

Research Report 2020

14 March 2021

ESS – ILL User Meeting – September 2020

For the second time, ESS and ILL held a joint user meeting in 2020: <http://www.neutrons4europe.com>. The first joint using meeting was hosted by ILL in Grenoble in 2018, and the 2020 meeting was set to welcome Europe's neutron users to Lund. Pushed by the pandemic into a virtual format, the meeting took on quite a different character.

The digital format lifted restrictions on numbers, and a record 777 participants registered. Over 600 unique viewers participated in the main meeting, and to date about 500 people have watched the sessions on YouTube afterwards.

In addition to the wide range of science covered in the programme, there were updates on the ILL, ESS and other LENS facilities, a presentation on PanOSC and how the neutron sources work with FAIR data and open data, an introduction to the international society for sample environment and a presentation about 'Where neutron scientists are and what they do' e.g. the analysis of the user community which ENSA performed and supported by brightness2. The meeting was wrapped up with a panel session, with lively discussions as the European community came together in this way.

A number of topical workshops were held in conjunction with the meeting, as always. These were Chemistry and Magnetism, Imaging, Materials and Engineering, Fundamental and Particle Physics, Polarisation, GISANS, and Atomic-Scale Simulations in Neutron Scattering. Again, the digital format allowed for more flexible scheduling and less timewise overlap of these workshops, and the attendance was high on all of them. Particularly the ESS - ILL Topical Workshop on Imaging, Materials and Engineering attracted an astounding 356 participants.

Although the chance to catch up in person was missed, the community made the best of the situation and seized this opportunity to come together and discuss important issues and meet old friends and colleagues on line. The high attendance and good discussions demonstrated the strength and resilience of the community, as well as showing how much can be achieved on line when necessary.

We look forward to welcoming our collaborators and friends to Lund and ESS for the next joint user meeting, to be held in 2022.

Key numbers for the User Meeting

Date for main conference 23-25/9 2020

Number of registrants 777

Number of unique viewers >600

This includes 491 unique email addresses using Zoom plus anonymous watchers on YouTube (at least 85 but more likely around 140)

Unique viewers per session >350

This includes approximately 275 on Zoom and approximately 85 on YouTube.

Replay viewers on YouTube appr. 500 as of January 2021.

For each session:

Session #1	2800 viewers (anomaly due to YouTube push)
Session #2	577 viewers
Session #3	457 viewers
Session #4	422 viewers

Topical workshops

ESS - ILL Topical Workshop on Chemistry and Magnetism

Date October 13,

Registrants 212

ESS - ILL Topical Workshop on Imaging, Materials and Engineering

Date October 14-15

Registrants 356

ESS - ILL Topical Workshop on Fundamental and Particle Physics

Date October 14

Registrants 66

ESS Polarisation Workshop

Date September 21-22

Registrants 87

ESS-ILL User Meeting - Topical Session on Atomic-Scale Simulations in Neutron Scattering

Date January 20-21, 2021

Registrants 221

Scientific Collaboration, Colloquia, Grant Execution and Sponsoring

Due to the pandemic we did not have our annual **ESS science day**. We have now started to move the ESS science day 2021 to a virtual format so it will continue to serve as a condensation point of our scientific network.

We shall mention the success of the **MaxIV ESS science colloquia** which have started in 2019 and continue in a virtual format using zoom, which attracts a wide audience :

March 2020 Jan Knudsen, Lund University
April 2020 Kristina Edström, Uppsala University
May 2020 Thomas Hellweg, Bielefeld University
June 2020 Poul Nissen, Aarhus University

Throughout 2020, the **ESS Science Focus Teams** continued in a similar format as in previous years providing a forum for scientific exchange - see the reports below. Participation in externally funded collaborations with other facilities such as 'accelerate' and 'BrightnESS2' took place throughout 2020. This enabled us to take an active role towards the collaborative LENS (League of European Neutron Sources).

In 2020 ESS financially supported the **Wolfram-Prandl Preis 2020** rewarding young scientists using neutrons for their research.

Update on Policies and Guidelines for the User Programme.

