Chemistry and Life Science Support

CLS

PRESENTED BY MONIKA HARTL

2023-04-26

Chemistry and Life Science Support - CLS

Structure of CLS with functional leads

Group Leader : Monika Hartl

DEMAX (Zoë)
Zoe Fisher, Anna Leung
Jia-Fei Poon, Hanna Wacklin-Knecht

Deuteration Service

SULF (Monika)
Monika Hartl, Katrin Michel, Melissa Sharp, CTA(Q2/23), Ghazaleh Roosteai, Damian Martin Rodriguez

Support laboratories
Installation / Spallation Chemistry

SCSE (Monika->Alice)
Alice Corani, Harald Schneider, Hannah Burral (Q4/23)

Soft Matter and Chemistry Sample Environment

Interaction to Science (Hanna)
Hanna Wacklin-Knecht, Melissa Sharp, Alice Corani, Monika Hartl

Interactions to science stakeholders (instrument, science community) on needs for DEMAX, SULF, SCSE

DEMAX Platform

Chemical Deuteration

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

Biological Deuteration

- Deuterated biomass from *E. coli*, *B. braunii*, *P. pastoris*
- Recombinant soluble proteins, plasmid DNA, "other"
- Yeast-derived lipids (total, phospholipid)

Protein Crystallization

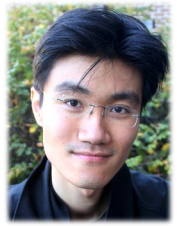
- High- and low-throughput screening
- Fine screening in large volumes
- Support for room temperature crystal mounting & data collection
- X-ray testing (LU BAG at MAX lab)

Extended team
(incl postdocs & tech support
From LP3/LU)


Zoë


Anna


Hanna


Jia-Fei


Jenny


Sophie

\+

0.75 FTE

LU/LP3

SULF Team

Areas of work

- Installation & Area Coordination
- Lab operations maintenance
- ESS Project support
- Neutron Guide Optics Support

Monika Hartl

Katrin Michel

Melissa Sharp

CTA (hiring process)

Ghazaleh Roostaei

Damian Martin Rodriguez

<u>internship</u>

(PhysTA Q3/23; CTA intern???

