



**EUROPEAN
SPALLATION
SOURCE**



Science Day 2021

Welcome and Introduction

June 2nd, 2021

PRESENTED BY ANDREAS SCHREYER

2021-06-02

Science Day 2021

A well-established forum to exchange on our scientific collaborations



Previous Science Days

- 2020: no science day ...
- 2019: <https://indico.esss.lu.se/event/1245/>
- 2018: <https://indico.esss.lu.se/event/990/>
- 2017: <https://indico.esss.lu.se/event/821/>
- 2016: <https://indico.esss.lu.se/event/564/>
- 2015: <https://indico.esss.lu.se/event/305/>
- 2014: June 10, Borgeby Castle, Bjärred
- 2013: May 16 and Oct 17, High Court, Malmö

Science Day 2021

A well-established forum to exchange on our scientific collaborations



Agenda 2021

- 2. June 2021 ; zoom video conference format
- <https://indico.esss.lu.se/event/2699/timetable/#20210602>
- 4 x 3 science talks (20min) by junior scientists
- covering many scientific topics are reflected by different SFTs
- inspires exchange and strengthens collaboration cross-discipline
- increases visibility for science using neutrons
- one day a year: science beats project
- however...

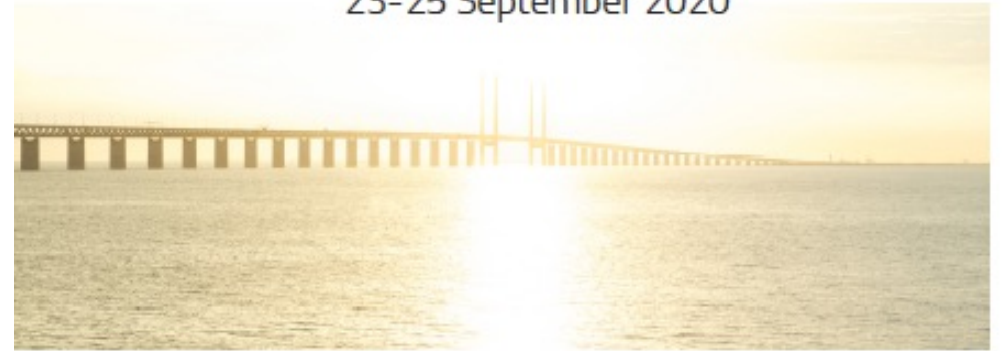
09:00	Andreas Schreyer: Zoom 09:00 - 09:30
	Josefin Martell: Neutron tomography in planetary science/water in Martian meteorites Zoom 09:30 - 09:50
10:00	Andrew McCluskey: Accurate uncertainty quantification and model selection for in-silico diffusion Zoom 09:50 - 10:10
	Sophie Ayscough: An investigation of the role of alkanes in cyanobacterial membranes Zoom 10:10 - 10:30
	Coffee break Zoom 10:30 - 10:45
	Emelie Wiklund & Anton Järild: Luminescence Materials for the ESS target Zoom 10:45 - 11:05
11:00	Manuel Morgano: Visualization of engineered residual strain in additive manufacturing materials Zoom 11:05 - 11:25
	Blahoslav Rataj: Simulation Studies for the ANNI beamline Zoom 11:25 - 11:45
	Lunch break Zoom 11:45 - 13:00
12:00	
13:00	Sofie Janas: Classical Spin Liquid or Extended Critical Range in frustrated antiferromagnet YMnO3 Zoom 13:00 - 13:20
	Swati Aggarwal: Towards Neutron crystallography of membrane proteins Zoom 13:20 - 13:40
	Mikhail Feygenson: Unravelling Magnetic Nanochain Formation in Dispersion for In Vivo Applications Zoom 13:40 - 14:00
14:00	Coffee break Zoom 14:00 - 14:30
	Johan Cedervall: High entropy alloys – magnetism and neutron diffraction Zoom 14:30 - 14:50
15:00	Pedro Leonidas Oseliero Filho: USING WIDE- AND SMALL-ANGLE X-RAY SCATTERING TO INVESTIGATE THE THERMOTROPIC BEHAVIOR OF EXOGENEOUS PULMONARY SURFACTANTS Zoom 15:10 - 15:30
	Sze Chun Yiu: The NNBAR experiment for the ESS Zoom 15:10 - 15:30
	Arno Hiess: Way forward for Science Zoom 15:30 - 15:45



ESS-ILL User Meeting

ESS ILL User Meeting 2020

Lund, Sweden
23-25 September 2020



Welcome to the second ESS ILL User Meeting

- Plenary talks about using neutron science to meet societal challenges
- Reports on recent achievements and ongoing work at ESS and ILL
- Focused parallel sessions on specific areas of neutron science

neutrons4europe.com



Bi-annual ESS-ILL user meetings



#1 10-12 October 2018, Grenoble

hosted by ILL

Focus sessions

- Scientific Potential for Combined or In-Situ Neutron Spectroscopy
- Laue Diffraction for Biology
- Laue Diffraction for Materials
- Spectroscopy in Biological Systems
- Imaging



