHE 1	**DREAM**	Hot Air Blower/Cryostream	10.24 – 03.25	ILL-Type furnace	07.25-03.26
	BIFROST	15T magnet / Wet cryostat	11.24-04.25		
	ODIN			Tortion/rotation rig	07.25-03.26
TRANCHE 2	**ESTIA**	2.5 T WBM/Flow cryostat	07.25-12.25		
	SKADI			Electromagnet	10.26-06.27
	BEER	60kN stress rig	07.26-12.26	Dilatometer	01.27-09.27
	MAGIC	8T magnet / Wet cryostat	04.26-09.26		
TRANCHE 3	**HEIMDAL**	ILL-Type furnace/Dry cryostat	10.26-03.27		
	T-REX	Wet cryostat	07.26-12.26	He3 insert	01.27-09.27
	MIRACLES	Dry cryofurnace	07.26-12.26	Wet cryostat	01.27-09.27
	CSPEC	Rotation stick	10.26-03.27	Spectro magnet	04.27-12.27
	VESPA	Dry cryostat	04.27-09.27		

MSPS workshops

B02: currently used by ECDC for testing of control integration

- will be used to test, safety check and integrate SE arriving at ESS

E03: Main MSPS SE workshop:

E03 SLIME lab:

- Installation started
- Currently used by instruments to test e.g. shutters
- Will be used from some SATs requiring space
- Will temporarily house high-pressure bunker
- Planned to support **BEER and ODIN** users for mechanical engineering/processing

Polarisation group has asked if MEOP station could be here

Chemistry and Life Science Support CLS

Main deliverables before end of 2027

SULF
Sample handling and user laboratory facilities

Finish installation of laboratories
Provide consumables and equipment for First science
Finalise user training, sample handling, chemical safety

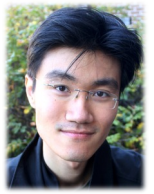
DEMAX
Deuteration and macromolecular crystallisation

Provide deuterated samples for First science experiments
Develop robust methodologies for user program

SCSE
Soft matter and chemistry sample environments

Provide/Support prioritized soft matter and chemistry SE for Loki, ODIN, ESTIA, SKADI, FREIA
Develop later SE with instruments










Zoe Fisher, Anna Leung, Jia-Fei Poon
Monika Hartl, Katrin Michel, Melissa Sharp,
Ghazaleh Roostaei, Nick Weisend
Alice Corani, Harald Schneider

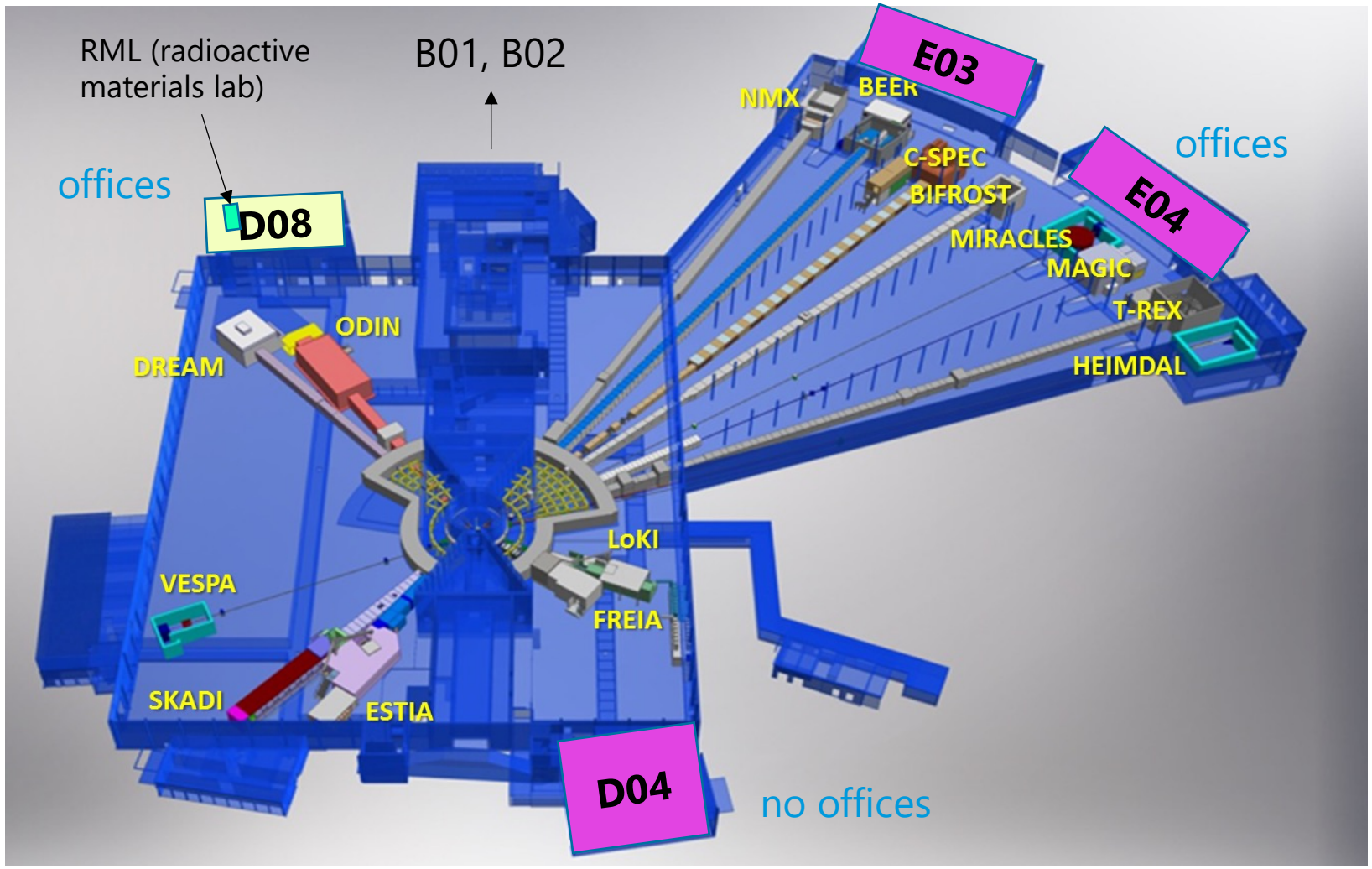
D04 soft matter/chem

D08 chemistry

D04 SCSE workshop

Chemistry and Life Science Support

news and locations



Chemistry and Life Science Supports :

- 1120 m^2, 25 rooms
- 4 buildings

E04 operational since 2019:
chemistry, life science, X-ray, cutting/polishing

D04 soft matter/chemistry lab:
commissioned for basic use
D04 DEMAX lab operational

D08 labs: chemistry, gas, thin-film, HP
furniture and electrical installation complete, tender for utilities evaluates
Plan: start in Q1/25 and end Q2/25.