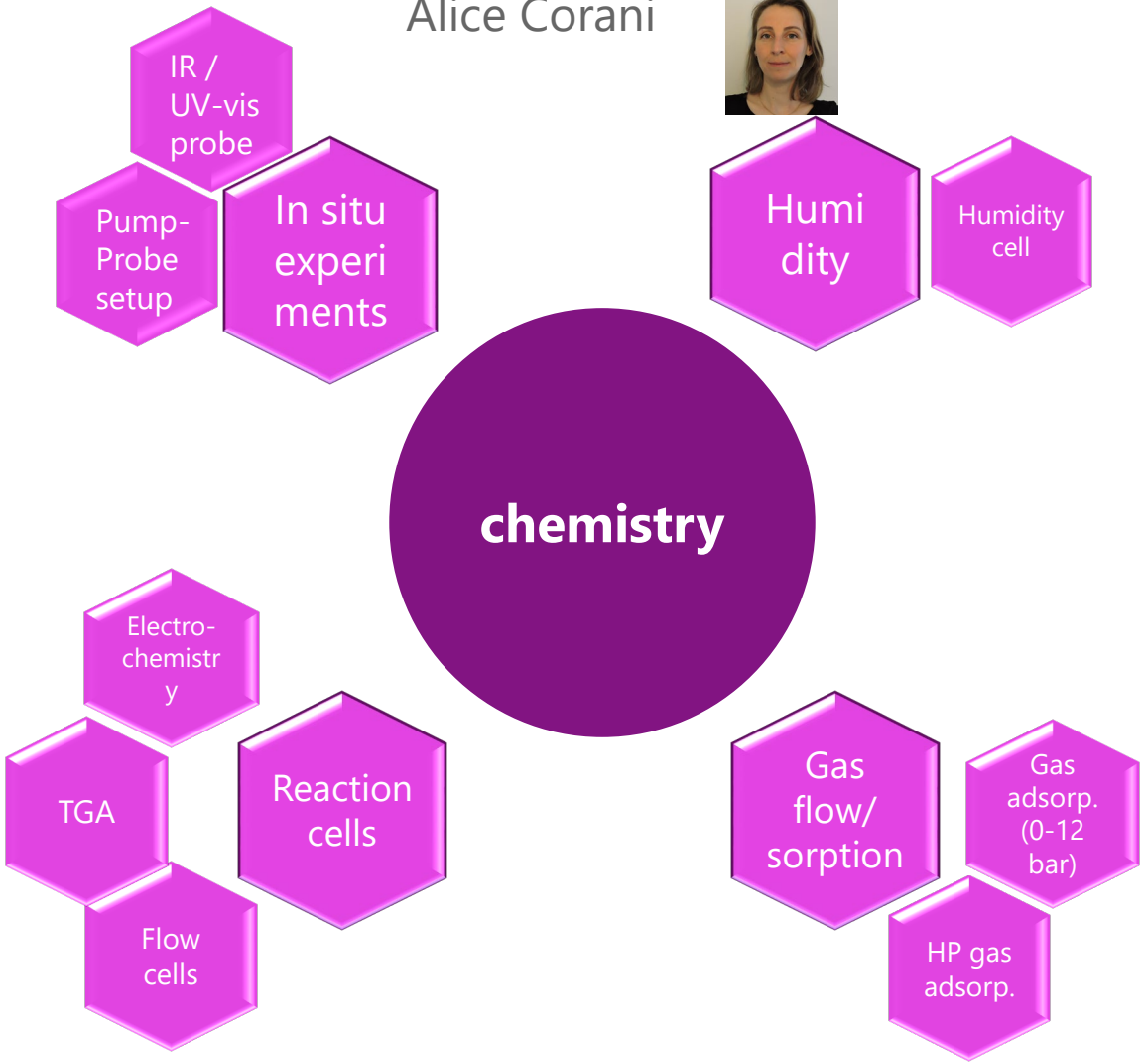
Soft matter and Chemistry Sample Environment

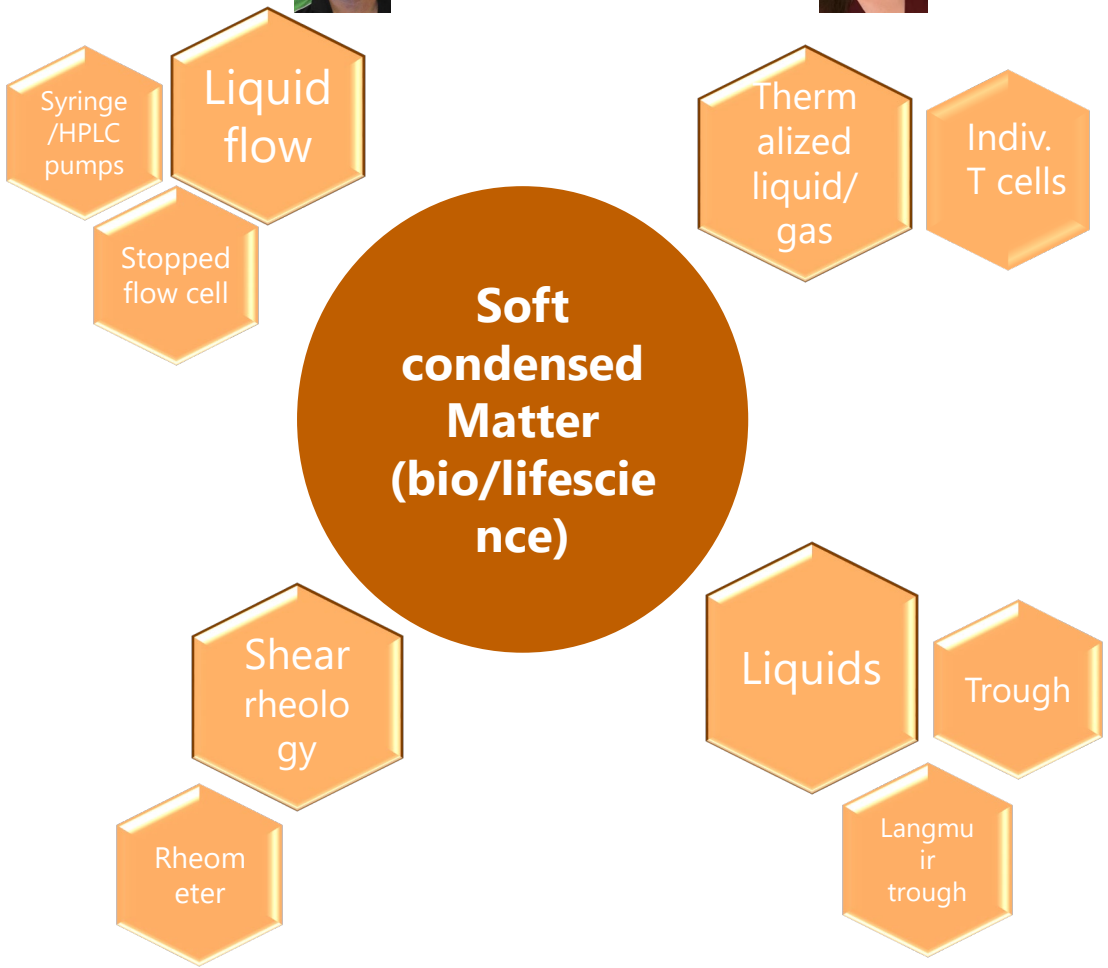
Provide sample environment systems and devices for:

Alice Corani

Harald Schneider

Hannah Burrall





I2S – Interfaces to Science in CLS

Strategy and interfaces in Chemistry, Soft Matter & Life Science

Work with all stakeholders to:

Capture scientific requirements and efforts

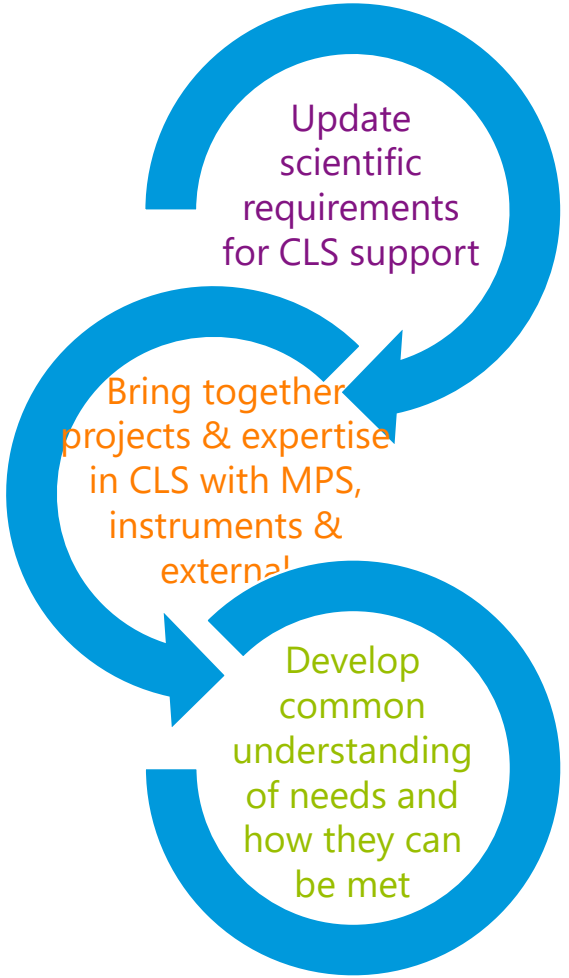
Create a strategy/prioritisation for:

- First Science
- First proposal call
- Towards Steady state Ops

Liase with external stakeholders

Leverage synergies with other actors

Interact with instrument teams/ scientific community on support needs for science in the areas of DEMAX, SULF, SCSE;



Hanna

Melissa

Soft matter/life science

Alice

Monika

Chemistry

I2S: Soft matter

Which materials will be measured?

Which instruments will be used?

What do we have? What is still needed? How do we fund it?

