Interface to Science I2S

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Summary

1. I2S – Interfaces to Science in CLS
2. Mission and brief history of how we got to where we are today
3. The way to First Science and towards steady state operations
4. Status and plans for soft matter/life science laboratories and sample environment
5. Solid-liquid cell in-kind project (UU) and in-situ ellipsometry/FTIR (LiU) collaborations

I2S – Interfaces to Science in CLS

Strategy and interfaces in Chemistry, Soft Matter & Life Science

Melissa Sharp
NSE/SANS, Soft Matter

Work with all stakeholders to:

Capture scientific requirements and efforts

Create a strategy/prioritisation for:

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

Update scientific requirements for CLS support

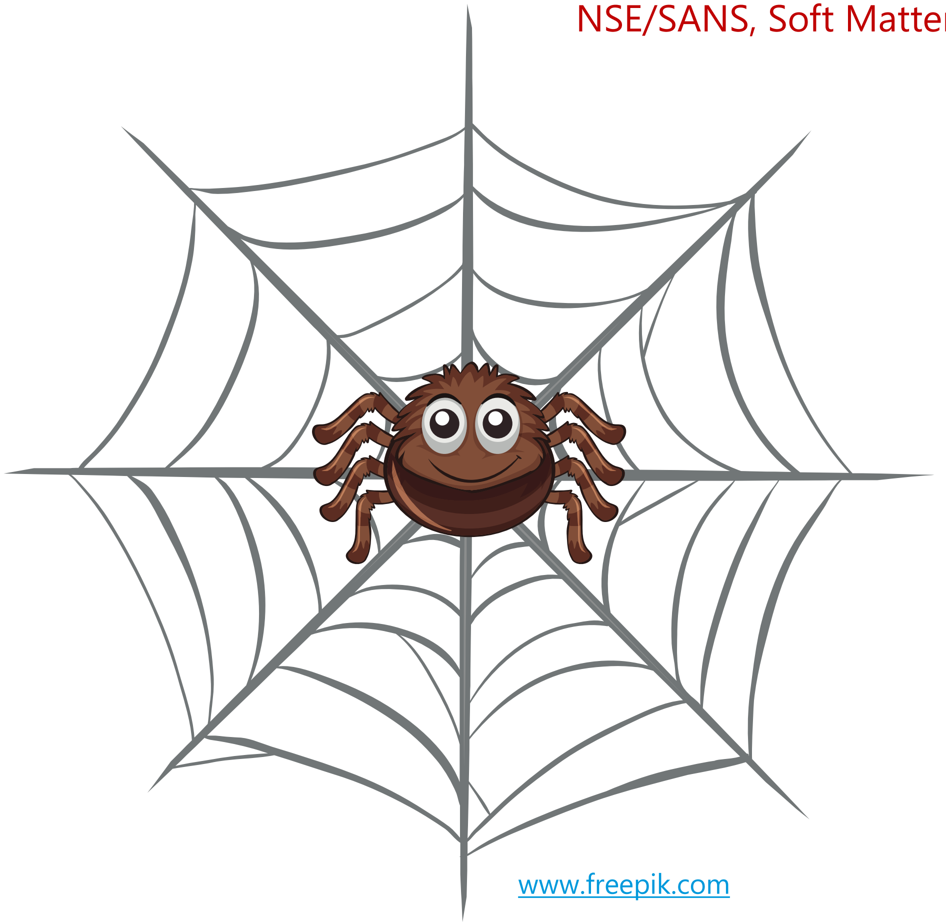
Liase with external stakeholders

Leverage synergies with other actors

e.g. in context of grant applications

Bring together projects and expertise in CLS, MPS, instruments and external projects

Develop common understanding of needs and how they can be met



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Friendly “spider-in-the-web”

Mission and short history

CLS support (DEMAX, SCSE, SULF) for neutron science at ESS

Mission:

From SAD mission statement: delivers the scientific and technical laboratories and sample environments to support the needs of the user program to enable research using neutrons in *chemistry, soft matter and life sciences.*

Prioritisation based on:

(i) the ESS science drivers, ensuring topical balance and addressing ESS-specific challenges

(ii) the construction schedule for the instruments

(iii) facility-wide integration aiming for streamlined user operation and most efficient use of beam time

Where we are today:

CLS formed in 2023 – coordination of support in chemistry, life science and soft matter

MPS supports materials engineering and physics experiments

History: SSS WP delivered by SAD

Organised in platforms, later groups.