Credit: Marie Ramparany, ILL

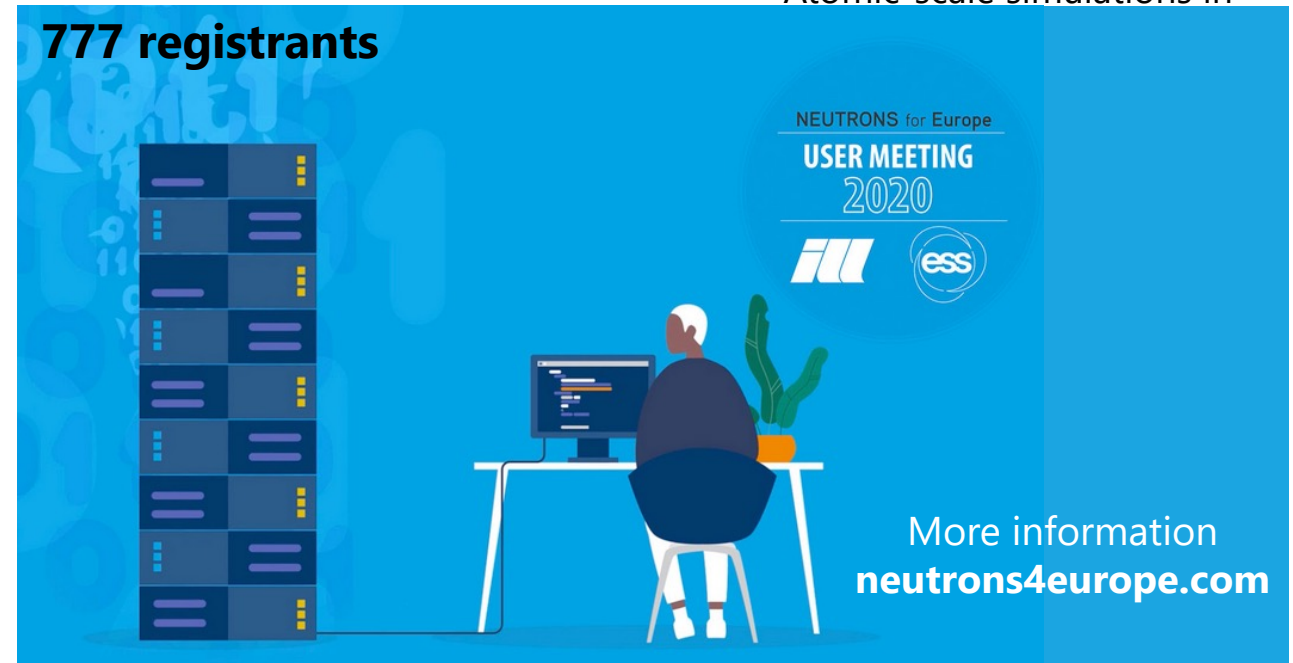
#2 23-25 September 2020, online

Jointly hosted by ESS and ILL

Topical workshops in Oct./Nov.

- ESS - ILL Topical Workshop on Fundamental and Particle Physics
- ESS - ILL Topical Workshop on Imaging, Materials and Engineering
- ESS - ILL Topical Workshop on Chemistry and Magnetism
- ESS Polarisation Workshop
- GISANS Meeting
- ESS - ILL Topical workshop on Atomic-scale simulations in

777 registrants



The next physical joint user meeting will be hosted by ESS in Lund in 2022

ESS/ILL Topical Workshop on Chemistry and Magnetism

13. October 2020,

<https://indico.ess.lu.se/event/1542/>



Zoom Webinar

a quantum liquid of magnetic octupoles

s, comparison to predictions for QSI monopoles ('two spinon contin...

212 registrants

Lingjia Shen (Lund Univ...)

Page 15

2021-06-02 PRESENTATION TITLE FOOTER

	Introduction: Link to the meeting; https://ill.zoom.us/j/94763977623?pwd=V2REeW5QOXFkZkUxV1JlVkdQUVNFQT09 Please note that the zoom public link directs you to a page where - if you don't already have a Zoom account in use - yo...
	Manila Songvilay, Institut Neel, CNRS, Grenoble. From one- to two-magnon excitations in the S = 3/2 magnet β -CaCr ₂ O ₄
10:00	09:30 - 10:05
	Lingjia Shen (Lund University). Hidden quantum critical point in SrCo ₂ V ₂ O ₈
	10:05 - 10:40
	Break
	10:40 - 11:00
11:00	Romain Sibille (PSI). Octupole ice in Ce ₂ Sn ₂ O ₇ quantum spin liquid
	11:00 - 11:35
	Matthew Coak (Warwick University). Tuning dimensionality, magnetism and conduction in van-der-Waals Mott insulators
12:00	11:35 - 12:10
	Lunch Break
	12:10 - 14:00
13:00	
	12:10 - 14:00
14:00	Matthew Rosseinsky, (Liverpool University) . Design of Advanced Materials?
	14:00 - 14:35
	Eleonora Vottero, (University of Turin). Inelastic neutron scattering spectroscopy applied to supported metal nanoparticles in catalysis.
15:00	14:35 - 15:10
	Break
	15:10 - 15:25
	Werner Paulus, (Institut Charles Gerhardt Montpellier). LOW-T OXYGEN DIFFUSION PATHWAYS EXPLORED BY SINGLE CRYSTAL NEUTRON DIFFRACTION METHODS IN NON-STOICHIOMETRIC OXIDES.
	15:25 - 16:00
16:00	Pascal Launois, (University of Paris Sud). SPECIFIC WATER STRUCTURE IN A GEO-INSPIRED NANOTUBE AND INTERRELATED DYNAMICS.
	16:00 - 16:35

ESS/ILL Topical Workshop on Imaging, Materials and Engineering

14./15. October 2020, <https://indico.esss.lu.se/event/1506/>



WEDNESDAY, 14 OCTOBER	
13:30 → 13:45	Instrument Updates: Engineering Diffractometers
13:30	SALSA Update 10m Speaker: Thilo Pirling SALSA@ILL 2020
13:40	BEER Update 5m Speaker: Premek Beran BEER@ESS reminder
13:45 → 14:45	Materials Science and Engineering - Overviews & General
13:45	Neutron diffraction in material science 30m Speaker: Martin Sahlberg
14:15	The Common Calibration Protocol and Neutron Quality Label for Neutron Strain Scanning instrumentation 30m Speaker: Ranggi S. Rhamadan Common Calibratio...
14:45 → 14:55	BREAK 10m
14:55 → 16:25	Materials Science and Engineering - Studies & Applications
14:55	Measurement of strain during fatigue crack growth by stroboscopic neutron diffraction 20m Speaker: Molly Probert
15:15	Development of new approaches for neutron diffraction 3D strain mapping in aluminium additive manufactured materials 20m Speaker: Anastasiia Mikheenkova
15:35	Residual stress measurement in dissimilar metal joints using neutron diffraction 20m Speaker: Taneshan Sapanathan Stress in metal joints
15:55	Studying granular mechanics with neutron diffraction 20m Speaker: Stefanos Athanasopoulos Granular mechanics