Radioactive Materials Lab (RML):
waiting for permit (INP)
used for non-active support tasks

Labs & workshops to install

D08 (next to ODIN)

Ready to move in by middle of 25

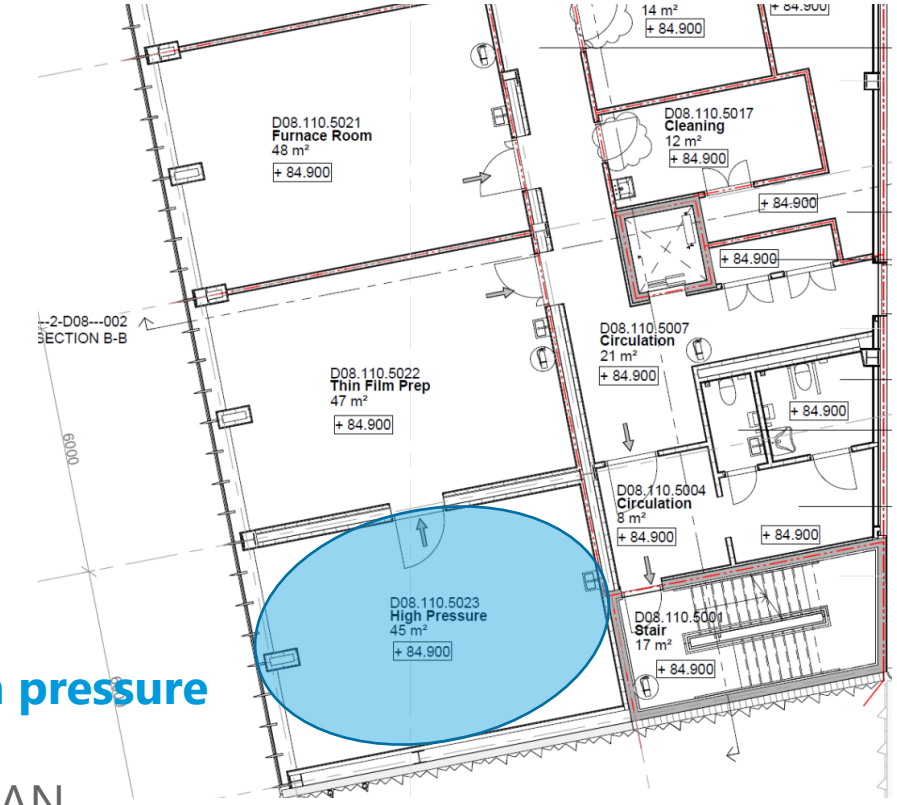
Sample environment
Maintenance and storage of cryos, magnets, furnaces for ODIN, DREAM, ESTIA,…

High Pressure
PE presses, Liquid, gas and clamp cells
Compressors

Ground floor

Sample storage

First floor



High pressure
DAC
RAMAN

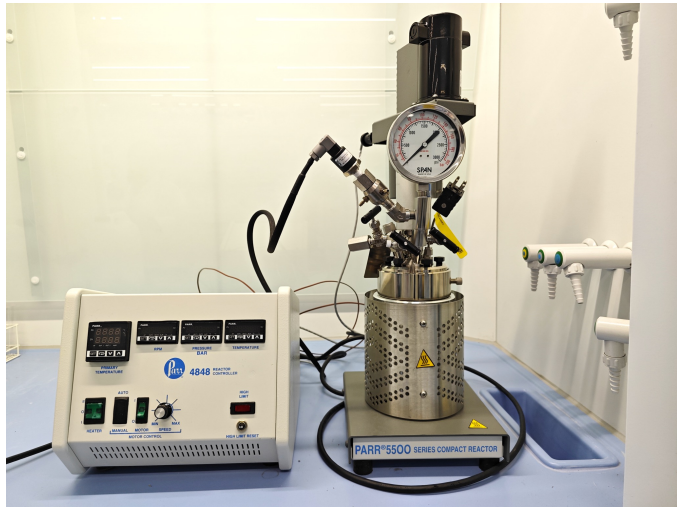
DEMAX: News & updates

> 100 users, 40 publications, rolling access since 2022 - 36 proposals requesting 62 molecules

New equipment installed at D04 chemistry labs expands out capabilities on site

Shimadzu NEXUS™ GS-MS

- Autosampler, 150 vials
- Helium as carrier gas
- Electron Ionisation (EI) MS with chemical ionisation (CI)
- columns for lipidomic analysis
- NIST library of MS data



Second Parr High Pressure Compact Reactor

- 450 mL vessel
- Max temp 350 °C, max pressure 200 bar
- For test reactions and method development

Main current challenges:
no NMR on-site
limited chemical storage

SCSE Priorities

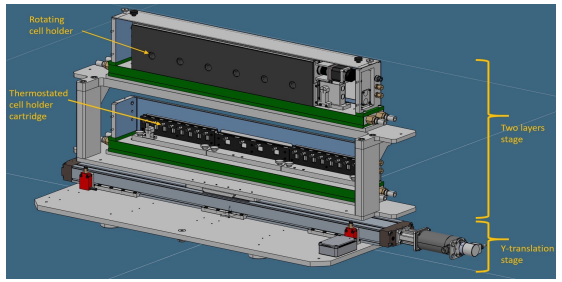
better collaboration with instruments is helping to prioritise and learn from new projects

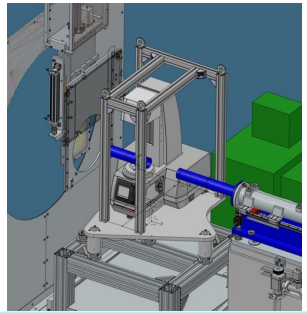
		Date CC	CC	Date HC	HC
Tranche 1	DREAM	Q1-2025	Cryofurnace/Quentin setup	Q1-2026	Vacuum furnace/ Quentin' changer
	LOKI	Q1-2025	SANS Sample changer	Q1-2026	Rheometer
	ODIN	Q1-2025	Syringe pump	Q1-2026	Robin stress rig
	TBL	Q1-2025	n/a		n/a
	BIFROST	Q2-2025	Wet cryostat / 15T magnet	Q1-2026	Wet cryostat / 15T magnet
	NMX	Q2-2025		Q2-2026	
Tranche 2	ESTIA	Q4-2025	Flow cryostat / Solid liquid sample changer		Flow cryostat / Solid liquid sample changer
	BEER	Q4-2026	Deformation rig	Q2-2027	Dilatometer
	MAGIC	Q3-2026	Cryostat/8T magnet		8T magnet
	SKADI	Q1-2026	Sample changer (temperature controlled)	Q2-2026	Electromagnet / Rheometer / Syringe pumps/mixing setup / Stopped flow if available
	CSPEC	Q1-2027	Cryofurnace + rotation stage	Q3-2027	High field magnet (6T)
Tranche 3	MIRACLES	Q4-2026	Dry cryostat	Q3-2027	8-Sample changer with CCR/ Wet cryostat Humidity chamber/ Laser pump-probe
	HEIMDAL	Q4-2026	Blue furnace / Cryostat		Blue furnace / Cryostat
	TREX	Q4-2026	Cryofurnace	Q3-2027	He3 insert
	FREIA	Q4-2026	Solid-liquid cell sample changer / Langmuir trough/ Julabos & temperature controllers / Static trough	Q3-2027	HPLC & syringe pumps
	VESPA	Q3-2027	Cryostat		running Cryostat