Interfaces to NID by single instrument contacts.

Emphasis on integrating 'readily-available' equipment provided as in-kind contributions. 'Highly-specialized' equipment is provided via facility- or   university-based expert groups.

The way to First Science and steady state ops

Strategy for supporting chemistry, soft matter and life science

Develop a common understanding of what these steps entail and include

Bring together CLS, MPS, instruments and external projects

Update scientific requirements for CLS support

Support for:
World leading science
Partnerships
Science Village
Industry

2025->

First science

24/7 essentials for common types of experiments

2027->

First proposal call

Support instruments coming online:

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

2028 ->

Towards steady state

- Advanced characterisation and sample prep facilities
- in-situ techniques
- automation!

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…

Prioritisation important for First Science and beyond

Labs: Create a strategy and plan for funding missing items for First Science

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

2. Map out requirements of instruments, status and plans for all projects

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)

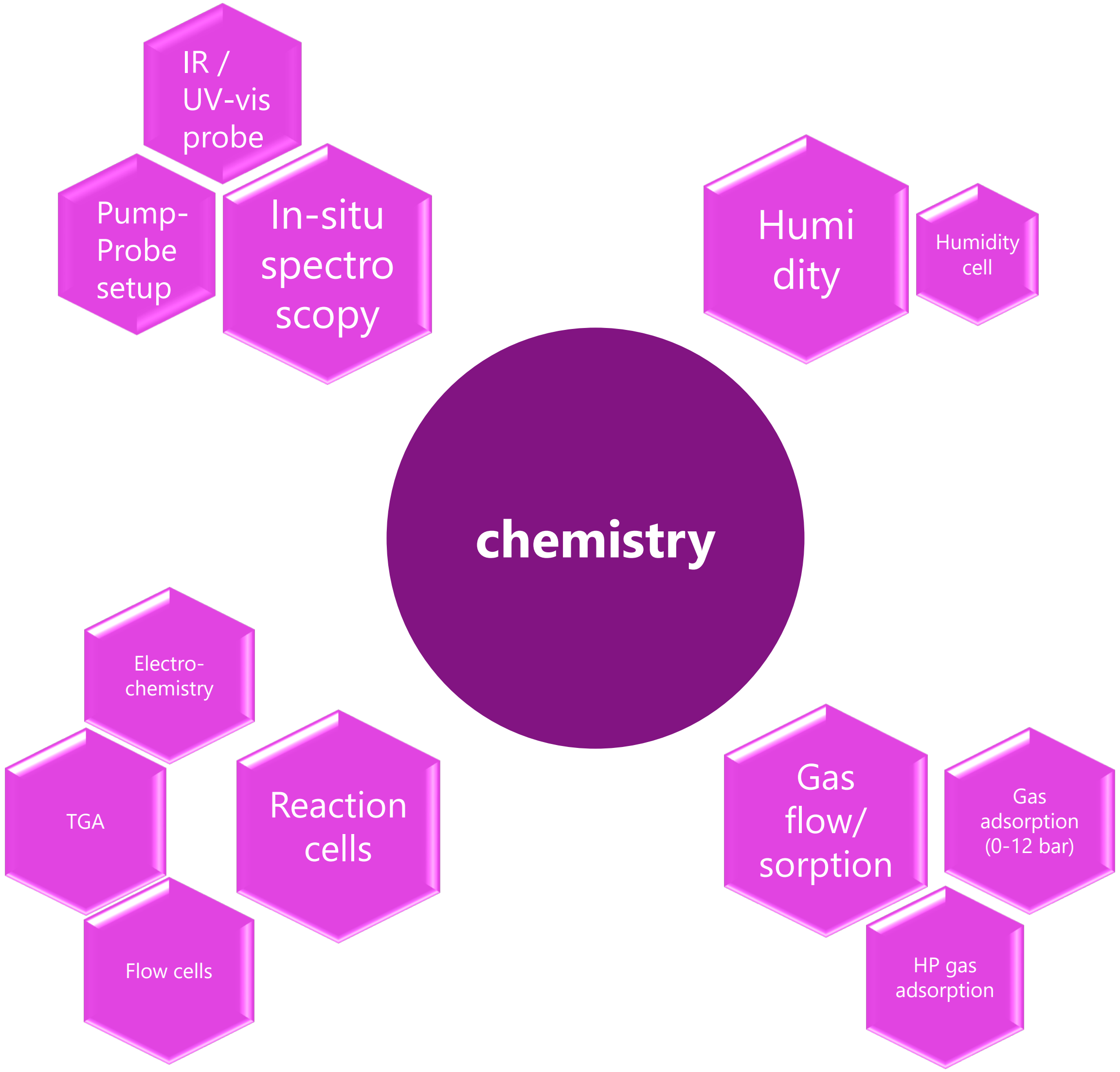
Diffraction/Imaging

- NMX ambient/cryogenic/humidity env.

what other SE is used for Soft/Bio samples?

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

Solid-Liquid Cells

ESTIA scope + project SREss3 from Tillväxtverket (Adrian Rennie, Uppsala University)

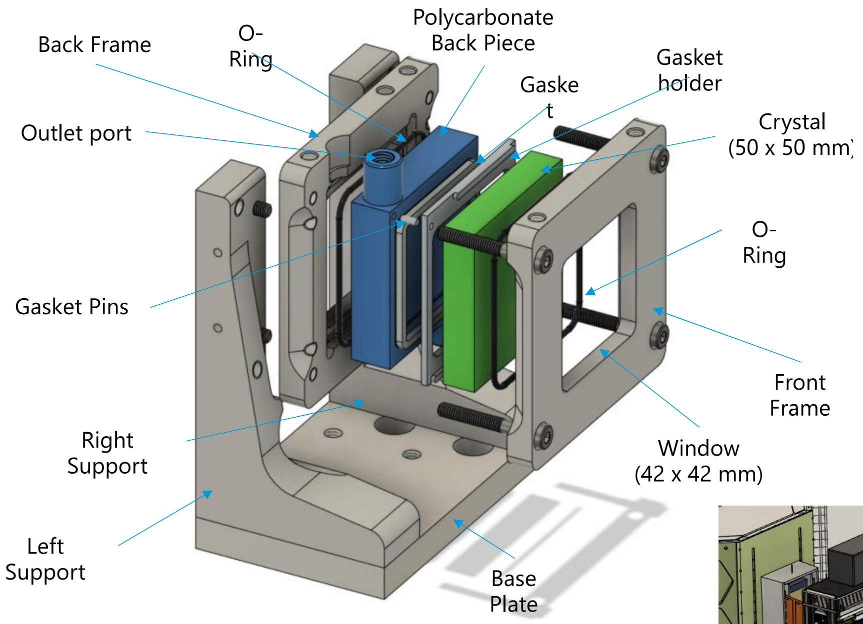
Main characteristics of the cell & changer:

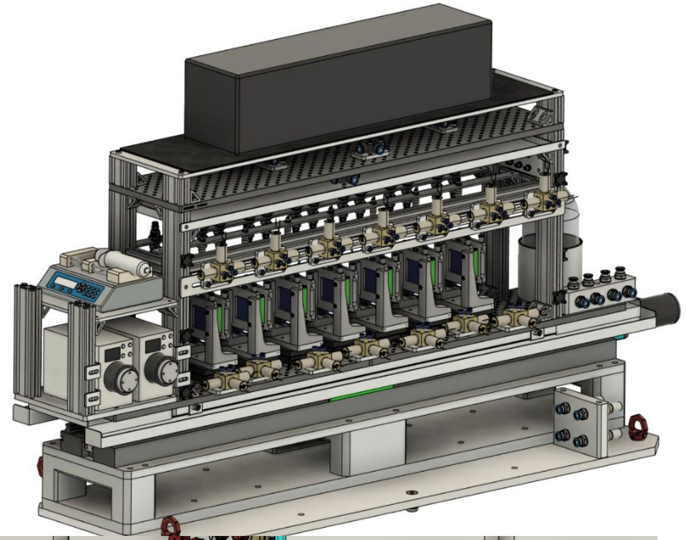
- *Compatible with both FREIA and ESTIA*
- *Low internal volume*
- *Transparent window on both sides (relevant for experiments requiring exposure to light, or SANS*)*
- *Changer can accommodate 7 cells, allows them to be filled from top or bottom using HPLC pump or 2 syringe pumps*
- *Water bath temperature control*

Collaboration between Tom Arnold (FREIA), Hannah Burrall (UU), Hanna W-K (CLS) and ESTIA (Alessandra Luchini -> University of Perugia).