THURSDAY, 15 OCTOBER	
13:00 → 13:20	Instrument Updates: Imaging Beamlines
13:00	NEXT Update 10m Speaker: Alessandro Tengattini
13:10	ODIN Update 10m Speaker: Aureliano Tartaglione, Manuel Morgano
13:20 → 14:50	Neutron Imaging - Overviews & General
13:20	Advanced imaging methods 30m Speaker: Nikolay Kardjilov
13:50	Cultural heritage metal artefacts tackled by neutron imaging and scattering 30m Speaker: Francesco Grazzi
14:20	Open source neutron imaging software 30m Speaker: Anders Kaestner Analyzing_NL_Data_...
14:50 → 15:00	BREAK 10m
15:00 → 16:30	Neutron Imaging and Diffraction - Studies & Applications
15:00	Bragg-edge imaging reveals local texture variations in additive manufactured samples 20m Speaker: Victor Manuel Pacheco Gimon
15:20	Neutron diffraction and imaging on battery systems 20m Speaker: Anatolij Senyshyn
15:40	Monitoring Li-ion batteries by advanced operando neutron techniques 30m Speakers: Claire Villeveille, Sandrine Lyonnard
16:10	Results from the GeoArchaeology try-out workshop 20m Speakers: Björn Nilsson, Burkhard Schillinger

ESS/ILL Topical Workshop on Imaging, Materials and Engineering

14./15. October 2020, <https://indico.ess.lu.se/event/1506/>



Recording

Participants (129)
Panelists (12) Attendees (117)
Find a panelist

Introduction

Contrast mechanisms + Time + Multi-Modes

	Diffraction	Phase	Magnetic	Attenuation
Metals	Strains	Phase transitions	Internal defects	Magnetic fields
Hydrogen in metals				Water uptake in plants
Device inspection: particle filters				Monolith Soot
Bone structures				Corrosion
Li transport in batteries				

Contrast mechanisms length scales: Å, nm, μm, mm, cm

Applic. Energy Storage Cultural Heritage Magnetism Hydrogen Metals

356 registrants

Nikolay Kardjilov, ESS - ILL Topical Workshop on Imaging, Materials and Engineering

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Q&A

Open Answered(1) Dismissed

AH Alan HEWAT 01:28 PM
Two very nice summaries of instruments that should start work in 2022. It is fascinating to see ILL competing with the two leading imaging labs, PSI and TUM at ESS. Thank you Alessandro and Aureliano. What will be the main advantages and disadvantages of ODIN vs NeXt-2? Constant wavelength vs Pulsed operation? Intensity? Resolution? Special techniques with wavelength selection?

Alessandro 01:34 PM
The flux should be essentially comparable between the two instruments (since the ESS flux is thus far only simulated, so the exact comparison is not available yet), and as you say the main difference is pulsed vs constant flux, with the usual pros and cons of both. As for the spatial resolution I can answer for the ILL part, we are below 4μm and pushing for more in the upgrade, and temporal resolution ~1s tomography, and also pushing for more (in low resolution mode, of course)

To: Panelists
Type message here...

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Type message here...

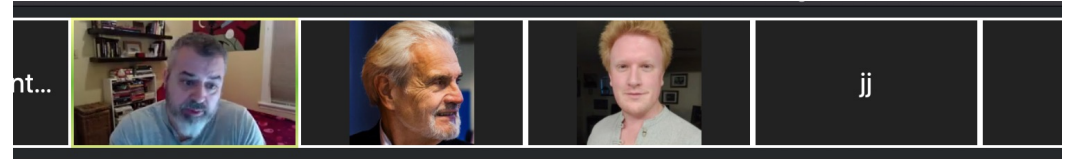
ESS/ILL Topical Workshop about Fundamental Physics



14. October 2020, <https://indico.ess.lu.se/event/1507/>

13:00	→ 13:10	Introduction Speaker: Valentina Santoro santoro.pdf	10m	
13:10	→ 13:35	The ESS neutrino Super Beam Design Study (ESSnuSB) and the High Intensity Frontier Initiative (HIFI) Speaker: Tord Ekelof (Uppsala University) ESSnuSB-HIFI pres...	25m	
13:35	→ 14:00	Coherent Elastic Neutrino-Nucleus Scattering at the European Spallation Source Speaker: Juan Collar ESS_CEVNS_Collar...	25m	
14:00	→ 14:25	New platforms for ultra cold neutron production: SuperSUN and beyond Speaker: Skyler Degenkolb 20201014_ILL-ESS...	25m	
14:25	→ 14:50	Neutron Beam EDM Experiment Speaker: Florian Piegsa piegsa_ess+ill.pdf	25m	
14:50	→ 15:05	Virtual Coffee Break	15m	
15:05	→ 15:30	Sterile Neutron Searches at ORNL Speaker: Leah Broussard ESS-ILL workshop ...	25m	
15:30	→ 15:55	The HIBEAM and NNBAR experiment Speaker: David Milstead (Stockholms Universitet) hibeam-ess-ill-ws-s...	25m	
15:55	→ 16:20	Antineutron optics Speaker: William Snow (Indiana University) nnbartalkWMESS...	25m	
16:20	→ 16:35	A combined paper on fundamental physics possibilities at ESS? Speakers: David Milstead (Stockholms Universitet), Valery Nesvizhevsky 2021-06-01 ESS overview paper...	15m	

