

## 1. General Comments

### Organisational Structure

In autumn 2022, based on a review carried out of all directorates, input gathered from division heads and considering the feedback from ESS advisory bodies, ESS management took decisions to delayer management positions and change the scope in certain areas. This organisational change affects the Scientific Activities Division and a consolidated group structure shall deliver scientific operation and support most efficiently. The change includes creating a 'Chemistry and Life Science Support Group' (CLS) led by Monika Hartl and a 'Materials and Physics Support Group' (MPS) led by Caroline Curfs. The functions related to 'Scientific Coordination and User Office' remain largely unchanged.

Specifically, the Chemistry and Life Science Support Group (CLS) ensures ESS' chemistry, life science, soft matter and biology support. It is responsible to

- Provide deuteration, chemistry, life science and crystallisation services as part of the ESS user programme and operate deuteration, chemistry and life science laboratories.
- Ensure sample management and provide support to the user in the on-site user laboratories when handling their samples in preparation or during their beamtime.
- Install, operate, calibrate, maintain and repair sample environment systems (together with the instrument teams) for physical chemistry, fluid control, surfaces & interfaces to enable experiments with multiple / combined parameters such as stabilized temperature, controlled humidity, gas loading, stopped liquid flow, excited states, conditioned fluids and free surfaces.
- Develop, procure, refurbish, integrate and commission new sample environment systems and lab equipment, ensure method development, and training of users and students.
- Provide neutron guide characterisation and simulations.

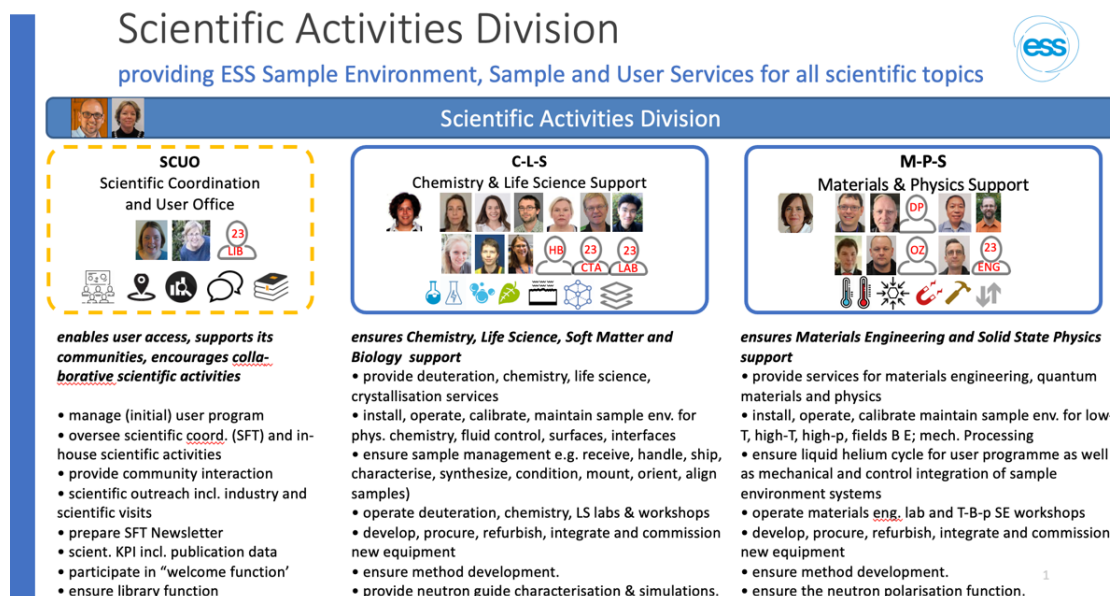
The Materials and Physics Support Group (MPS) ensures ESS' materials engineering and solid-state physics support. It is responsible to

- Provide services for material engineering, quantum materials and physics as part of the ESS user programme and operate materials engineering labs and T-B-p workshops.
- Coordinate the liquid helium cycle and additional sample environment related supplies for experiments.
- Install, operate, calibrate, maintain and repair sample environment systems (together with the instrument teams) to enable experiments with multiple / combined parameters such as low and high temperatures, electric and magnetic fields, high pressures and mechanical constraints.