With regards to the user programme we have prepared the Policy for Science Evaluation & Access and the Policy for User Scientific Publications. The Policy for Science Evaluation and Access has been approved by SAC and awaiting ESS Council approval. The Policy for User Scientific Publications has been approved by SMT and shall soon be presented to SAC and ESS Council. Also the matching guidelines for Science Directorate Sponsorship and Science Directorate Publications and Affiliations have been updated and approved by the Science Management Team (SMT). The STAP for Samples and User Services have assisted in this work. DMSC is working on an update of the data policy to reflect the commitment to open and fair data.

Attachments

- Reports from the ESS Science Focus Teams
- Publication Report 2020 as one key element for anchoring ESS in society:
<https://europeanspallationsource.se/article/2020/12/16/anchoring-ess-society>

SFT DaSNeT

Students and post docs (co-supervised by ESS staff)

- TH Rod has supervised Post Doc Thomas Farmer at ISIS, STFC
- DRAM group: Pernille Lous, DTU-Management, studied how the group managed development of software for her master thesis.

Grants and other Funding Applications with related ESS/in-kind partner participation

Participation in grant applications that were not granted:

1. Post doc application for Lundbeck foundation (TH Rod)
2. "A new method to model inelastic and quasielastic neutron scattering data by molecular dynamics simulations", (J. Swenson, A. Markvardsen, H. Bordallo, [T.H. Rod](#)) Tillväxtverket SREss3 programme at ESS
3. "A new method to model inelastic and quasi-elastic neutron scattering data by molecular dynamics simulation" (M. López Vidal, sponsor [T.H. Rod](#)) NordForsk - Nordic Neutron Science Programme - Post Doc Call 2020
4. "Automated software pipeline for NMX data processing" (U. Ryde, E. Oksanen, [T.H. Rod](#)) Tillväxtverket SREss3 programme at ESS
5. "Automated data processing and refinement pipeline for neutron macromolecular crystallography" (O. Caldararu, sponsors E. Oksanen, [T.H. Rod](#)) NordForsk - Nordic Neutron Science Programme - Post Doc Call 2020
6. "Improving Neutron Macromolecular Crystallographic Data quality - from collection to refinement" H2020-MSCA-IF-2019 (O. Caldararu, E. Oksanen, [T.H. Rod](#))
7. "Comprehensive Improvements to NeutronScattering Data Analysis Software for Biological Applications", [Essential Open Source Software for Science, Cycle 2](#), [Chan Zuckerberg Initiative](#) (W Potrzebowski, P Rozyczko, TH Rod)

Participation in grant applications that were granted:

- SSF utilization project (P Rozyczko & TH Rod)
- Vetenskapsrådet - Research Infrastructure Grant - VR - Accessibility to infrastructure: "Making neutron crystallography easy and precise – a software pipeline for realising the full potential of the NMX diffractometer at ESS" U. Ryde, E. Oksanen, [T.H. Rod](#)
- Tillväxtverket SREss3 programme at ESS: "A new method to model inelastic and quasielastic neutron scattering data by molecular dynamics simulations" J. Swenson, H.N. Bordallo, F.J. Villacorte, P.P. Deen, D. Meferini, [T.H. Rod](#)
- Tillväxtverket SREss3 programme at ESS: "Automated software pipeline for NMX data processing" U. Ryde, E. Oksanen, [T.H. Rod](#)
- Tillväxtverket SREss3 programme at ESS: "Managing and mining small-angle scattering and complementary spectroscopic data" J. Houston, W. Potrzebowski, C. Dicko, A. Reanie.
- SwednESS PhD project: "Framework for modeling neutron spectra of liquid chromophores" P. Erhart, Müller, Börjesson, H.N. Bordallo, [T.H. Rod](#)

Networks and Committees

- TH Rod: Speaker for LENS Work group 4 subgroup 3 on Computing, Data-Processing & -Analysis
- DM Rodriguez Member of LENS Working Group 3, subgroup Neutron Delivery Systems
- T Richter & TH Rod: Member of PaNOSC Project Management Committee (T Richter WP leader for WP3 and TH Rod for WP8)
- TH Rod: Member of PhD Committee for Lili Cao, Lund University
- A Sazonov: Member of the ILL Subcommittee: Evaluation of Scientific Proposals (College 5B, Magnetic structures)