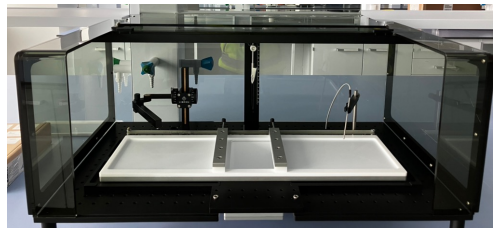
Instrument

SCSE

Current status

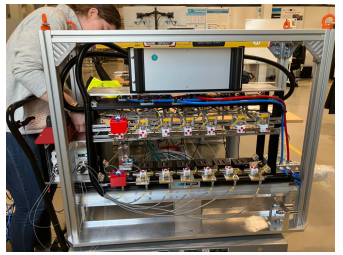


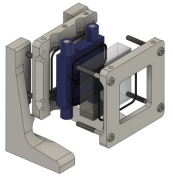


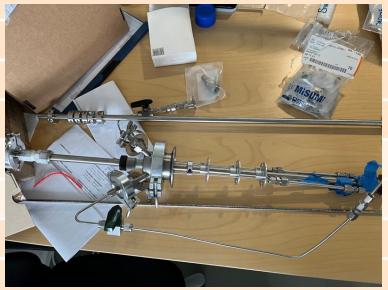


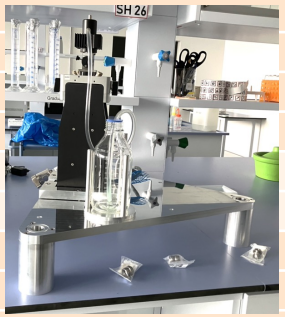
LOKI		
Sample changer CC		Follow the project and support the mechanical and control integration if needed
Rheometer HC	✓	Support the control and the mechanical integration
Odin CC		
Syringe pump	✓	Done, Tubing, connectors
Estia		
Sample changer CC		Get a functioning setup for CC
SKADI		
Sample changer CC		Follow the project and support the mechanical and control integration
FREIA CC/HC		
Solid liquid cell sample changer		Adapt the ESTIA sample changer to FREIA
Troughs		Static air-liquid troughs Langmuir troughs
In-situ Ellipsometry/ATR-FTIR		Grant project - follow and support the project – CDR completed Sep 2024
Stopped flow LOKI FS		
Humidity chamber FS		
Electrochemsitry FS		
Gases manifold FS		
- Up to 200 bar isorb		
- 0 to 30 bar		
LPP		test and development
Sample stick		For gases and EC
Julabo		Maintenance scheme, trolley