66 registrants

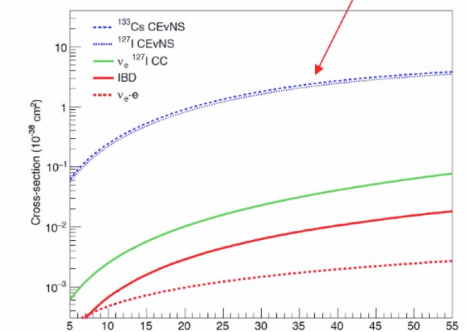


CEvNS: the advent of "miniature" neutrino detectors



CEvNS has largest ν x-section

The catch: low-E NRs are the only detectable signature



ESS/ILL topical workshop on Atomic-scale simulations in NS



20./21 January 2021 (<https://indico.ess.lu.se/event/2411/>)

Wed 20/1

13:00	Welcome		13:00 - 13:15
	Unraveling water dynamics and restructuring upon α -synuclein fibril formation by neutron spectroscopy and molecular dynamics simulations	Dr. Kevin Pounot	
	Short-time diffusive dynamics of proteins in a naturally crowded environment	Hender Lopez-Silva	13:40 - 14:05
14:00	Sucrose and trehalose as agents of protein stability: a systematic molecular dynamics simulations	Dr. Inna Ermilova	
	Structure and Dynamics of Huntingtin. A Segmental Labelling Approach	Mr. Xamuel Loft Lund	14:30 - 14:55
15:00	Solution Structure of the Gloeobacter violaceus Ligand-Gated Ion Channel Probed by Small Angle Neutron Scattering	Marie Ly	
	Coffee Break		15:20 - 16:00
16:00	An investigation of 3He in C60: A DFT, theoretical and INS study	Mohamed Aouane	16:00 - 16:25
	Neutron scattering and MD simulation of protein-ligand interactions	Arianna D'Angelo	16:25 - 16:50
	Water dynamics in carbon nitride	Karolina Lisowska	16:50 - 17:15
17:00	THE STRUCTURE OF WATER IN CALCIUM-SILICATE-HYDRATES STUDIED BY NEUTRON DIFFRACTION WITH ISOTOPIC SUBSTITUTION.	Mrs. Zhanar Zhakiyeva	
	Neutron reflectivity and MD simulation study of ionic liquids and deep eutectic solvents at a solid electrode	Nebojsa Zec	
18:00			

Biology

Nano-particles & liquids

Thu 21/1

13:00	Enhancing refinement with quantum mechanics in neutron protein crystallography	Octav Caldararu	13:00 - 13:25
	New on-line DFT approach to analyse neutron diffraction crystallography and SANS data	Luigi Genovese et al.	13:25 - 13:50
14:00	Diffusive motions in a solvent free myoglobin-polymer hybrid revealed by neutron scattering and MD simulation	Yann Fichou	
	OpenMP Parallelized Neutron Scattering Experiments	Yanqin Zhai	
	Molecular modeling and neutron scattering experiments to investigate F10FAM microgels	Letizia Tavagnacco	14:40 - 15:05
	Coffee Break		15:05 - 16:00
16:00	A combined computational and experimental approach to studying structure-property relationships in complex oxide ion conductors	Chloe Fuller	
	Lattice dynamics and thermal conductivity in complex metallic alloys with atomic simulations in neutron scattering	Pierre-Francois Lory	
	Reproducing Anharmonicity in INS Measurements	Stella d'Ambrumenil	16:50 - 17:15
17:00	Tunable bonding in the incipient metal thermoelectric material	Dr. Simon Kimber	17:15 - 17:40
	Persistent homology for magnetism	Mr. Bart Olsthoorn	17:40 - 18:05
18:00	Closeout		18:05 - 18:30

221 registrants

Soft matter incl. Biology

Hard condensed matter

ESS ILL User Meeting 2022



First thoughts only

2018 (in person)

10-12 Oct (WE-FR, 3 days), Grenoble WTC, 500 participants

Programme: 5x plenary sessions (3x talks), parallel workshops (5x 2h), posters, exhibition

2020 (virtual)

23-25 Sept (WE-FR, 3 days), zoom, >700 main event participants, 70-350 workshop participants

Programme main event: 4x plenary sessions only (4x talks each); no poster sessions

Separate workshops: 4x scientific topics, 2x methodological topics; different format.

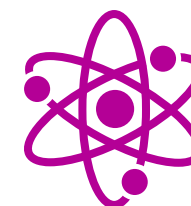
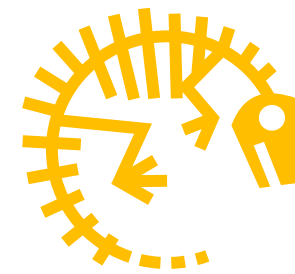
2022 (hybrid format: in-person in Lund, possibility for remote participation)

date and duration: 3 days (WE-FR) in September or October 2022

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Input welcome

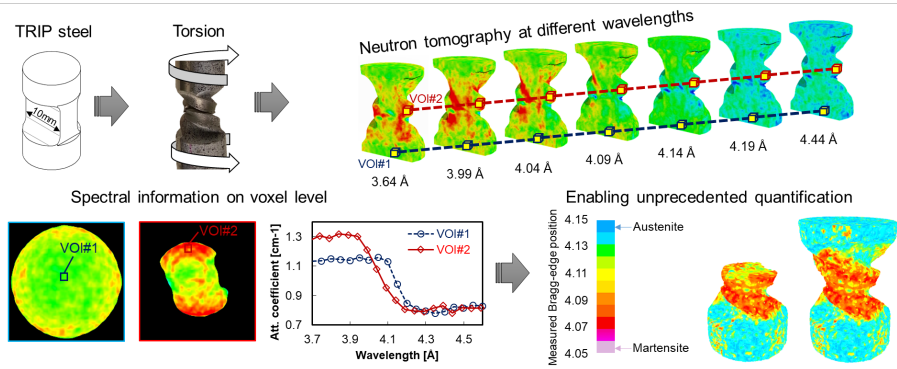
Science Output



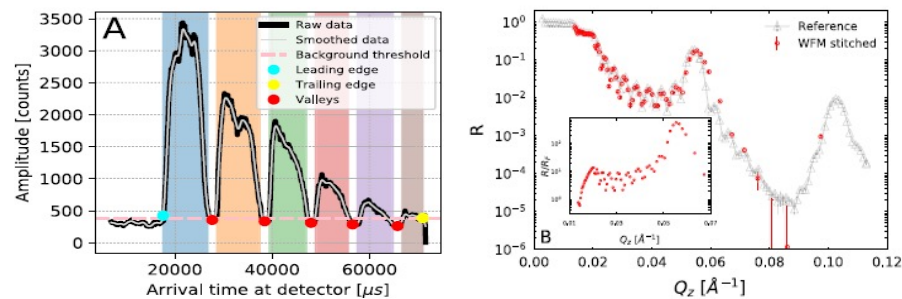
Neutron Instruments Division



Papers, PhDs, and Prizes!