Industry Relations

- IceT development in SSF utilization project where Sandvik is partner (P Rozyczko & TH Rod)

Seminars and Conferences

1. "McStas GPU Hackathon" [Mads Bertelsen](#) [Torben Roland Nielsen](#) [Peter Willendrup](#) (27 Jan 2020 - 31 Jan 2020, DTU)
2. "scipp hackathon" [Neil Vaytet](#) [Simon Heybrock](#) (11 Feb 2020 - 13 Feb 2020, ISIS)
3. "SasView virtual code camp" [Wojciech Potrzebowski](#) [Piotr Rozyczko](#) (18 Mar 2020 - 24 Feb 2020, <https://github.com/SasView/sasview/wiki/VirtualCodeCamp/>)
4. "DMSC, ESS and data analysis", [Thomas Holm Rod](#), AI workshop on quantitative 3D microscopy - MAX IV (31 Jan 2020 QIM, DTU, Denmark) ([slides](#))
5. "Impact sensitivity of energetic materials – theory and experiment", [Piotr Rozyczko](#), 60th Sanibel Symposium - University of Florida (18 Feb 2020 St. Simon, GA)
6. "PYTHON WORKSHOP for women in science" [Celine Durniak](#) [Wojciech Potrzebowski](#) (11 Feb 2020 Lund University)
7. Python training for ESS and in-kind partners. Entire DRAM group (27 Feb 2020 <https://indico.esss.lu.se/event/1375/>)
8. "Dive into atoms" LINXS webinars: [Andrew Sazonov](#) [Thomas Holm Rod](#) [Wojciech Potrzebowski](#)
9. LINXS Webinars: Let's dive into the atoms! <https://www.linxs.se/educational/> -
 - a. Science and data analysis at the European Spallation Source [Thomas Holm Rod](#) (15 Jun 2020)
 - b. [Small Angle Scattering Data Analysis with SasView](#) [Wojciech Potrzebowski](#) (22 Jun 2020)
 - c. [EasyDiffraction: new easy-to-use software for analysis of diffraction data](#) [Andrew Sazonov](#) (29 Jun 2020)
10. McStas GPU presentation at "OpenACC Summit 2020" [Peter Willendrup](#) (31 Aug 2020 , <https://www.openacc.org/events/openacc-summit-2020> and <https://youtu.be/HDU-WRJUZxs>)
11. PaNOSC presentation at ORSO meeting [Thomas Holm Rod](#) (26 May 2020)
12. ESS/ILL User meeting 2020 - topical session on Atomic-scale simulations in Neutron Scattering [Thomas Holm Rod](#) [Danielle Adonis](#) [Miguel Gonzalez](#) (20 Jan 2021 - 21 Jan 2021)
13. PaNOSC & ExPaNDS Annual Meeting 2020, plenary talk "Update On PaNOSC WP 5: Simulations" [Mads Bertelsen](#) (10 Nov 2021)