- Develop, procure, refurbish, integrate and commission new sample environment systems and lab equipment, ensure method development, and training of users and students.
- Ensure the neutron polarisation function.

Finally, the Scientific Coordination and User Office Function (SCUO) enables user access to beam time based on scientific merit and others (innovation, proprietary) incl. industrial access, supports its scientific communities by ensuring community interaction and encourages internal collaborative scientific activities. SCUO is responsible to

- Manage the user programme, community interactions incl. user meetings, support scientific outreach and visits; organise access for and outreach to industry and industrial users.
- Oversee scientific coordination and in-house scientific activities; participate in an envisaged ESS-wide “welcome function”
- Provide scientific key performance indicators including publication data and ensure the ESS library function.



### Team:

Though line management has changed in some cases, overall the individual role of the SAD team members remained largely unaffected by the organisational change. As part of the re-organisation it is our pleasure to welcome Joanna Lewis (Scientific Communication, Outreach and Public Engagement), Hal Lee (Polarisation), Joël Hagman (Polarisation) and Damian Martin Rodriguez (Guide Characterisation) as new members to the SAD team. After his PostDoc deuteration project, Jia-Fei Poon joined as CLS scientist for deuteration. Two MPS research engineers for low-temperatures (Oleksiy Zadorozhko) and for high-pressure (Damian Paliwoda) as well as a CLS research engineer for soft matter (Hannah Burrall) will join the team shortly. Recruitment is ongoing for a librarian, a CLS lab technician and a CLS technical support (2years). One more MPS research engineer is foreseen to start in 2023.

### Project Execution

Having established an amended baseline scope in 2022 for the whole period until end 2027, all SAD activities are part of the Science Directorate project. We are now routinely using the same planning and reporting tools making our achievements and challenges more visible in the organisation. We continue to improve the cross links to other teams, not least with the instrument teams and their delivery schedule. To keep our plans up-to-date, change requests have been presented on the library function, scientific communication, creating of CLS and MPS work packages, move of polarisation function and guide characterisation, deuteration move to site. We shall prepare additional change requests related to IK2Cash conversion of several sample environment systems, lab fit-out as well as an updated estimate for user reimbursement.

### Collaboration

The new organisational structure creates groups with well-matched team sizes and similar competences / subject matter experts. This ensures well-balanced scientific support in operations and reduces single points of failure. Matching laboratories / workshops, lab instrumentation and sample environment by scientific topic reduces the risk for duplication-of-effort and eases consistent ways-of-working as well as integration. The change has been well-received by the instrument teams and they work even more closely with the subject matter experts within CLS and MPS related to their needs related to sample services and sample environment.

Though the new organisational structure creates more multi-faceted links to external partners by dissolving (well-known) technical functions. This is mitigated by continued exchange with (new or existing) networks (such as ISSE, DEUNET, ...). The number of several technical interfaces has also increased. This will be mitigated by keeping excellent links to (new) ESS central services: facility management (lab fit-out, operation, maintenance), EHS&Q (samples), ICS/ECDC/MCA/DMSC (control integration, fair data), NSS/EIS (mechanical integration), AD/TD (material analysis, cryogenics, vacuum), ....

Specifically, we have support from ECDC for control integration (Anders Pettersson) and from accelerator division for the Helium management (Jaroslaw Fydrych). The central design team is currently recruiting a mechanical design engineer (largely) dedicated to sample environment mechanical integration compensating the gap created by the NSS mechanical engineer (Tobias Quispe) focusing on NSS-related topics only.

### Infrastructures

Laboratories and workshops in the E buildings are well-used by the various teams and interfaces to central services (such as facility management) are well-established. Fit-out activities for the spaces in the D buildings faced some delays during the tender process and a (significant) cost increase is now confirmed. We are looking into mitigating both and fit-out of the core D04 labs has started. This ensures that the move of the deuteration function from Medicon Village to the on-site labs can proceed as planned.