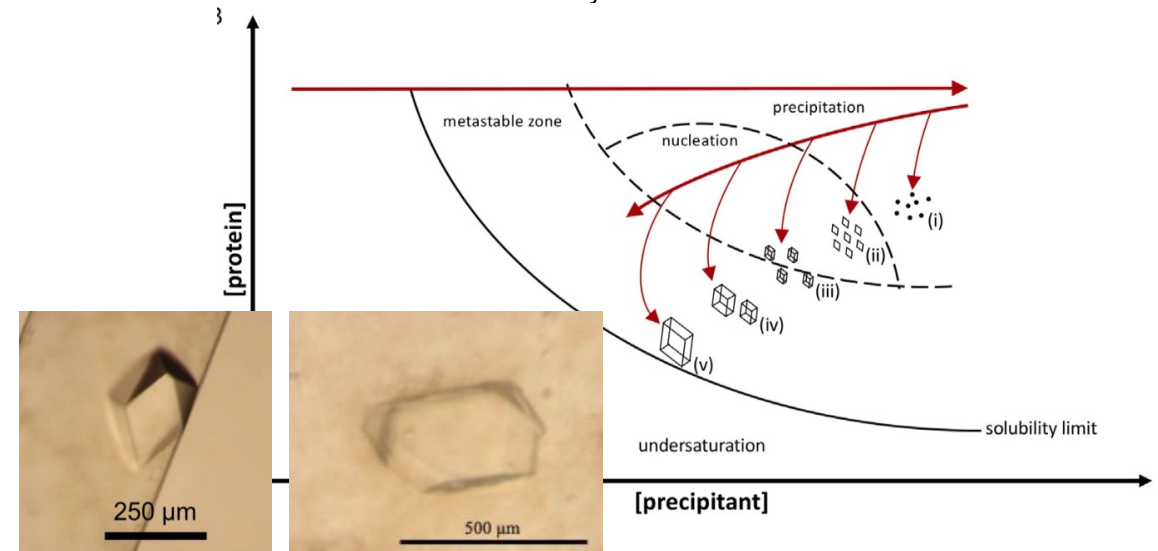
"Spectral neutron tomography" Tran, Woracek, et al, *Materials Today Advances*, 9 (2021)



"Wavelength frame multiplication for reflectometry at long-pulse neutron sources." Löhmann, et al, *Review of Scientific Instruments* 91 (2020)



German Materials Society Werner Köster Prize

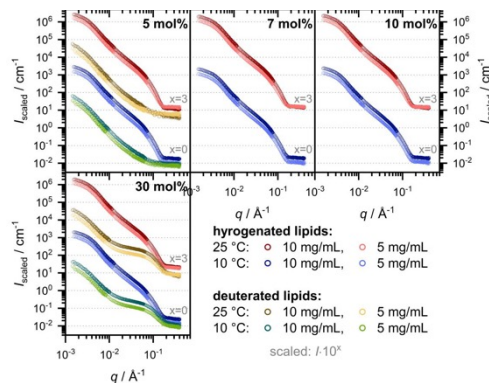


Sam Hjorth-Jensen PhD defence - Co-supervisor Esko Oksanen

User Science enabled by DEMAX proposals

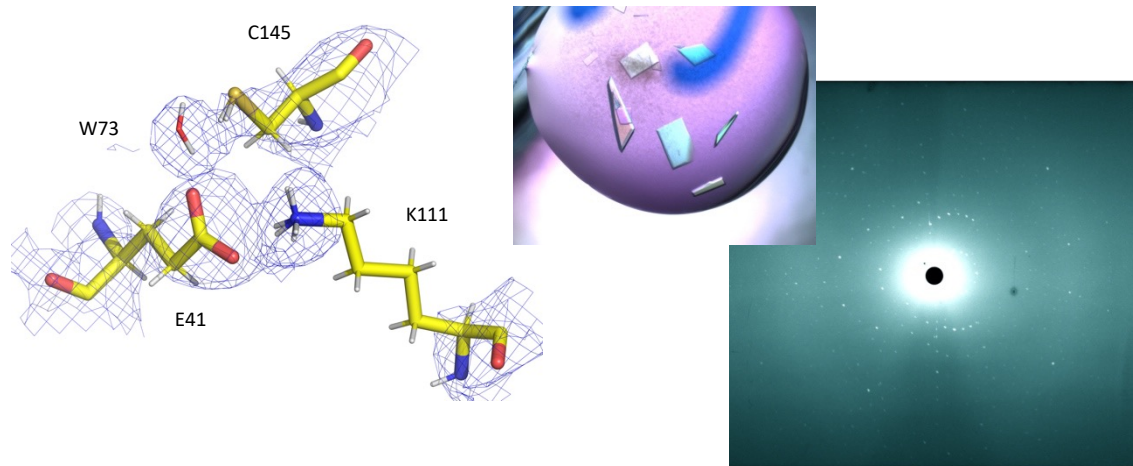
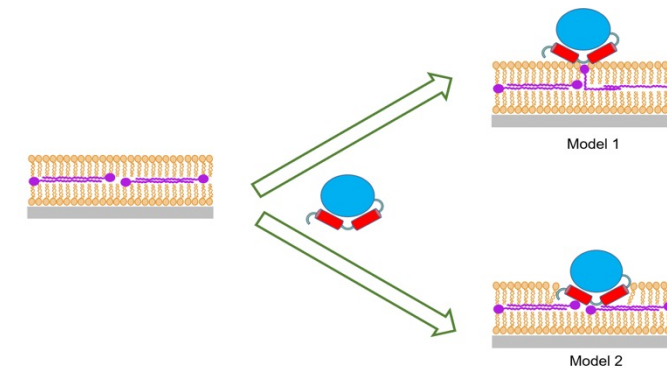


Effect of the saponins on hydrogenated and deuterated phospholipid membranes from yeast *P. pastoris* – SANS on D11 (ILL) Sep 2020.