Publications

1. Carminata, C. *et al.* [Bragg edge Attenuation Spectra at Voxel Level from 4D Wavelength-Resolved Neutron Tomography](#), *Journal of Applied Crystallography* **53**, 188-196 (2020)
2. Pospelov, G. *et al.* [BornAgain: software for simulating and fitting grazing-incidence small-angle scattering](#), *Journal of Applied Crystallography* **53**, 262-276 (2020).
3. Heybrock, S. *et al.* Scipp: Scientific data handling with labeled multi-dimensional arrays for C++ and Python, *Journal of Neutron Research*, DOI: 10.3233/JNR-190131
4. 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).
5. Albani, G. *et al.* High-rate measurements of the novel BAND-GEM technology for thermal neutron detection at spallation sources. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **957**, doi:10.1016/j.nima.2020.163389 (2020).
6. Cai, X. X. & Kittelmann, T. NCrystal: A library for thermal neutron transport. *Computer Physics Communications* **246**, doi:10.1016/j.cpc.2019.07.015 (2020).
7. Mauri, I. Apostolidis, M.J. Christensen, A. Glavic, C.C. Lai, A. Laloni, F. Messi, A. Lindh Olsson, L. Robinson, J. Stahn, P.O. Svensson, R. Hall-Wilton, and F. Piscitelli "The Multi-Blade Boron-10-based neutron detector performance using a focusing reflectometer", *JINST* **15** P03010 (2020), doi: doi.org/10.1088/1748-0221/15/03/P03010
8. F. Piscitelli, G. Mauri, A. Laloni, R. Hall-Wilton, "Verification of He-3 proportional counters fast neutron sensitivity through a comparison with He-4 detectors", *European Physical Journal Plus* **135**, 577 (2020), doi: doi.org/10.1140/epjp/s13360-020-00600-8
9. Oliver RC, Potrzebowski W, Najibi SM, Pedersen MN, Arleth L, Mahmoudi N, and André I "Assembly of Capsids from Hepatitis B Virus Core Protein Progresses through Highly Populated Intermediates in the Presence and Absence of RNA", <https://pubs.acs.org/doi/10.1021/acsnano.0c03569>
10. DD DiJulio, I Svensson, XX Cai, J Cederkall, PM Bentley, [Simulating neutron transport in long beamlines at a spallation neutron source using Geant4](#), *Journal of Neutron Research* **22** (2020) 183-189,
11. P. M. Bentley and U. Filges, [Metaheuristic layout design of a 2 billion euro science facility](#), *J. Phys. Commun* **4** (2020) 055011
12. P. Bentley, [Accurate Simulation of Neutrons in Less Than One Minute Pt. 2: Sandman—GPU-Accelerated Adjoint Monte-Carlo Sampled Acceptance Diagrams](#), *Quantum Beam Science* **4** (2020), 24
13. P. M. Bentley, [Instrument suite cost optimisation in a science megaproject](#), *J. Phys. Commun* **4** (2020) 045014
14. A. Addazi *et al.*, [New high-sensitivity searches for neutrons converting into antineutrons and/or sterile neutrons at the European Spallation Source](#), arXiv 006.04907v1
15. A. Pietropaolo, M. Angelone, R. Bedogni, N. Colonna, A. J. Hurd, A. Khaplanov, F. Murtas, M. Pillon, F. Piscitelli, E. M. Schooneveld, and K. Zeitelhack, "Neutron detection techniques from ueV to GeV", *Physics Reports* **875**, 1-65 (2020), doi: doi.org/10.1016/j.physrep.2020.06.003
16. A. Morozov, L. M.S. Margato, I. Stefanescu, "Simulation-based optimization of a multilayer ¹⁰B-RPC thermal neutron detector", [arXiv:2002.02284](#), *JINST* **15** (2020) P03019, doi:10.1088/1748-0221/15/03/p03019.
17. Thomas O Farmer, Anders J Markvardsen, Thomas H Rod, Heloisa N Bordallo, Jan Swenson, "[Dynamical Accuracy of Water Models on Supercooling](#)", *The Journal of Physical Chemistry Letters* **11** (2020) 7469-7475. <https://doi.org/10.1021/acs.jpclett.0c02158>
18. Peter K Willendrup, Kim Lefmann "[McStas \(i\): Introduction, use, and basic principles for ray-tracing simulations](#)", *Journal of Neutron Research* vol. 22, no. 1, pp. 1-16, 2020. <https://doi.org/10.3233/JNR-190108>
19. J. C. E. A. Hafner, T. Kluyver, M. Bertelsen, M. Upadhyay Kahaly, Z. Lecz, S. Nourbakhsh, A. P. Mancuso, C. Fortmann-Grote, [VINYL: The Virtual Neutron and x-ray Laboratory and its applications](#), *Proceedings Volume 11493, Advances in Computational Methods for X-Ray Optics V*; 114930Z, 2020

20. Asla Husgard, Martin A. Olsen, Rebekka Frøystad, Jonas P. Hyatt, Mads Bertelsen, Rasmus Toft-Petersen, and Kim Lefmann, [Effects of ground movements on realistic guide models for the European Spallation Source](#), Phys. Rev. Accel. Beams 23, 103501, 2020
21. J. Jeong, B. Lenz, A. Gukasov, X. Fabrèges, A. Sazonov et al., [Magnetization Density Distribution of Sr₂IrO₄: Deviation from a Local \$j_{eff}=1/2\$ Picture](#), Phys. Rev. Lett. 125, 097202 (2020)
22. I. A. Zobkalo, A. N. Matveeva, A. Sazonov et al., [Direct control of magnetic chirality in NdMn₂O₅ by external electric field](#), Phys. Rev. B 101, 064425 (2020)

Misc

1. [DTU student Pernille Lous](#)
2. Gerald Kneller (24/1 & 28/1)
3. 2 x icaleps conference proceedings - issued in 2020 but conference in 2019 and thus listed in 2019 report.