## 2. Chemistry and Life Science Support Group

The CLS group in its current state was formed in January of 2023 after the ESS-wide reorganization. It consists of the former deuteration services DEMAX and the user laboratories SULF. The sample environment for soft matter and chemistry SCSE (former FLUCO) has been added. Even though the main task for a large number of the group members remained the same, the reorganization had and still has a large impact on the way the CLS group is working as a whole.

The CLS group supports the ESS users in chemistry, life science, soft matter and biology and is organized in the following way (four "functions"):

- Sample and User Laboratory Facilities (SULF) providing the user laboratories
- Deuteration and Macromolecular Crystallography (DEMAX) providing deuteration services
- Soft Matter and Chemistry Sample Environment (SCSE) providing sample environment
- Interactions towards science (I2S) capturing the requirements of the instruments and science community towards CLS

The functional lead for SULF and DEMAX lies as before with Monika Hartl and Zoe Fisher, respectively. Monika Hartl currently is the functional lead for SCSE until a member of the SCSE team is ready to step up. Hanna Wacklin-Knecht has taken over the I2S functional lead role.

### User laboratory support (SULF)

The operations in E04 are going smoothly and we were able to add some smaller equipment. We are now waiting on the CHN elemental analyser procured at the beginning of the year. The SULF team under functional lead by Monika Hartl has completed commissioning the Radioactive Materials Lab (RML) and is now waiting on the hand-and-foot monitor and the permit to handle activated materials. The collaboration with the beam diagnostics group at ESS is continuing and we will host their testing device in the RML for testing activated beam diagnostics parts.

SULF is still very active in the Spallation Chemistry Team that supports the ESS construction project. Since April 2023, Damian Martin Rodriguez, responsible for neutron optics and neutron guide/substrate characterization, is part of the SULF team. Damian will continue supporting the instruments during reviews with regard to neutron optics, and with identifying ppm levels of strongly activating elements (e.g. Co, Ag) in delivered guide components. While this broadened the SULF scope, we are confident that it will also give us an extra pair of hands in the laboratory.

The tender for the framework agreement for laboratory fit out has been completed after long negotiations. The installation of the labs in D04 has started as of March 29th, 2023. The scope was reduced due to the large cost increase for the fit out. The two large laboratories in which DEMAX will occupy 50% of the space, and the sample

environment laboratory needed for the SCSE team will be installed. Estimated date of completion is after summer with the ground floor lab ready in time for DEMAX to move in. The accelerated hire of a lab technician, originally planned for 2026, is ongoing. The technician will help to support the move of the DEMAX team and consequently operation of D04. Furthermore, we are in the process of hiring a technical admin on a two-year limited term contract to support the documentation, work permits, training records and day-to-day tasks related to the installation work.

SULF hosted a chemical technical assistant for three months last fall. This worked out extremely well and was a true support to our lab operations. We have since visited two vocational schools in Berlin, Germany to look for further possibilities to host interns. We are planning to host a physical technical assistant in fall 2023 and hoping to get a chemical technical assistant as well.

The main issue for the SULF team in the past three months has been the fallout of restructuring in the division and consequently the disruption of the planned work and lack of personnel. The team already has one member on sick leave and a second one (Harald Schneider) moved over to support the SCSE function. That leaves two persons for the user lab support and planning, one of which is the group leader of CLS. This results in very little time to keep operating the labs in E04 while at the same time scientifically supporting the ESS project with material analysis and expertise.

#### Deuteration Activities (DEMAX)

The deuteration team DEMAX under the functional lead of Zoë Fisher is well on track: the team has completed 70% of the accepted proposals from the last call and a 'rolling access' call is now open for deuteration proposals. It is foreseen that DEMAX will finish the syntheses for the current call before the move from their current lab in Medicon Village to site is starting in May.

The on-site lab installation has started and is almost on time, so that the move from Medicon Village to ESS is foreseen to take place as planned. The move will still result in a downtime of 3-6 months for the DEMAX team until all services can be established at ESS. The hiring of a chemical technical assistant (see SULF) to support the setting up of the new labs will reduce the downtime. There are several benefits for the CLS group when the DEMAX team works on-site as it will integrate the DEMAX team members into the CLS group and the whole groups can share tasks of operating labs, both for deuteration as well as general user laboratories.