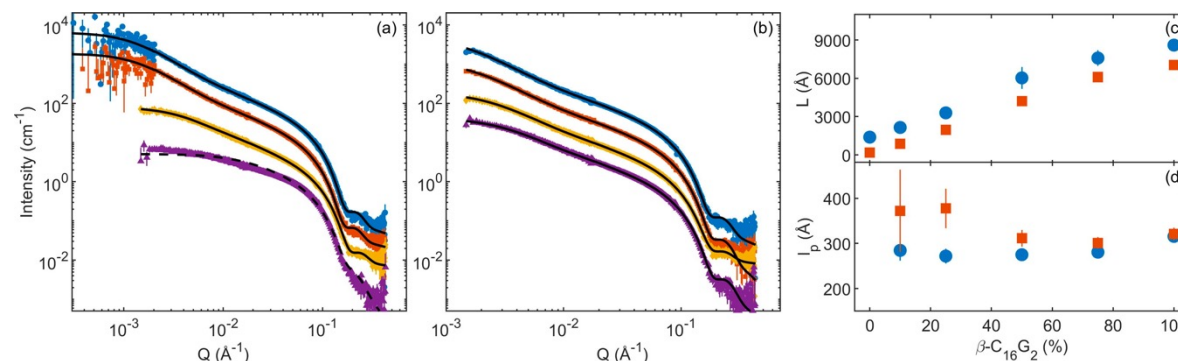
New insights into the interaction of Class II dihydroorotate dehydrogenases with ubiquinone in lipid bilayers as a function of lipid composition

d_{63} POPC used to resolve Q_{10} location in centre of bilayer - moves up to bind to enzyme



Large crystals of NitN amidase from Antarctic polyextremophile to study enzymatic mechanism; NPX data collected at LADI (ILL), X-ray data from BioMAX (MAX IV)

Molecular structure of maltoside surfactants controls micelle formation and rheological behavior; SANS data collected at D11 (ILL)



<https://doi.org/10.1016/j.jcis.2020.08.116>

Scientific Activities Division: Chemistry Services SULF



Work during C19 at E04 continues with masks and collaborations ...



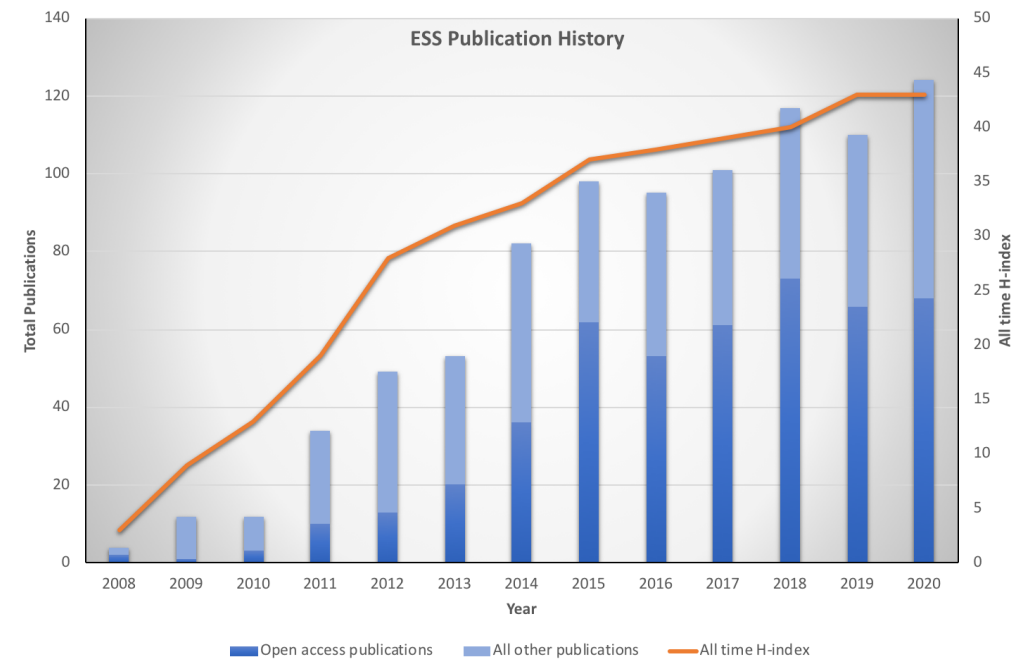
- + Preparing multi-annual framework for future fit-out of technical / scientific spaces in D04 and D08
- o Only few UK contractors back to finish E04 but accepting some delay on E03; D08 and D04 need to start.

Publication Report 2020

Tracking KPIs for the user programme

2020 – Number of Publications

- 124 publications in core collection Web of Science
- 68 published open access (several kinds)
- 67 publications include SD staff and affiliates
- Most cited ESS publication cited 355x up to now
- Most cited 2020 publication cited 22x already.
- Andersen, K. H. et al., The instrument suite of the European Spallation Source. Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment 957, 39, doi:10.1016/j.nima.2020.163402 (2020).