SFT Engineering Material, Geosciences, Archeology and Heritage Conservation

(Coordinator: Premek Beran)

(Note: Non-ESS SFT members are not fully represented here)

Grants, Networks, and Committees

- Vinnova “Increasing the competence of PhD students regarding industrially relevant neutron and synchrotron-based analytical methods – Spring 2020” (12-month collaboration with KTH involving Robin Woracek)
- Two SAKURA programs (R. Kiyonagi visiting, M. Neikter going, both involving R. Woracek; *postponed due to Covid*) Reviewer for journals from within this SFT field: Robin Woracek (Journal of Applied Crystallography, Metallurgical and Materials Transactions A, Materials Characterization, Journal of Imaging, International Journal of Solids, Plant and Soil, Journal of Nuclear Materials, Nuclear Instruments and Methods), Premek Beran (Intermetallics, Materials, Metals, Materials Chemistry and Physics, Crystals)
- SFT members are a reviewer for beamtime proposals: Robin Woracek (ORNL - SNS/HFIR for Engineering and Materials between 2017-current; J-PARC MLF between 2018-current; ILL College 1, Applied Materials Science, Instrumentation and Techniques, between 2019-current), Premek Beran (J-PARC MLF between 2018-current)

Awards

The publication from 2019 (see below), was awarded in November 2020 by the Werner Köster Prize.

Since 1992, the German Materials Society (DGM) has been awarding the Werner Köster Prize together with Carl Hanser Verlag. It honours an outstanding article published in the International Journal of Materials Research (IJMR), formerly Zeitschrift für Metallkunde. Each year, the editorial board of the IJMR selects a publication from the previous year “that focuses on fundamental, original work in the field of materials science”.

The award-winning publication deals with a cobalt-rhenium alloy with nickel and chromium – a promising material for stationary gas turbines and aircraft turbines.

In the DGM’s explanation for the award, the “consistent application of a broad spectrum of complementary experimental and theoretical methods” is particularly emphasized. Furthermore, it says that what the scientists discovered in their experiments is an important basis for future materials design.

Original Publication:

Katharina Esleben, Bronislava Gorr, Hans-Jürgen Christ, Christian Pritzel, Debahis Mukherji, Joachim Rösler, **Premysl Beran**, Pavel Strunz, Markus Hoelzel, Ralph Gilles. (2019). *Effect of Cr and Ni on the microstructural evolution in Co–Re–Cr–Ni alloys*. International Journal of Materials Research. 110. 1092-1104. DOI: [10.3139/146.111855](https://doi.org/10.3139/146.111855).



Seminars, Conferences and Outreach

Nordic Residual Stress Group meeting (March 2020)

The Nordic Residual Stress Group meeting (March 2020) – a semi-regular meeting of the group of researches and industry-related people dealing with the residual stress measurement and evaluation. It was held in ESS premises with the following program.

The Nordic Residual Stress Group meeting, March 10th, 2020

Date: March 10th, 2020.

Place: ESS, European Spallation Source, Odarslövsvägen 113, Lund

Agenda.

08:30	Tour at ESS
10:00	Coffee
10:15	Opening of the Nordic residual stress group meeting 2020, Per Lundin
10:20	"ESS and the engineering diffractometer BEER", by Premek Baren, ESS
11:00	"Full field synchrotron X-ray and neutron strain microscopy", by Hanna Leemreize, Danish Institute of Technology
11:40	"Residual stress measurements on compression springs after different shot peening procedures", by Stefan Musslinder, Lesjöfors
12:20	ESS invites us for a light lunch at ESS
13:20	Leaving ESS for a 10 min walk to MAX IV
13:30	Arrival to MAX IV. Brief general overview: MAX IV a unique tool with many applications run by experts. How to access?
14:15	Experimental hall, accelerators/beamlines, specific beamline/scientist. NanoMAX,
15:30	Visit ends

Register to the meeting to Rasha or Per, no later than Friday February 14th.