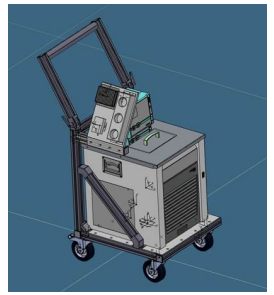
automation RÅC grant Kiel/Lund Uni

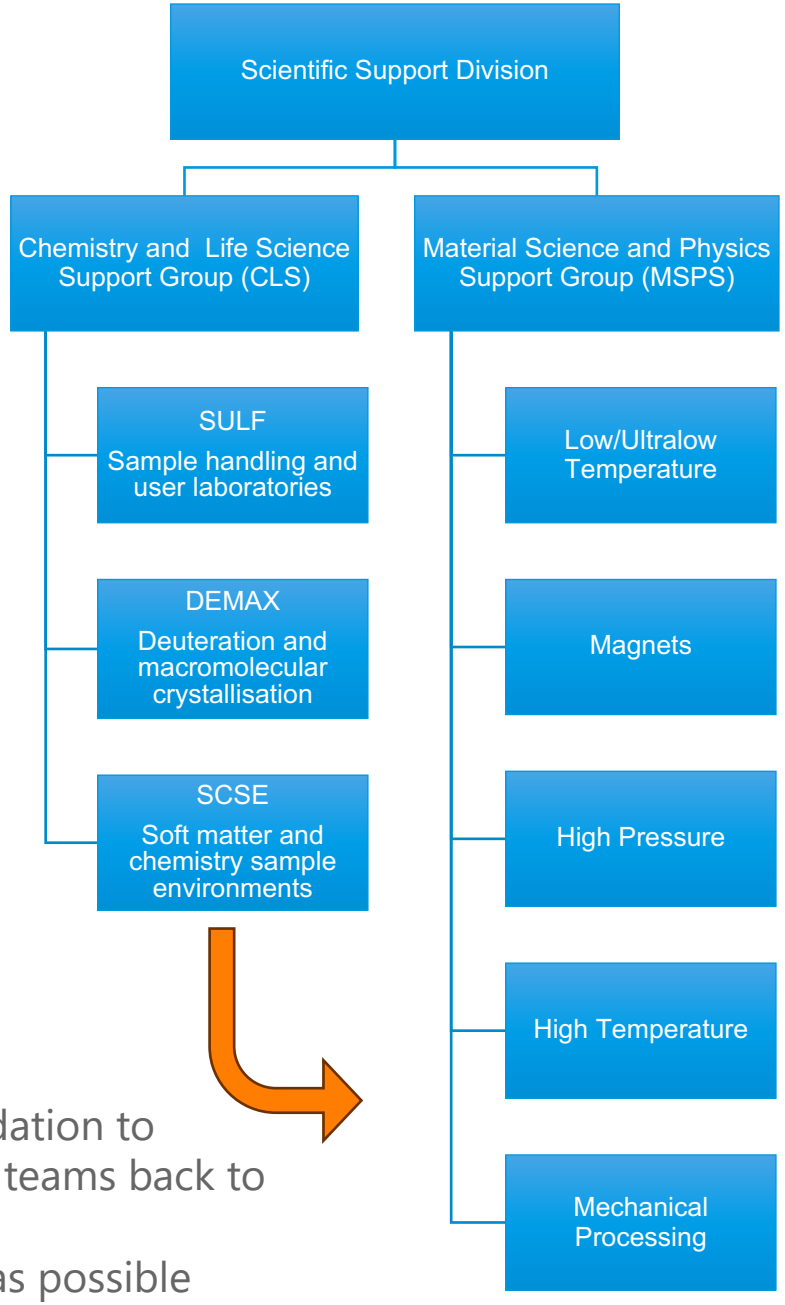






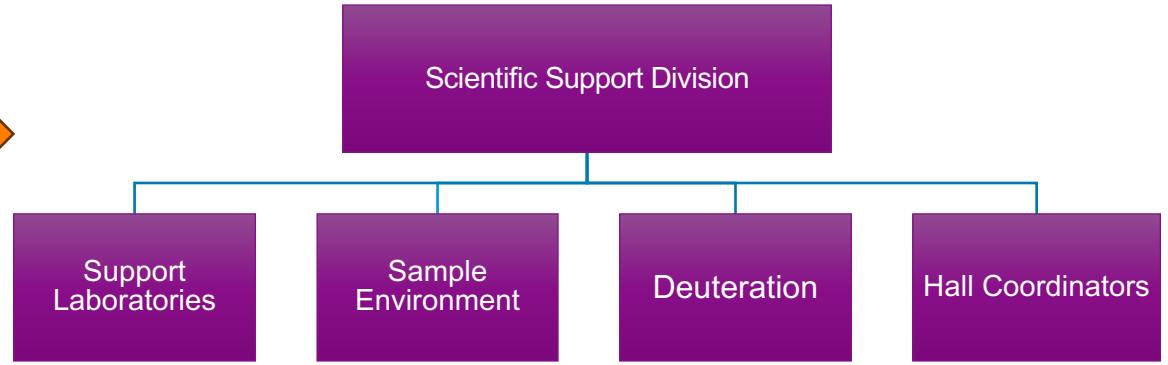






Recommendation to combine SE teams back to one group
-> as soon as possible

SSO proposed structure:
(not necessarily final)



Clear mission and identity for each group

Questions?

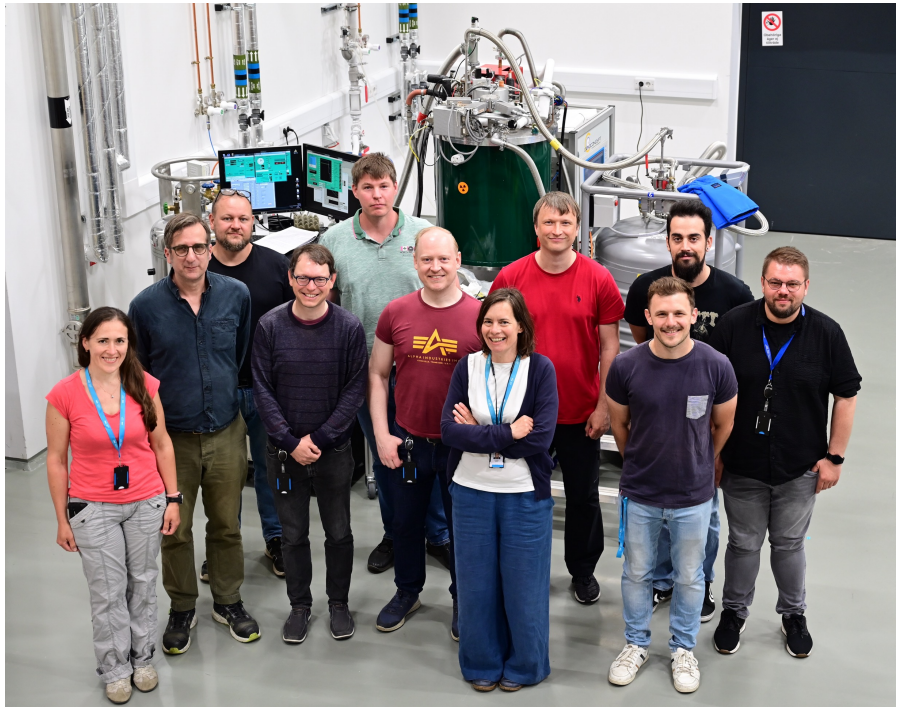
Additional details from SE an Labs

Material Science and Physics Support

STAP summary from spring 2024:

understoon, work in progress

- We see very good progress for the sample environment projects, integration, and tests.
- Many visits to other facilities have been made to improve knowledge and we encourage a continuation with e.g. internship and participation in experiments.
- We endorse the SSO review recommendation that CLS and MSPS should be joined into a a single sample environment support group. The split into two groups is somewhat artificial. However, at this point yet another change of the organisation may be very disruptive to the ongoing work by the teams.
- Possibly change the organisation to a new division under the Science Director with a division leader, including groups for sample environments, chemistry laboratories, deuteration, and sample handling (radioactive, post experiment).
- Centralised sample environment support is important for standardisation, standard operation procedures, and maintenance. It makes it easier to train the existing and new staff, as well as to build a large pool of experience in operations support.
- The spilt of the group creates a contact problem when complex sample environments experiments using combination of e.g. gas, pressure, and heat.
- Make procedures and rules for user-supplied sample environments.
- The staff plan ramp-up plan to 2027 seems to be lean on controls and integration.
- The number of engineers planned for 2027 seems sufficient (at a minimum level).
- Try to break barriers between the support groups and instruments to increase the possibility for successful experiment support.
- Review the instrument needs in regular intervals and and try to make short- and long-term plans for the sample environment needs and development (1 – 10 years). Management should give support to surveys into the sample environment requirements for all instruments.
- We expect that sample environments required for the first experiments are identified and trained upon.
- Continue the work on team building, roles and responsibilities.
- Provide technical training for all sample environment to staff involved in 24/7 on-call duties.
- The plan for cold commissioning is supported by us but could be proceeded by mock-up experiments to train on sample environments at the instruments.
- Focus on the workflows is needed for effective sample environment and lab support to instruments. (well documented procedures).
- Consider a ticket system for sample-environment support.