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2020 – Number of Publications and H-index

- 124 publications in core collection Web of Science
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- H-index: h papers have been cited at least h times.
- Indication of scientific impact
- All time H-index over all years for ESS is $h = 43$
- Asymptotic nature: each publication needs lot of citations

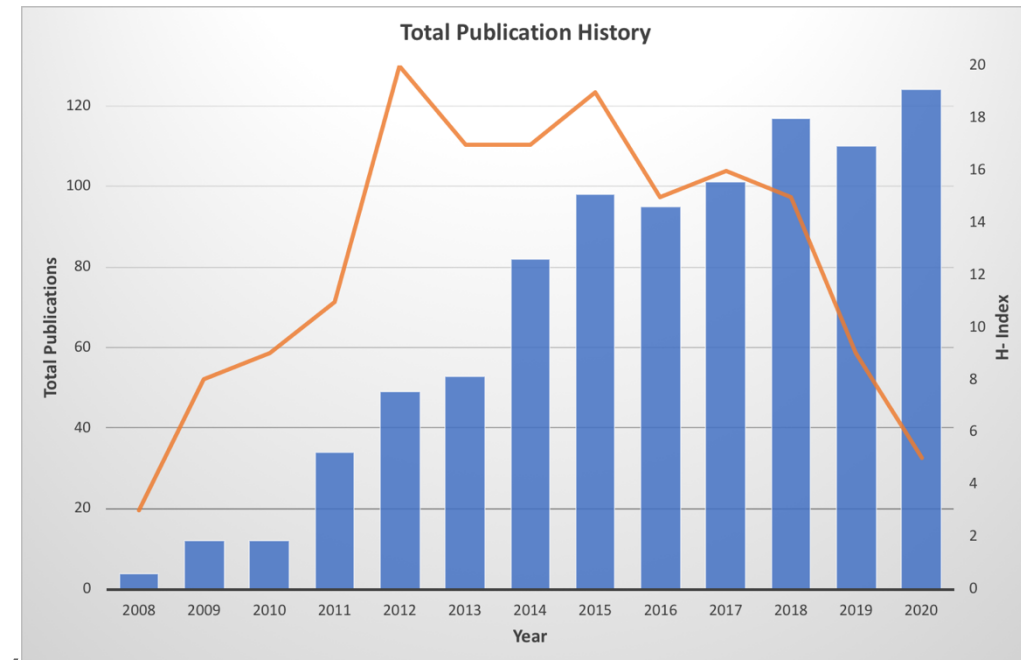
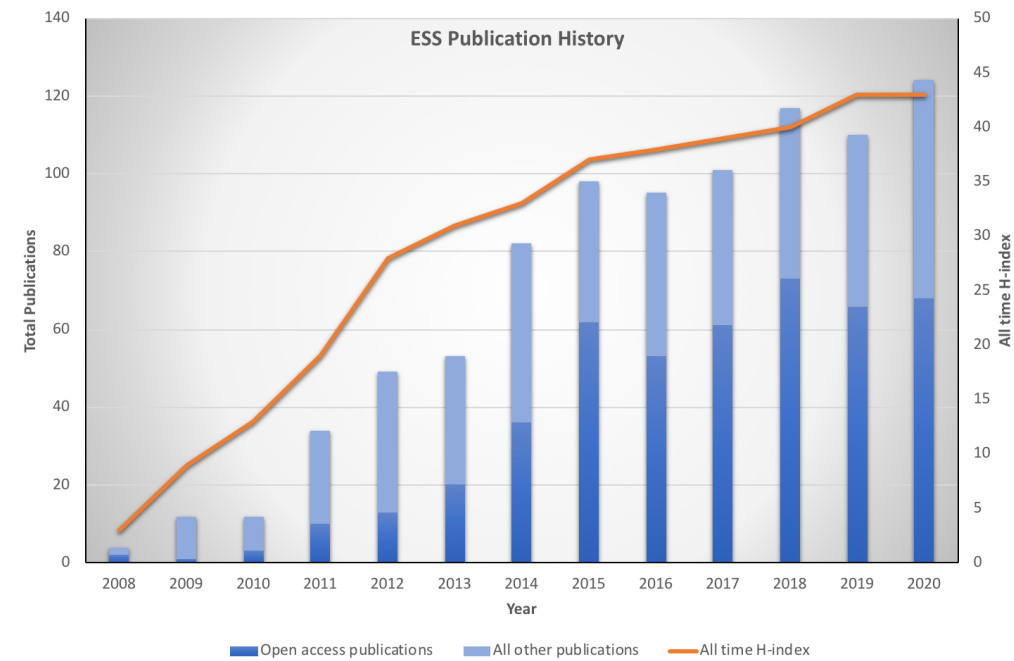


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- All time H-index over all years for ESS is $h = 43$
- Asymptotic nature: each publication needs lot of citations
- Annualized H-index: H-index resulting from publications in selected year
- Example: Today 17 out of the 53 publications from 2013 have been cited 17 times or more.
- Lag as H-index requires publications to be cited