Soft Matter and life science experiments at ESS

Soft matter/life science experiments: types of materials and samples

Materials: surfactants, lipids, polymers, RNA/DNA, amino acids, proteins, peptides, cells, tissues, blood, toxins, drugs, ionic and DU solvents, oils, food, resins, minerals, glue + 100 other things…

LSS:

- solutions of molecules, aggregates, micelles, bicelles, vesicles, nanoparticles, fibres, cells
- nano/microemulsions, gels, clays, nanotubes, composites, microfluidics
- thin films made in-situ by adsorption, or ex-situ by LB/LS, spin coating on liquid and solid interfaces, porous/patterned/coated or magnetic solid surfaces

Spectroscopy:

- solutions of molecules, aggregates, vesicles, nanoparticles, fibres, cells
- nano/microemulsions, gels, composites, powders
- oriented films, spin coated/evaporated/ hydrated

Diffraction:

- crystals, fibres and powders of proteins, DNA, cellulose, amyloids etc.

Other?

- samples for imaging (?) – e.g. tissues, plants, bones, wood, implants, films, bulk materials, food…

SE for Soft matter and life science

Reflectometry

- Solid-liquid cells for each instrument
- Multiwell-solid-liquid cells (ESTIA)
- HPLCs + syringe pumps/switches
- Small + Large Langmuir trough
- Air-liquid troughs + box
- Small volume/cooled + multi-well troughs
- Humidity cell, WLS, GISANS (Flexiprobe)
- Julabos
- Temperature controllers
- Antivibration table
- Laser interferometer (Keyence)
- Liquid-liquid cells
- Electrochemical cells + potentiostat
- In-situ ellipsometry/FTIR cells + mount (design)
- Ellipsometer/FTIR spectrometer
- Furnace
- overflowing cylinder
- Automation/autosamplers

SANS

- Temp controlled cuvette changer (LOKI)
- Sample tumbler
- Hugginn 5 position changer (finished)
- Sandwich cells
- Flow cell (LOKI)
- In-situ fluorescence/UV set up (NURF)
- In-situ DLS/foam cell (Flexiprobe)
- Stopped flow rig(s)
- Rheometer (cylinder + cone-plate)
- In-line size-exclusion chromagraphy (SEC)
- Autosampler
- Skadi?
- GISANS/GINSES multilayer resonator/Prism?

Other/Synergies with Chemistry:

Spectroscopy:

- Humidity cell (Estonia)
- Laser Pump Probe (Estonia)

what other SE is used for Soft/Bio samples?

Diffraction/Imaging

- NMX ambient/cryogenic/humidity env.

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CLS Lab equipment for Soft/bioscience

Sample prepration, characterisation

Items on-site (E04):

DLS (Zetasizer)
DSC/Thermogravimetry
Uv-vis
FTIR incl. h-ATR
Raman
Autoclave
small shaker-incubator
pH meter
MilliQ
Vortex
Benchtop centrifuge
1 tip + 1 bath sonicator
Potentiostat
Optical microscope
Vacuum oven
Balances
XRD
Rheometer (Loki)
Glass drying oven?
Elemental analysis:
XRF, CHN+S, ICP-OES
Polishing machine

At LP3:

Nanodrop
pH meter (microtip)
Akta LC (basic)
mini-centrifuge
Gel electrophoresis
LED/CO_2 shaker-incubator
Xtallisation equipment
Thermofluor, NanoDSF
DLS, SEC-MALS

DEMAX (MV -> D04)):

Freeze-dryer -> LU Fkem1
Sample prep robot
Flash chromatography
TLC + UV chamber
glass drying + vacuum oven
HPLC (analytical/prep.)
2 rotavaps, vortex
GC-FID, bath sonicator (S)
Sample concentrator
Shaker-incubator
pH-Stat titrator
Benchtop centrifuge (new)

Priority (day 1, 24/7):

Analytical microbalance
LN2 storage Xtals (NMX)
Density meter
Spin coater
UV-vis nanodrop
Tip sonicator(s)
Freeze dryer and rotavap(s)
Microwave

XRR slits for Rigaku XRD
QCM-D
LB/LS dipping trough
UV-O3 cleaner(s)
Surface tensiometer
SEC/GPC for proteins

Later/specialised/€€€ equipment:

GC-MS (DEMAX)
Ellipsometer (ESTIA/FREIA)
MALS (goniometer)
CD/LC spectrometer
(GI) SAXS
NMR (DEMAX)
LC-MS (DEMAX)
FPLC for protein purification
Floor centrifuge

At other facilities also:
Brewster angle microscope
Contact angle
Differential refractometry
Plasma cleaner
Diffusion NMR
Foam analyser
AFM

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Deuteration – covered through DEMAX & Deunet

I2S: Chemistry

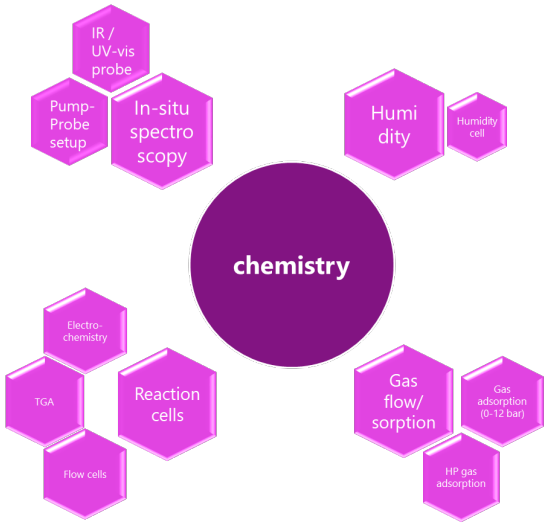
Which materials will be measured?

Which instruments will be used?

What do we have? What is still needed? How do we fund it?

CLS- Interactions to Chemistry (A. Corani, M. Hartl)