You are most welcome!

Volvo GTT, Göteborg
Rasha Alkaisee
rasha.alkaisee@volvo.com
Tel. 031-322 06 63

Schlumpf Scandinavia AB
Per Lundin
per.lundin@schlumpf.se
Tel. 070-368 60 48

SNSS Seminar series – Seminar 1: Neutron Imaging (Nov 2020)

SNSS Seminar series – Seminar 1: Neutron Imaging

Tuesday, November 17, 2020

13:00 – 15:00



Programme

13.00 - 13.05. Welcome - **Maths Karlsson**, Chair SNSS

13.05 - 13.40 "An introduction to Neutron Imaging with a focus on Geomechanics" - **Alessandro Tengattini**, Università Grenoble-Alpes / ILL

13.40 - 14.00 "Dual modality neutron and X-ray tomography data from skeletal tissues with a metallic implant" - **Elin Törnquist**, Division of Biomechanics, Lund University

14.00 - 14.25 "Revealing localized microstructure and temperature variations by wavelength selective neutron imaging" - **Robin Woracek**, ESS

14.25 - 14.50 "Neutron imaging and applications in archaeology" - **Anna Fedrigo** (STFC, ISIS Neutron and Muon Source)

ESS - ILL Topical Workshop on Imaging, Materials and Engineering (October 14-15, 2020)
 The “satellite” remote meeting to the main ESS&ILL user meeting focused on materials science and imaging was organized. There were in a maximum of around 250 participants from all over the world, which provided very constructive discussion and feedback.

Wednesday 14 October 2020

Instrument Updates: Engineering Diffractometers (13:30-13:45)

time	[id] title	presenter
13:30	[1] SALSA Update	PIRLING, Thilo
13:40	[2] BEER Update	BERAN, Premek

Materials Science and Engineering - Overviews & General (13:45-14:45)

time	[id] title	presenter
13:45	[3] Neutron diffraction in material science	SAHLBERG, Martin
14:15	[4] The Common Calibration Protocol and Neutron Quality Label for Neutron Strain Scanning instrumentation	RHAMADAN, Ranggi S.

BREAK (14:45-14:55)

Materials Science and Engineering - Studies & Applications (14:55-16:25)

time	[id] title	presenter
14:55	[5] Measurement of strain during fatigue crack growth by stroboscopic neutron diffraction	PROBERT, Molly
15:15	[6] Development of new approaches for neutron diffraction 3D strain mapping in aluminium additive manufactured materials	MIKHEENKOVA, Anastasiia
15:35	[7] Residual stress measurement in dissimilar metal joints using neutron diffraction	SAPANATHAN, Taneshan
15:55	[8] Studying granular mechanics with neutron diffraction	ATHANASOPOULOS, Stefanos

Thursday 15 October 2020

Instrument Updates: Imaging Beamlines (13:00-13:20)

time	[id] title	presenter
13:00	[9] NEXT Update	TENGATTINI, Alessandro
13:10	[10] ODIN Update	MANUEL MORGANO, Aureliano Tartaglione,

Neutron Imaging - Overviews & General (13:20-14:50)

time	[id] title	presenter
13:20	[11] Advanced imaging methods	KARDJIOV, Nikolay
13:50	[12] Cultural heritage metal artefacts tackled by neutron imaging and scattering	GRAZZI, Francesco
14:20	[17] Open source neutron imaging software	KAESTNER, Anders

BREAK (14:50-15:00)

Neutron Imaging and Diffraction - Studies & Applications (15:00-16:30)

time	[id] title	presenter
15:00	[15] Bragg-edge imaging reveals local texture variations in additive manufactured samples	PACHECO GIMON, Victor Manuel
15:20	[13] Neutron diffraction and imaging on battery systems	SENYSHYN, Anatoliy
15:40	[14] Monitoring Li-ion batteries by advanced operando neutron techniques	VILLEVIEILLE, Claire LYONNARD, Sandrine
16:10	[16] Results from the GeoArchaeology try-out workshop	NILSSON, Björn SCHILLINGER, Burkhard