The demand for deuteration is growing and requests to synthesize new types of deuterated molecules are continuing to come in frequently. These expressions of interests are a good possibility to perform research and development before the user program starts and time becomes scarce.

DEMAX as part of DEUNET successfully conducted a micro symposium at the ECNS 2023. Staffing is still low with two team members on leave and others with health issues. However, this is mitigated by two new hires: Jia-Fei Poon has started as deuteration chemist in February 2023, and the postdoc Sophie Ayscough that has started in November 2022 and is supporting the lipid deuteration.

### Soft matter and chemistry sample Environment (SCSE)

This part of sample environment refers to systems for physical chemistry, fluid and gas control, surfaces & interfaces. This team and its tasks was formed in January by reuniting the former "FLUCO" team members Alice Corani and Harald Schneider after the restructuring at ESS. The functional lead is currently Monika Hartl but this will change as soon as one of the team members is ready to take over this role. A new engineer, Hannah Burrall, will join this team in September 2023 and will strengthen the soft matter sample environment aspect especially the focus on the neutron reflectometers.

The past three months have been spent on identifying the status of ongoing projects and establishing a work plan in "Kanban" style. This has allowed us to gain an overview of what needs to be done and what might be missing from the plan. We have also started gathering and submitting documentation, drawings and manuals of the completed and ongoing projects to store them in the correct location in the ESS document system CHESS. This helps on short term to gain an overview of what might be still be needed and long term to have a place where we can find everything.

The physical equipment has moved from its previous location in E03 to one of the labs in E04 where integration testing is ongoing. The Estonian in-kind projects for sample environments will end this year and several site-acceptance-tests are expected. We are currently finalizing the stopped-flow-cell and are expecting the laser-pump-probe system and two electrochemical cells to arrive in summer.

The SCSE workshop in building D04 is currently being installed and should be finalized after summer. Then the team will commission the workshop, move the equipment into the room and establish an optical workbench for aligning the laser of the pump probe system.

### Interactions towards science (I2S)

The interactions towards science is a team with Hanna Wacklin-Knecht as functional lead that will gather the requirements in the areas of soft matter/life science and chemistry from the instruments and the science community. The I2S team will communicate these priorities to the respective CLS teams (support labs, deuteration, sample environment) as input for planning the next steps in the respective team. In turn, I2S will present information on the status of capabilities from the respective CLS teams to the instruments and science community explaining what can and cannot (yet) be achieved with what has been provided. This interaction team will assist greatly in streamlining interactions and maximizing transparency of what will be in the plan for commissioning, first science and beyond.

### 3. Material and Physics Support Group

MPS Team and scope: Following the reorganisation, the overall scope of the MPS group has been slightly modified and the group is now in charge of delivering Sample Environment Systems (SES) for low and high temperatures, magnetic and electrical fields, high pressure and mechanical processing only. The group is also in charge of the mechanical and control integration of all the SES, including SES for soft matter and physical chemistry, as well as supporting users in the fields of materials engineering, quantum physics and high pressure.

The MPS group is now composed of 1 group leader (also in charge of the mechanical processing), 1 subject matter expert (cryo and magnets), 2 engineers for the control (electronics) and control integration and 2 technicians. 2 new research engineers (subject matter experts) will arrive in May. They correspond to 2 of the 3 positions included in the project plan for 2023 (initially 4 were included in the plan). Damian Paliwoda will take care of the high pressure from the 1<sup>st</sup> of May and Oleksiy Zadorozhko of the low and ultra-low temperature SES from the 29<sup>th</sup> of May. Alex Holmes, will then be able to concentrate on delivering the magnets. A 3<sup>rd</sup> research engineer will be recruited before the end of the year.

In addition to the 6 (+2) MPS members, we have support from ECDC for the control integration (Anders Pettersson) and from the accelerator division for the Helium management (Jaroslaw Fydrych). Tobias Quispe from NSS (Neutrons Scattering Systems) was supporting the sample environment group until 31<sup>st</sup> of December 2022. EIS (Engineering and Integration Support) is now recruiting a mechanical designer to replace him. The recruitment is ongoing.