Caroline Curfs, Niklas Ekström, Andreas Hagelberg, Alex Holmes, Damian Paliwoda, Yulia Pedersen, Luca Sagliano, Lauritz Saxtrup and Oleksiy Zadorozhko; Richard Ammer (-> ODIN IOE)

already being addressed or planned

Division Updates

Summary of STAP comments spring 2024

SULF
Sample handling and user laboratory facilities

- There is pressing need for a sample handling/storage lab
- Develop a plan and budget for capital equipment to address the most pressing needs as ESS progresses toward SSO

DEMAX
Deuteration and macromolecular crystallisation

- No NMR/MS spectrometer on-site a risk
- Increasing D2O costs - Consider recovery and purification
- Own appropriate lab for DEMAX to free D04 user lab

SCSE
Soft matter and chemistry sample environments

- Currently roles/responsibilities between beam lines and SCSE for SE development are not clear enough
- SCSE should finish a few sample environments to demonstrate capabilities.
- SCSE should sit in on large scale structures meetings to increase visibility and communication
- Do not neglect chemistry sample environment

Zoe Fisher, Anna Leung, Jia-Fei Poon
Monika Hartl, Katrin Michel, Melissa Sharp,
Ghazaleh Roostaei, Nick Weisend
Alice Corani, Harald Schneider

Progress MSPS

Magnets in scope

15T for BIFROST (2nd hand from HZB)
- Done: Tested, basic control integration (Octopy)
- Next step: Mechanical integration

6.5T for ESTIA (2nd hand from HZB)
- Tested up to 6.5 T with new electronic racks
- Next step: Control (via Octopy) and mechanical integration

15T for POOL (2nd hand from HZB)
- Leak tested at room temperature
- Next step: test at field and integration

2.1T WBM for ESTIA
- HTS 110 compatible with flow cryostat and polarisation
- SAT done
- Design for mechanical integration done
- Next step: Control integration and mechanical integration

15T magnet for BIFROST

2.1T WBM for ESTIA

8T for Diffraction for MAGIC
- Large aperture magnet
- Production to start Jan 25
- Planned to arrive at ESS Q4/25-Q1/26

Magnet for Spectroscopy
- Design study done for a 14T
- Next step: Call for tender – *would like to understand user base for 14T vs e.g. 10T ?*

1T Electromagnet
- For SANS, DREAM and ESTIA
- Simulation for polarisation done
- Requirements set
- Procurement on going

17T magnet (Lund University)
- Control integration done (Octopy)

From instrument's wish list:

\+ **10T horizontal SANS magnet**

5T magnet for SANS and second 2.1 T WBM replaced by a 10T horizontal split pair magnet for SANS as the next one.

Progress MSPS

Low Temperatures

Pools cryostats and cryofurnaces

- 3 wet cryostats, 3 dry cryostats, 3 wet cryofurnaces and 1 dry cryofurnace for MAGIC, BIFROST, LOKI, SKADI, DREAM, HEIMDAL, T-REX and MIRACLES
- **Tender awarded to AS scientific**
- Detailed specifications for each system on-going

Cryofurnace for Electro-chemistry (DREAM)

- Dry cryofurnace dedicated to electrochemistry and diffraction
- Large sample space (100 mm)
- In Production, delivery planned Q4/24

Cryostat for MAGIC (2nd hand from FRMII)

- Leak test done

Pumping cart

Automatic pumping cart

- includes pumps, temperature control and He and N2 level meters
- 6 in production

Wet cryostat for MAGIC

Dilution fridge (2nd hand from HZB)

- Refurbished and successfully tested down to 27 mK
- Next step : control integration

Others:

- 1 for 8T magnet (previous IK) + 1 for Pool
- Tender and specifications on going

HZB dilution fridge

a pool wet cryostat

Progress MSPS

High-Pressure (all instruments)

Gas, Liquid and clamp cells

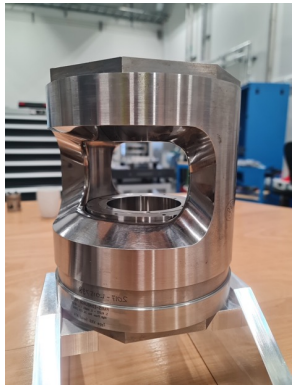
- Received at ESS and some tested without beam
- Training to manufacture more done

10kBar compressor for gas cells

- Received at ESS
- SAT done

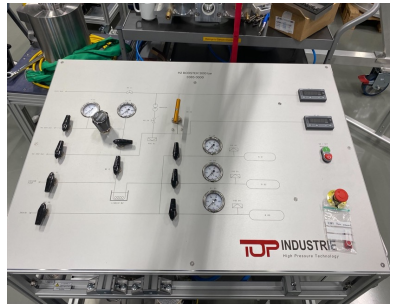
Other compressors

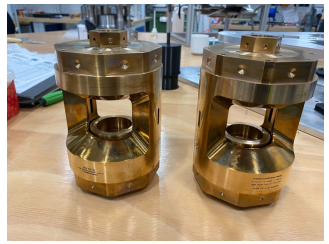
- Vinci pump and PACE 5000 control integrated



PE presses and gas loader

- 3 PE presses at ESS
- Gas loader: SAT done





Diamond anvil cell (DAC)

- available for the Lab single X-tal XRD

Cryostat for High-Pressure (IK)

- Custom-made wet cryostat built by ILL
- Construction finished
- FAT planned 11.24
- Planned to be ready in 2025

Progress MSPS

High Temperature and Mechanical processing

ILL-Type furnaces (DREAM and HEIMDAL)

2 Niobium 1650 C and 1800 C (2nd hand)

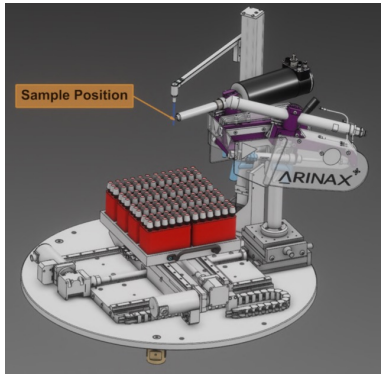
- Transfer from LLB still delayed
- Refurbishement needed

1 Vanadium 1100 C

- Specifications on going

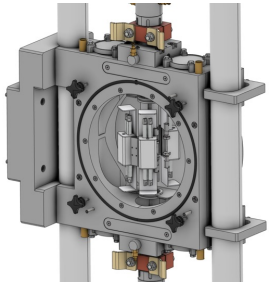
Hot Air Blower/Cryostream (DREAM and HEIMDAL)

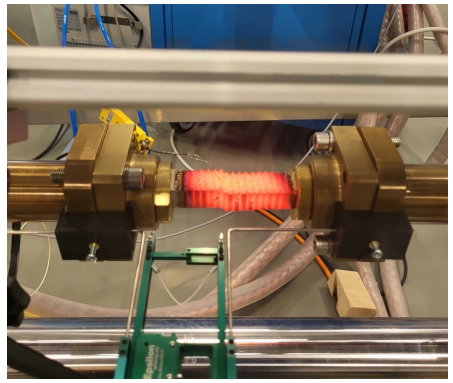
- From 100 K to 800 C
- Sample changer
- Design completed
- Mounting on going
- Control box on going
- Planned to be available Q4/24-Q1/25

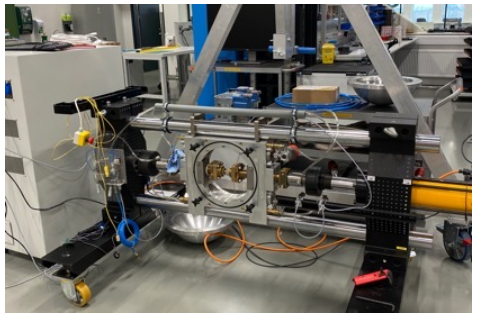


UHT furnace (BEER)