Provide labs/sample environment and deuteration for Chemistry

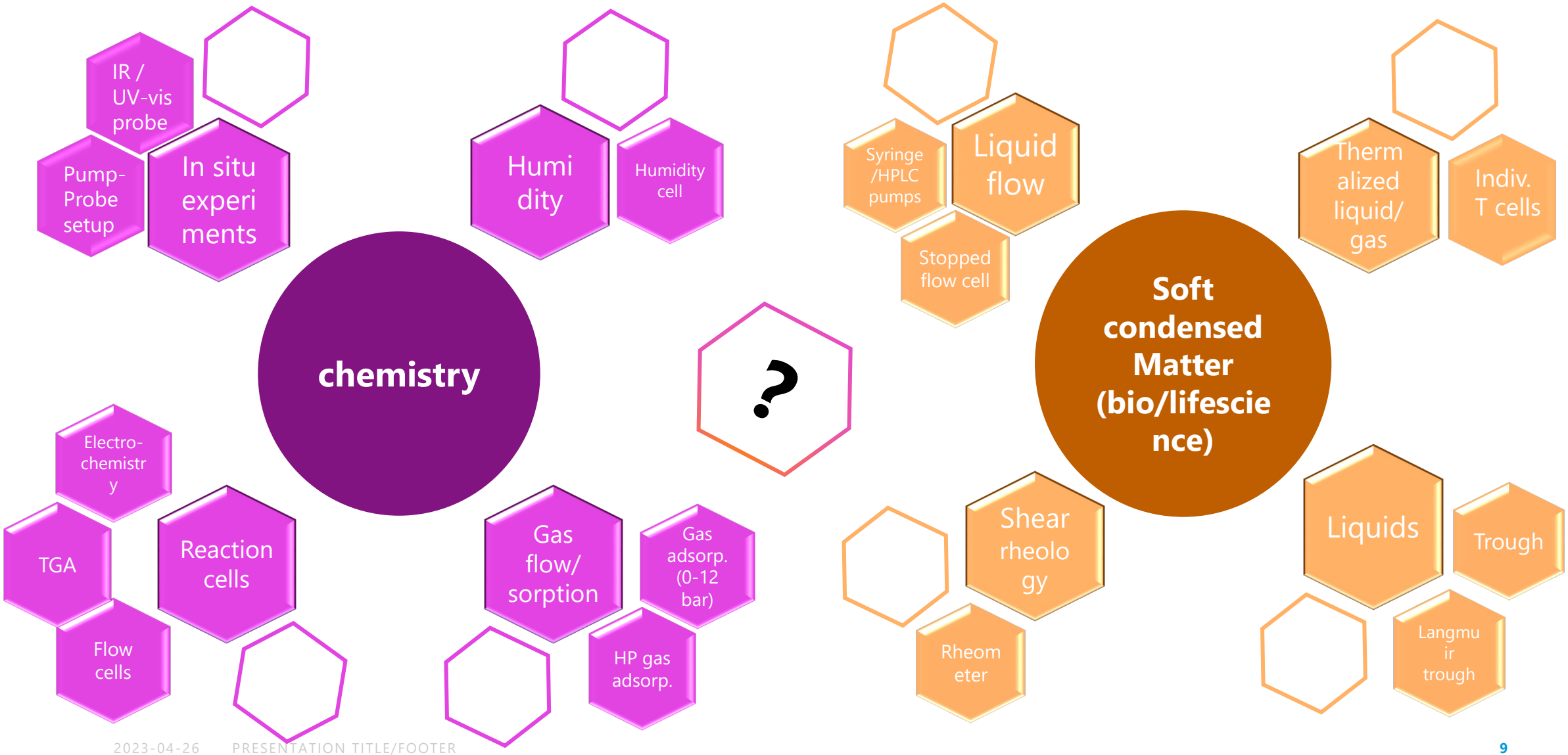


DEMAX:
-'organic' chemistry covered *(excl. polymer and peptide synthesis)*
-inorganic materials, e.g. lead salts for battery research started

SULF:
- chemical synthesis covered (inorganic, organic, hydrothermal, solid state)
- analytical equipment:
  - Spectroscopy (UV/VIS, RAMAN, FTIR, DLS)
  - Diffraction (XRD powder & single crystal)
  - Elemental analysis (XRF, ICP-OES, CHN)
  - Microscopy (optical, SEM)
  - Thermal (DSC low/high temp, DTA/TG)
  - Gas adsorption (BET/ HP-adsorp)
  - Sample prep for analysis (microwave/ fusion furnace)
  - Cutting, polishing

Soft matter and Chemistry Sample Environment

Provide sample environment systems and devices for:



SCSE – STATUS OVERVIEW

In-Kind and In-House

	Sample Environment System (SES)	Design/select	Test/adapt I	Software integration	Test/Adapt II	Adapt on instrument
LOKI	Stopped-flow cell	Done		On going		
Spec./ Diff.	Isorb gas sorption High pressure	Done				
Spectro	Laser pump probe	Done	At ESS Q3 2023			
POOL	Humidity chamber	Done	At ESS Q3 2023			
POOL	Humidity Generator	Done		On going		
POOL	2 EC/Battery cells	Done	At ESS Q3 2023			
Reflect.	Troughs (various)	plan				
SANS	Rheometer	Done		On going		
SANS	Huginn cuvette rack	Done		Done		
POOL	Syringe pumps	Done		Done		Documen-tation
POOL	HPLC pumps	Done		Done		Documen-tation
POOL	Potentiostat	Done		1st level		
POOL	Julabos	Done		done		Documen-tation

Design/select (manufacture/procure) → Test/adapt I → software integrate → Test/adapt II → Adapt on instrument

SCSE – STATUS OVERVIEW

Instrument budget and Instrument grant

	Sample Environment System (SES)	Design/select	Test/adapt I	Software integration	Test/Adapt II	Adapt on instrument
LOKI	Thermoslistated sample changer for quartz cuvettes (part of SANS Mag)	Done				
LOKI	Cell tumblers/rotating sample holders (Part of SANS mag)	Done				
DREAM	EC/Battery cell	Ongoing				
ODIN	EC/Battery cell					
DREAM	TGA					
LOKI	Flow cell (including HPLC pumps, Part of the NURF for LOKI)	Done		Done		
LOKI	In situ spectroscopic measurements for the flow cell (NURF for LOKI)	Done				
Reflect.	Solid liquid cell	Done				
SANS	Flexiprobe	Done				

Design/select (manufacture/procure) → Test/adapt I → software integrate → Test/adapt II → Adapt on instrument

Finish presentation