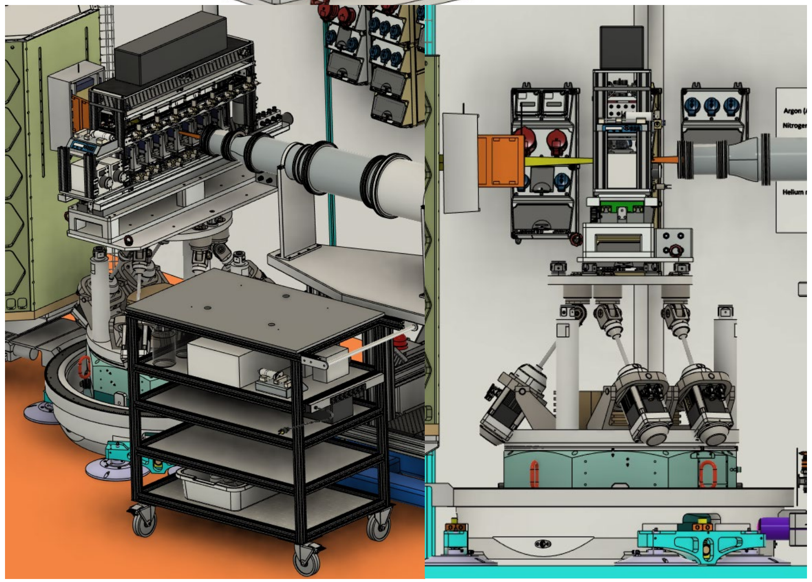
Prototypes ordered from local workshop, test beamtime at PSI in June.

** with transparent trough (Quartz, sapphire)*





Desing for FREIA frames/sample changer carried out in parallel.



Multi-channel Solid-Liquid Cells

Nordforks postdoc project (Nico Paracini, Malmö University -> FIGARO @ ILL)

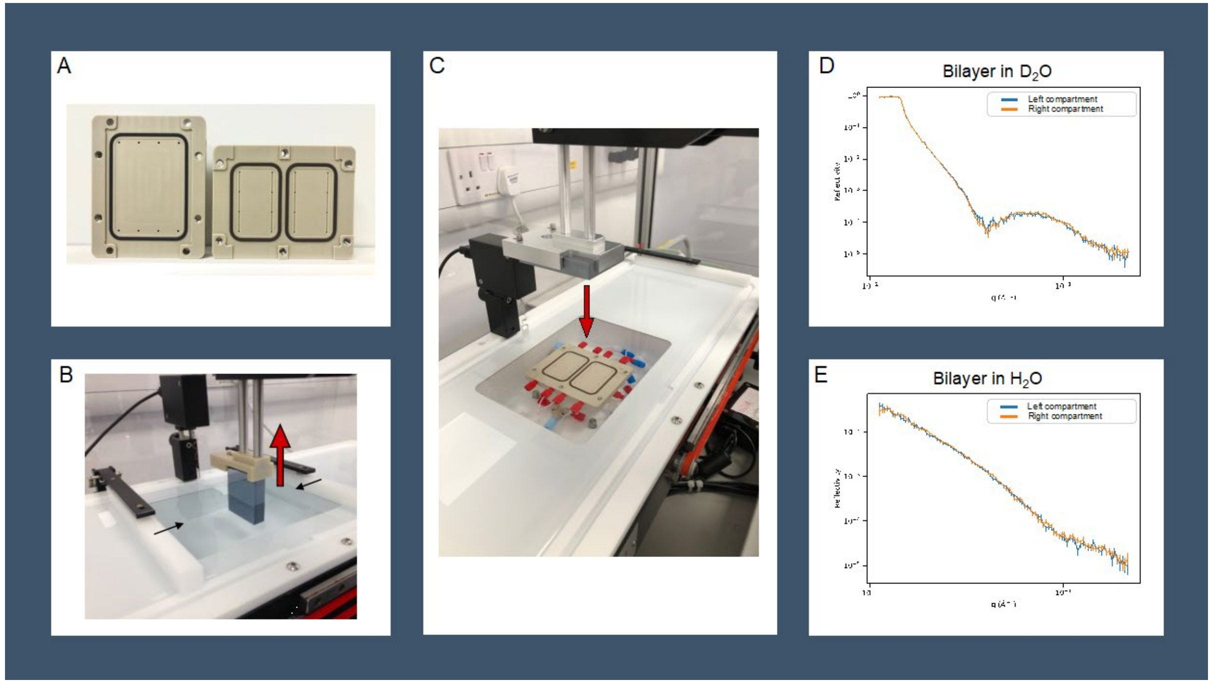
SPLICS** - **Scientific application:

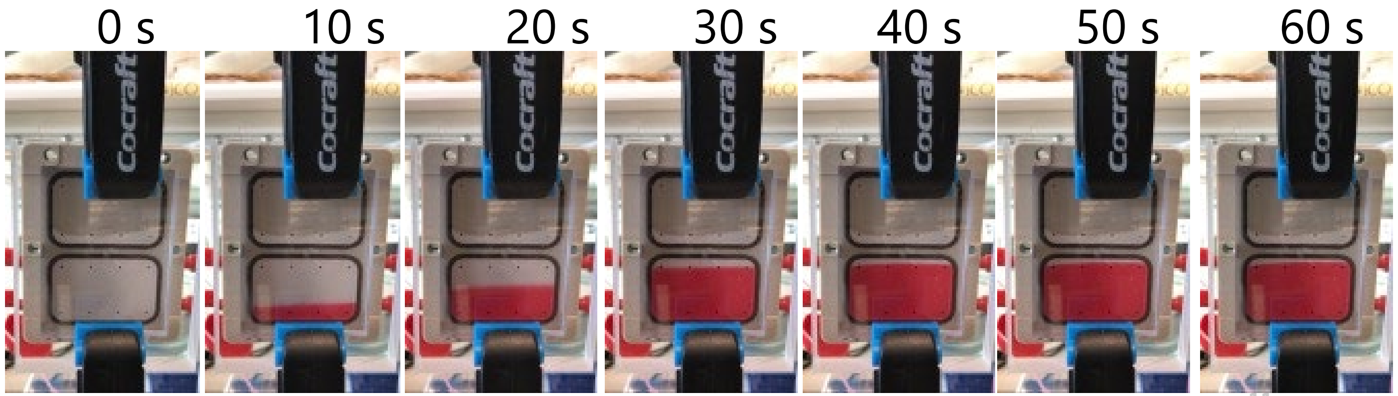
Monitor two different conditions (etc. temperature, pH, ligand) on the sam e(LB/LS) sample or on two different samples formed in-situ.

Relevant for ESTIA & compatible with solid-liquid cell changer

With the small beam available on ESTIA, SPLICs enables to investigate two different samples within the same cell. This will increase the number of samples that can simultaneously be placed on the sample stage.

Prototypes ordered from MV with UU solid-liquid cells.