From the 1<sup>st</sup> of April 2023, the polarisation group (Wai Tung Lee, scientist, and Joel Hagman, technician) will join the MPS team.

#### Training, conferences and collaborations:

To prepare for operation, the MPS team is encouraged to participate in experiments at other large facilities: Niklas and Alice participated to an experiment with the 17T magnet at ISIS during fall 2022 (Lund University), Caroline at DESY in March 23 and Andreas, Lauritz and Caroline will take part in a magnet experiment at MAX IV with the ESS-DREAM team.

Alex attended the ECNS conference in Garching, Germany, in March 23 to present his poster entitled "A wide aperture high field asymmetric magnet for diffraction at ESS" and Caroline's poster on "Materials and Physics Support at ESS".

The MPS group is also directly involved in several project and proposals:

- Ongoing projects: SRESS for the design of a torsion/rotation rig and the development of a 3D Digital Image and Volume Correlation system (Lund and Malmö Uni) and SRESS-ISIS grant on a Ultra High Temperature furnace (ISIS and Chalmers and Linköping Uni)

- Starting projects: VR Infrastructure grant on Hydrogen embrittlement (KTH and Lund Uni)
- Proposals: NEXT competence center (KTH, Linköping Uni and many Industries) and HMS@NS High Field Magnet (ILL, FRM II)

Workshops: The SE workshop is now fully operational and the installation of the SLIME lab (Support lab for Imaging and Mechanical Engineering) in E03 will start once it has been emptied and cleaned. Discussions are on-going to see how to best use the different labs and workshops.

### Sample Environment systems:

#### *Magnets:*

- **8T magnet:** the procurement has started and the CDR is planned within the next month. The PDR for the **dilution fridge** will start in May.
- **2.5 T WBM:** after a design study with HTS-110, whose results have been received beginning of 2023, an open call for tender has been written and is now in the hands of the procurement team at ESS.
- **15 T HZB magnet:** The refurbishment of the second-hand magnet is finished. It has been vacuum leak tested at room temperature and, recently, a first attempt to cool it down using liquid nitrogen occurred. We were unable to fully cool the entire system to 77K with the quantity of LN2 available at the time, and were relying on generic calibrations for the diagnostic thermometry so decided to improve the setup and carry out another attempt, which is currently under way. Once cooled down, another leak test will be performed. We had considered moving the magnet to the cold box hall, where helium recovery is already available, for the full cooldown (but not running to field). A dry run with the magnet warm was not entirely satisfactory (it is quite a long distance and the forklift rebooted during the test run!), therefore we decided to wait for a provisional connection to the helium recovery line in E03. Cooling down with liquid helium is pending the installation of an He recovery line in the SE workshop. This part is on-going and should be available very soon. Works on the software and integration of the power supply and controllers in Octopy are still going on. The Risk Assessment for the magnets has been finalised.
- **Spectroscopy Magnet:** A kick-off meeting was held with the CSPEC and TREX scientists to agree on a range of specifications to be explored in a design study. Oxford Instruments have been contacted and preliminary discussions have started with them on this project. After the design study is complete an open tender is planned.
- **Force magnetic testing rig:** the design is finalised and a search for a manufacturer is on going



### *Cryostats:*

- **BIFROST cryostat:** the SAT has successfully passed, as well as the installation test on the instrument.
- The **automatic pumping cart** prototype has been successfully tested. The ESS vacuum group has started to list all the items needed and will make 4 of them using the same model. More will follow. The control system, using Beckhoff, is built by the MPS group. Its main design and building of the first prototype is done. It has automation of flushing of the sample space, and control loop for the cold valve using the same basic algorithm as HZB uses on their Cryostats.
- **Dry cryofurnace for electrochemistry:** The specifications are set and the call for tender documents is being written.
- **Cryostats:** A framework agreement to procure the cryostats planned (3 dry cryostats, 5 wet cryostats and 3 cryofurnaces) is still envisioned, but no work has been done yet.
- **DREAM cryofurnace:** due to several failed open calls for tender, a sole source procurement has been initiated at the end of 2023. After discussions with the envisioned manufacturer, quotation including options is pending and should arrive within the next month.