- Lamp furnace up to 1800 C
- Vacuum or inert atmosphere
- Adapted to the NPI
- Design on going with ISIS





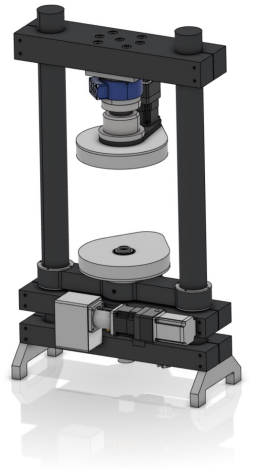


NPI stress rig (BEER)

- 60 kN unixial deformation rig: tension and compression
- Conductive heating (800 A / 15 V)
- At ESS
- Software update on going
- Collaboration with Alfa Laval for use case started

Tortion/rotation rig (ODIN)

- Design finished – PDR done
- Off-the-shelf pieces arrived at ESS
- Construction planned Q4/24-Q1/25



Dilatometer (BEER)

- Specifications on going

CLS Lab and workshop Installation 2024

D08 laboratories/workshops and two small rooms at D04

D08 furniture and electrical installation complete

Tender being evaluated

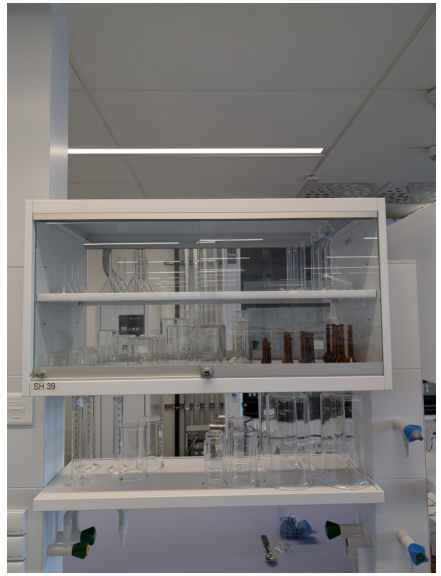
(a) utilities (water, DI water, cooling water, ventilation)

(b) gas/vacuum

Plan: start in Q1/25 and end Q2/25.

CLS D04 lab commissioning

D04 soft matter lab is ready for general users



Added: small-scale equipment
- Tip sonicator
- Vacuum furnace
- UV/VIS
- Balances

Glassware/consumables in place
Procedures, safety, PPE in place

SCSE lab D04:

E04 chemistry laboratories: operational since 2 years
- instrument teams invited to safety induction
- Support provided for project users with analysis and testing of materials, unknown substances and other issues
- Support instrument teams for beamtime preparations at other facilities

CLS Radioactive Materials Lab (RML)

Waiting on permission to use as controlled zone

- Radiation monitoring equipment: infrastructure installed, monitors will arrive soon -> Radiation Protection Group is responsible

The RML will be used to support the machine directorate in material analysis when starting up.

The RML will be for neutron users handling samples that have higher activation or when activated samples need to be modified in a system that cannot be contained.

<u>Current use:</u>

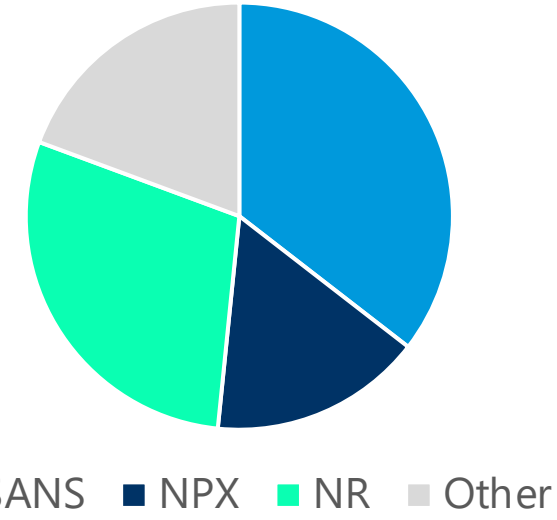
- RML will house GC system for Target Division to check He gas for target cooling (Helium circulator): installation November
- Tensile testing of Proton beam window successfully completed in spring (Accelerator Division, Engineering)
- Filling of catalyst into vessel for target cooling water completed in spring

CLS DEMAX

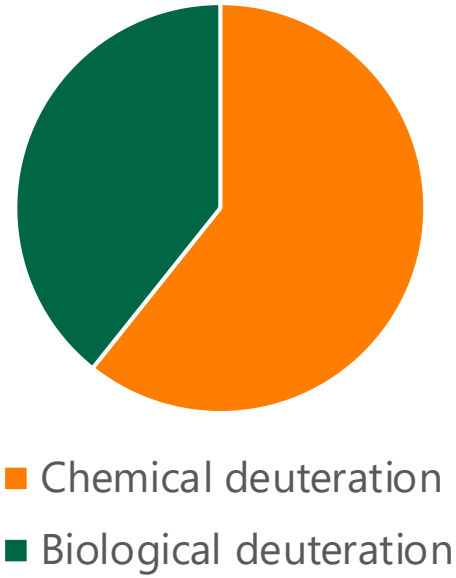
Proposal statistics

- over 100 unique users since starting (2019)
- 40 papers in peer-reviewed journals published or has under review
- In last proposal call (2022) + Rolling Access (-> Sep 2024) 36 proposals requesting 62 molecules/services

Intended neutron scattering technique



Type of deuteration required



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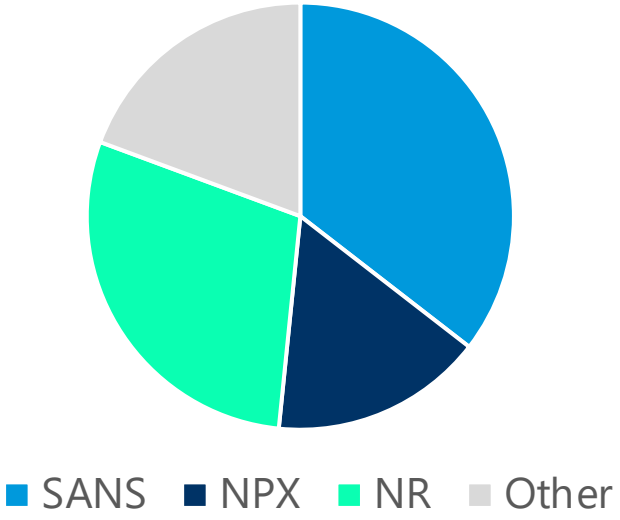
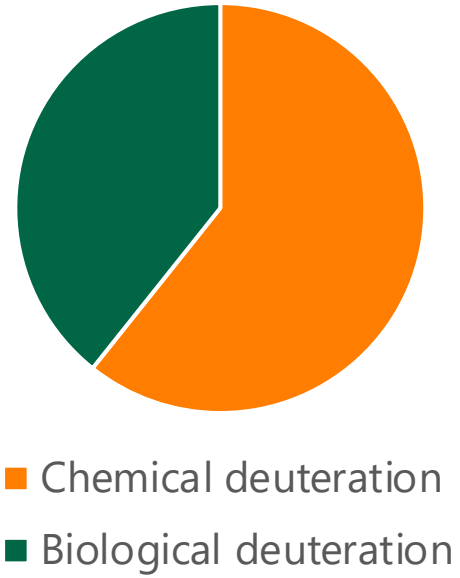