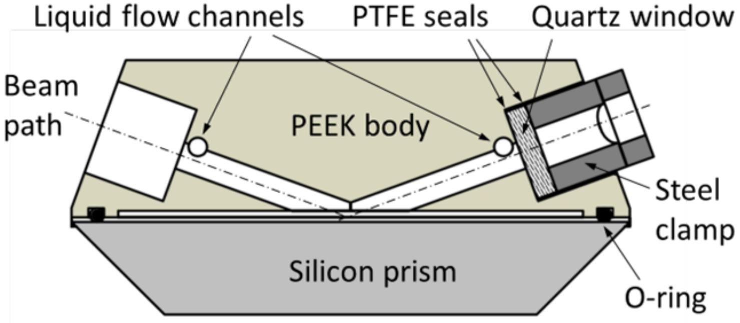


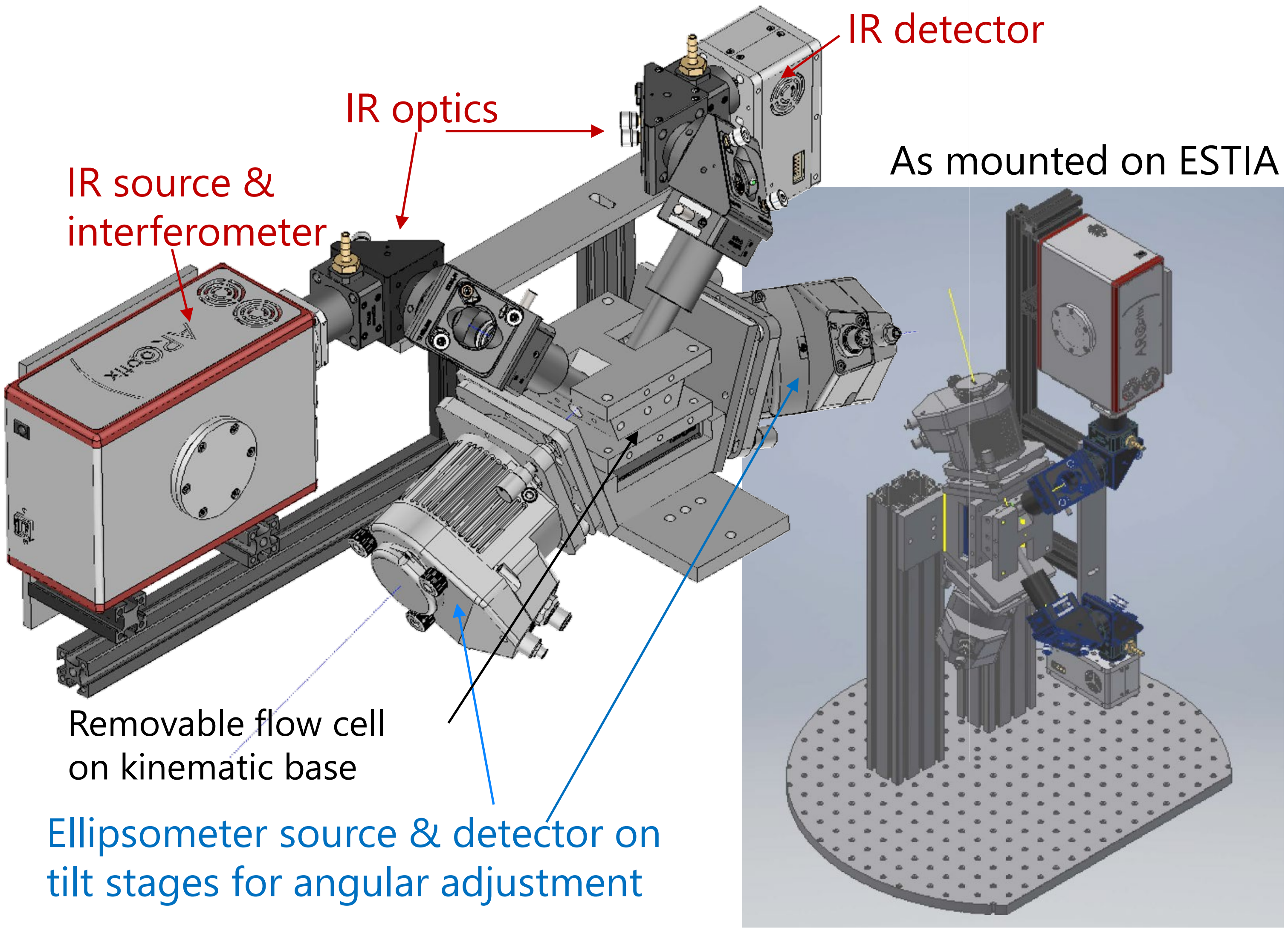


A combined IR and ellipsometry setup

As part of project SREss3 from Tillväxtverket (Thomas Ederth, Linköping University)

- *Builds on an existing Röntgen-Ångström Cluster (RÅC) project*
- *Adapting the design of existing equipment at Liu to be compatible with both ESS reflectometers*
- *Includes design to allow sample changer (translation change) i.e. change sample without moving the optics.*





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