### *High-Pressure:*

- Pressure tests of the **gas, liquid and clamps cells** were successful, as well as the **SITEC compressor FAT**.
- The **PE press VX1** has been received at Sorbonne University and successfully tested.
- A collaboration agreement, between ILL, CNRS, CEA and ESS, has been written and its signature is ongoing. This will enable ESS technicians to participate in the assembly of the **HP cryostat** at ILL.

### *Mechanical Processing:*

- **Uniaxial deformation rig:** The 60 kN (100 kN) stress rig developed by NPI, CZ has been delivered at ESS in December and the SAT was successfully performed in January. Improvements on the control software are still needed and our partners are working on it with us. The mechanical integration will start soon as well as the development of new grips to be able to reach 60 kN and to accommodate other samples geometries.
- **Dilatometer:** The discussion with Dmytro Orlov from LTH, Lund, on the possibility to procure it as a Swedish In-Kind contribution has not come to a successful conclusion. Therefore, the procurement will be done by ESS. A meeting with the interested instruments is planned before summer to start discussing the size constraints for the CFT.
- **Tortion/rotation rig:** an updated design is currently being done by Lund University through a SRESS project. The new drawing should be ready before the end of 2023 and once finalized, a new rig can be built.

### *High Temperature:*

- **ILL-type furnace (x2):** The administrative procedure to allow their discharge from the reactor (LLB) is still ongoing. We hope that they will be shipped to ESS before the end of 2023. The niobium foils have been ordered and the refurbishment of the furnaces will be done at ESS by the MPS technical team under the supervision of Florence Porcher (CEA/DREAM).
- **Induction furnace:** During fall, this project was discussed with Martin Sahlberg from Uppsala University to have it as an In-kind contribution from Sweden. However, he finally decided to withdraw his interest: The cost book value (90 kEuros) is not sufficient to cover for the manpower. It is envisioned to apply for additional funding from the Swedish Research Council (VR) When an appropriate call will open. In the meantime, the parts already purchased (power supply, coils and induction generator) have been received at ESS.
- **Hot air blower/cryojet system:** in addition to a commercial hot air blower and cryojet, the original project included a glass chamber specifically designed. Since ESS does not have a glass blower, it has been decided, with the instrument scientists (DREAM and HEIMDAL), to provide a much simpler system: a series of samples placed on a translation stage and the hot air blower (already purchased) and the cryostream pointing toward one them. An additional rotation under the sample could be added for homogeneity of the temperature.
- **UHT furnace:** ISIS is in charge of the design which is well advanced. They will make a prototype for their own use and once tested, Chalmers University is in charge of making one for ESS. The UHT furnace is a lamp furnace which can be used with or without the 60 kN stress rig from NPI. End of February, the project partners visited ESS to see the stress rig and have their regular meeting.

### *Control Integration:*

- **Octopy:** its development is progressing and a successfully demonstrated at the SECoP meeting at HZB. The 15T magnet is currently being integrated with Octopy.
- **General Purpose I/O-box (aka the MacGyver box):** This device is designed to enable multiple analog and digital inputs and outputs for general purpose temporary use. The first prototype is done and integrated to EPICS.
- **Solartron Potentiostat:** a possible viable solution has been found: the three auxillary outputs from the potentiostat are routed to NICOS via EPICS. The potentiostat runs the experiment using its own program, but can synchronize the instrument via custom NICOS scripts. The electronic box and integration are mostly done.

### *Mechanical integration*

- The **vacuum chamber/pot** to test the top loading equipment has been designed. Discussions with potential manufacturers are still ongoing.

### *Helium management*

- The first delivery for the Helium management has been received from HZB. It includes some Helium level meters, some communication bases. The software has been installed and tested locally.
- The **pipe work** for the helium recovery is continuing and an end pipe has been connected to the main one in E03 SE lab.