Type of deuteration requirec



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ARTICLE

Stabilization of Non-Native Folds and Programmable Protein Gelation in Compositionally Designed Deep Eutectic Solvents

Adrian Sanchez-Fernandez,* Jia-Fei Poon, Anna Elizabeth Leung, Sylvain François Prévost, and Cedric Dicko

Contents lists available at ScienceDirect

Journal of Colloid And Interface Science

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ELSEVIER

Modulating protein unfolding and refolding via the synergistic association of an anionic and a nonionic surfactant

Johanna Hjalte [a], Carl Diehl [b], Anna E. Leung [c], Jia-Fei Poon [a,c], Lionel Porcar [d], Rob Dalgliesh [e], Helen Sjögren [f], Marie Wahlgren [a], Adrian Sanchez-Fernandez [g,*]

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[g] Center for Research in Biological Chemistry and Molecular Materials (CIQUS), Department of Chemical Engineering, Universidade de Santiago de Compostela, Santiago de Compostela 15705, Spain

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ELSEVIER

Botryococcus braunii **autolysate for the production of deuterium-labeled recombinant protein**

K. Koruza [a,1], E. Krupinska [b], C. Sele [b], Á. Végvári [c], W. Knecht [b], S.Z. Fisher [a,d,*]

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[b] Lund Protein Production Platform (LP3) & Protein Production Sweden (PPS), Department of Biology, Lund University, Sölvegatan 35, SE-223 62 Lund, Sweden
[c] Division of Chemistry I, Department of Medical Biochemistry & Biophysics, Karolinska Institute, Scheeles väg 2, SE-171 77 Stockholm, Sweden
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ARTICLE INFO

Keywords:
Microalgae
Autolysate
Perdeuteration
Neutron scattering
Deuterium-labeling

ABSTRACT

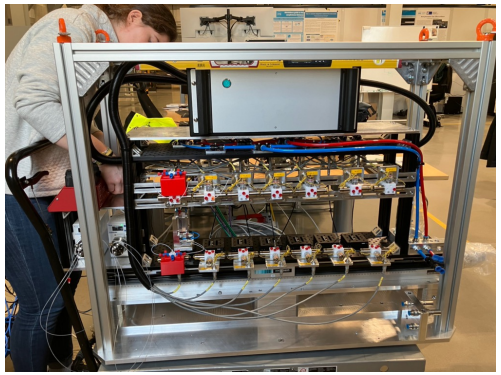
Deuterated biomolecules such as proteins, lipids, and DNA are widely used in neutron scattering experiments. This is due to the unique scattering properties of ^{2}H, including a strong positive neutron scattering length while contributing very little background compared to the more abundant ^{1}H isotope. Deuteration is therefore an indispensable component in the study of structure, function, and dynamic behaviour of biomolecules by neutron scattering. In the past we compared multiple microalgae species for their ability to grow under deuterated conditions and in our hands *Botryococcus braunii* proved the easiest and most resilient to long-term culturing in D_2O. In this study we describe how to culture *B. braunii* cells under deuterated conditions followed by preparation of an aqueous extract. The procedure is based on autolysis where cells are incubated at 50 °C for 24 h and clarified by centrifugation and filtration. The product, deuterated algal autolysate, is then used in minimal media for deuterated recombinant protein production in bacteria. We demonstrate that in-house produced deuterated algal autolysate can fully substitute for glycerol-d8 in minimal media without a reduction in expressed protein yield while obtaining ~98 % deuterium incorporation in the final product, suitable for neutron scattering and other types of experiments.

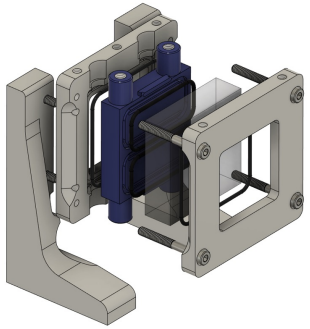
CLS SCSE News

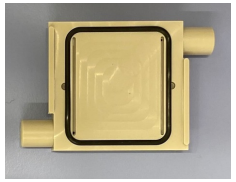
Instrument projects supported by SCSE

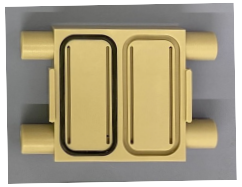
Reflectometry Solid liquid cell (ESTIA/FREIA):

Sample changer solid/liquid cell ESTIA is completed. Final test at PSI (H.B.): 7 cells, 50x50 mm, 5-50 ˚C.





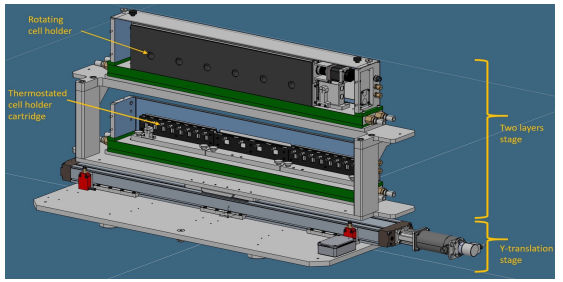




Cells successfully tested at PSI in sept.

- Fast assembly
- Quick change from horizontal to vertical orientation

SANS Loki :



SANS sample changer, thermalized and rotating cell holder, 2 rows of cells holders, 24 narrow cells/row:

- Temperature read out box done (outsourced)
- Translation stage received
- Test with B4C coating ongoing
- Parts are ordered and/or being manufactured

NURF cell insitu optical probe setup for flow cell, done.

CLS – SCSE News

SCSE projects soft matter

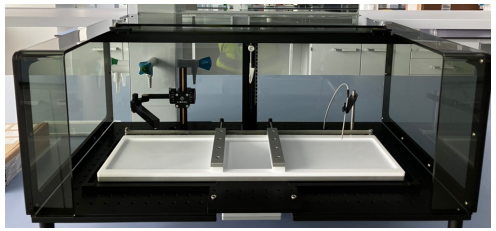
Reflectometry (ESTIA /FREIA):

Sample changer solid/liquid cell FREIA:

- Ongoing, waiting for ESTIA sample changer final test feedback.