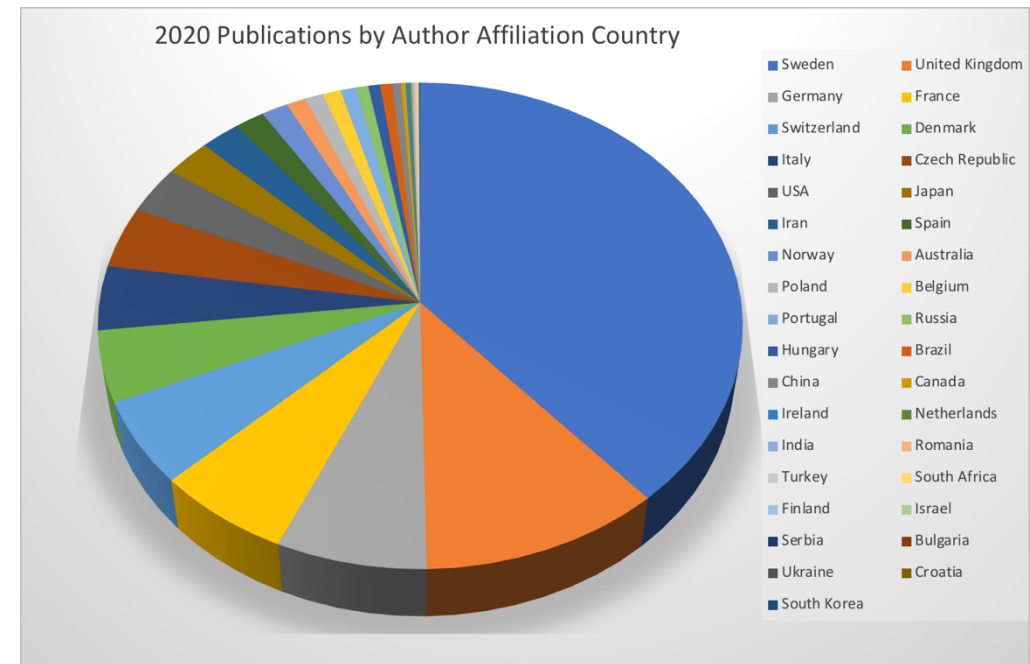
Publication Report 2020

Tracking KPIs for the user programme



2020 – Author Affiliation

- More than 70% of authors in ESFRI countries
- More than 80% of authors in ESS member countries
- Large SE (and DK) share as ESS affiliation is included



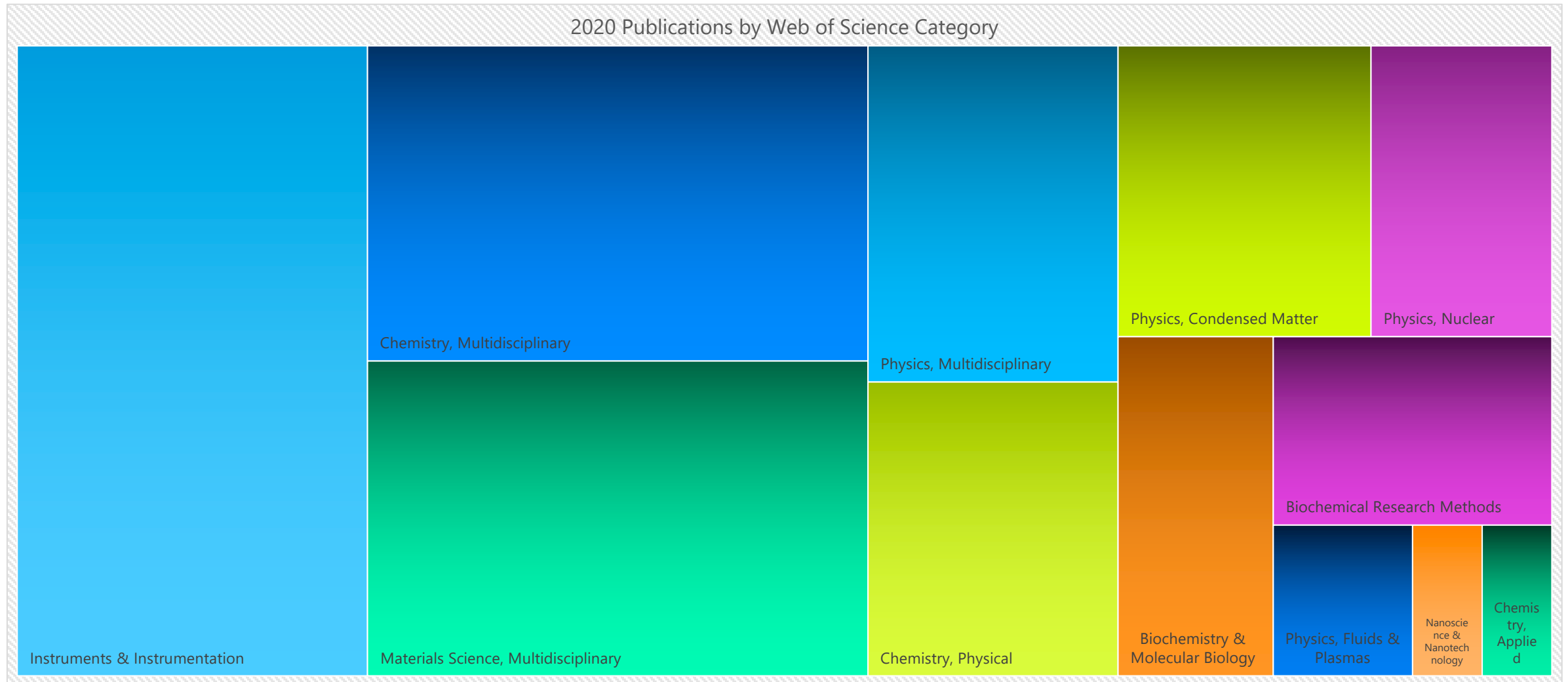
Publication Report 2020

Tracking KPIs for the user programme



2020 – Science Categories

2020 Publications by Web of Science Category



Discussion



ESS ILL User Meeting 2022



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Input welcome

Science Day 2021 and Beyond

A forum to exchange on our scientific collaborations



Considerations for Science Day 2022

- in-person meeting (only)
- consider topical sessions, external keynote speakers
- link closer to ESS project & future operation – not only from science directorate but also other ESS entities
- ensure complementarity with User Meeting – especially in 2022
- *Liaise with Carina, Bea, Arno or your SFT coordinator to provide input!*



Pascale



Premek



Esko



Valentina



Søren

09:00	Andreas Schreyer: Zoom 09:00 - 09:30
	Josefin Martell: Neutron tomography in planetary science/water in Martian meteorites Zoom 09:30 - 09:50
	Andrew McCluskey: Accurate uncertainty quantification and model selection for in-silico diffusion Zoom 09:50 - 10:10
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	Arno Hiess: Way forward for Science Zoom 15:30 - 15:45