Combined Ellipsometer/IR setup: Swedish IK with Linköping University:

- Critical design review done
- procurement of the IR and ellipsometry instruments ongoing.

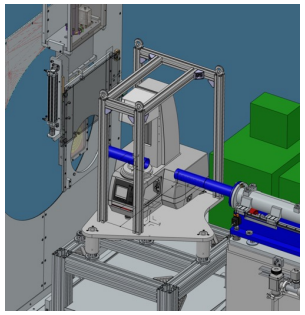


LB/LS Dipping trough D04

Troughs: RÅC grant with Kiel University, Lund University and ESS:

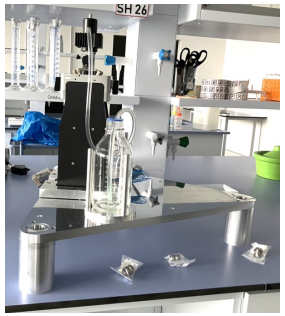
- Automatisation design of static troughs started July ’24
- Langmuir troughs (Kiel U.): includes laminar flow Langmuir troughs for subphase exchange, started July ’24

SANS:



Rheometer:

- Mechanical integration, manufacturing ongoing
- Final test for the control integration



Stopped Flow:

Mechnical integration done, test and control integration ongoing. Parts for the control box ordered.

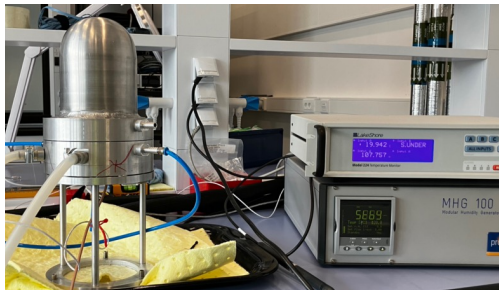
CLS – SCSE news

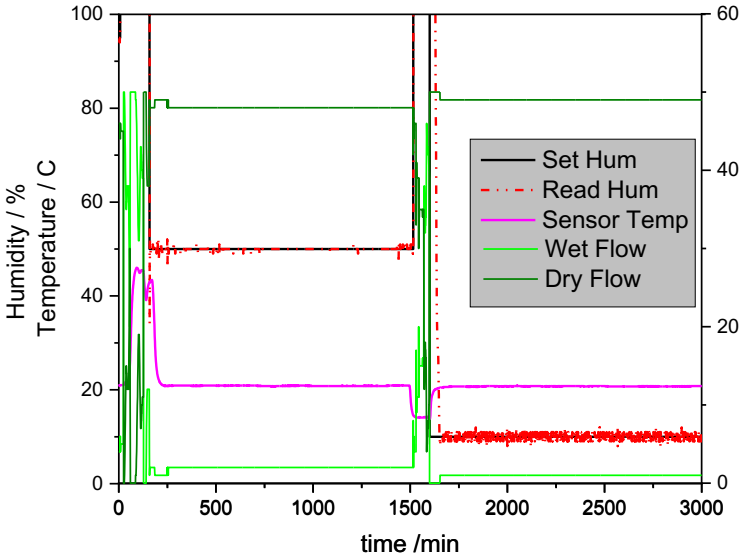
Advice from relevant insturment STAPs on day 1 priorities for wet electrochemistry/battery SE and lab equipment would be appreciated

SCSE projects - Chemistry

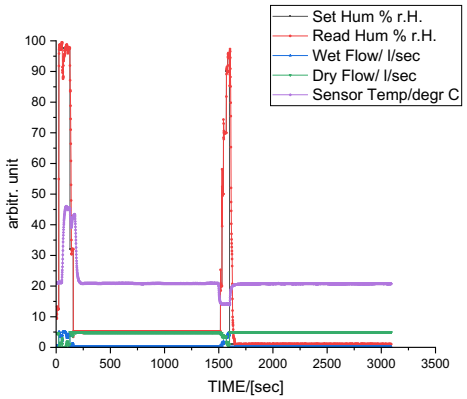
Humidity chamber

Tested and improved, still need to test Al sample chamber with neutrons.





Stable at various % humidity (shown here 2%, 5%, 10% and 50%

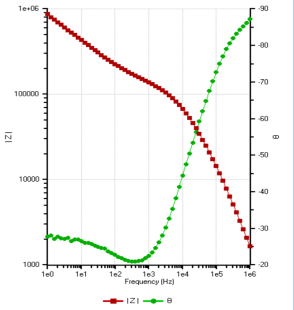


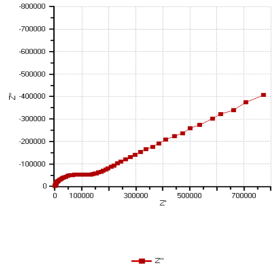
Electrochemistry/Battery cells:

Tested in the lab ongoing, impedance measurements

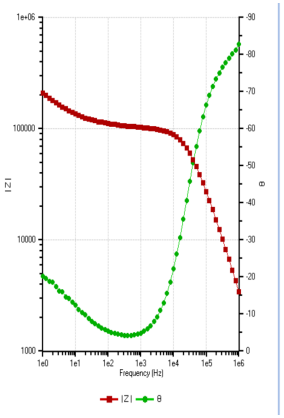
- Versatile Cell, Spectroscopy:

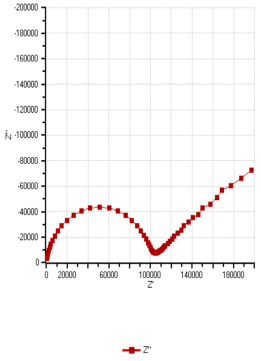
To be tested at SNS in Nov.





- Battery cell, diffraction :



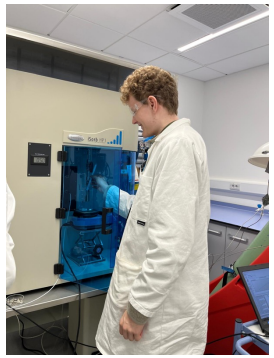


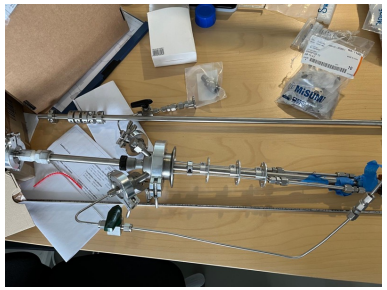
CLS - SCSE

SCSE projects - Chemistry

Gas manifold high pressure <200 bar

Project with Intern Philipp M., sample stick for gases (200 bar) from 10K to 673K





Low pressure Manifold 30 Bar:

- Gas lines and parts received
- Pressure gauges and flowmeter specification undergoing.

Julabo trolley :

Prototype done, part has been ordered

Small accessories and others

Syringe pumps

HPLC pumps

Potentiostat

Julabos

Drop levitator

Reaction and flow cells