Students and PostDocs

Not directly supported, co-supervised by ESS staff, working on neutron projects:

- Tran Van Khan (HZB/TU Berlin, "Diffraction contrast tomography with neutrons") (Robin Woracek)
- Nancy Elewa (NPI, CZ-ESS-OP, R. Woracek)
- Victor Manuel Pacheco Gimon (Uppsala, "Additive manufacturing") (Premek Beran)
- Josefine Martell (Lund, "Impactor determination with neutrons– Towards a better understanding of solar system dynamics and the impact cratering process"; R. Woracek)
- Fernando Vieira Lima (Lund, "rock-mechanics") (Robin Woracek)

Supported by ESS:

none

Publications

- [1]
- P. Strunz, L. Kunčická, **P. Beran**, R. Kocich, C. Hervoches, *Correlating Microstrain and Activated Slip Systems with Mechanical Properties within Rotary Swaged WNiCo Pseudoalloy*, Materials. 13 (2020) 208. <https://doi.org/10.3390/ma13010208>.
- [2]
- P. Strunz, R. Kocich, D. Canelo-Yubero, A. Macháčková, **P. Beran**, L. Krátká, *Texture and Differential Stress Development in W/Ni-Co Composite after Rotary Swaging*, Materials. 13 (2020) 2869. <https://doi.org/10.3390/ma13122869>.
- [3]
- A. Michalcová, D. Vojtěch, J. Vavřík, K. Bartha, **P. Beran**, J. Drahokoupil, J. Džugan, J. Palán, J. Čížek, P. Lejček, *Structure and Properties of High-Strength Ti Grade 4 Prepared by Severe Plastic Deformation and Subsequent Heat Treatment*, Materials. 13 (2020) 1116. <https://doi.org/10.3390/ma13051116>.
- [4]
- J.J. Marattukalam, D. Karlsson, V. Pacheco, **P. Beran**, U. Wiklund, U. Jansson, B. Hjörvarsson, M. Sahlberg, *The effect of laser scanning strategies on texture, mechanical properties, and site-specific grain orientation in selective laser melted 316L SS*, Materials & Design. 193 (2020) 108852. <https://doi.org/10.1016/j.matdes.2020.108852>.
- [5]
- M. Koller, M. Vilémová, F. Lukáč, **P. Beran**, J. Čížek, H. Hadraba, J. Matějčík, J. Veverka, H. Seiner, *An ultrasonic study of relaxation processes in pure and mechanically alloyed tungsten*, International Journal of Refractory Metals and Hard Materials. 90 (2020) 105233. <https://doi.org/10.1016/j.ijrmhm.2020.105233>.
- [6]
- F. Damay, J. Sottmann, F. Lainé, L. Chaix, M. Poienar, **P. Beran**, E. Elkaim, F. Fauth, L. Nataf, A. Guesdon, A. Maignan, C. Martin, *Magnetic phase diagram for $Fe_{3-x}Mn_xBO_5$* , Phys. Rev. B. 101 (2020) 094418. <https://doi.org/10.1103/PhysRevB.101.094418>.
- [7]
- P. Beran**, D. Mukherji, P. Strunz, R. Gilles, M. Hölzel, M. Hofmann, L. Karge, J. Rösler, *In Situ Neutron Diffraction Study of Ni Addition in Co–Re–Cr High-Temperature Alloys and Influence on Phase Transformations*, J. Synch. Investig. 14 (2020) S179–S184. <https://doi.org/10.1134/S1027451020070071>.
- [8]
- K.H. Andersen, D.N. Argyriou, A.J. Jackson, J. Houston, P.F. Henry, P.P. Deen, R. Toft-Petersen, **P. Beran**, ... **R. Woracek** ...et al., *The instrument suite of the European Spallation Source*, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment. 957 (2020) 163402. <https://doi.org/10.1016/j.nima.2020.163402>.
- [9]
- K.V. Tran, **R. Woracek**, N. Kardjilov, H. Markötter, A. Hilger, W. Kockelmann, J. Kelleher, S. Puplampu, D. Penumadu, A.S. Tremsin, J. Banhart, I. Manke
Spectral neutron tomography
Materials Today Advances, in production. (2021)
- [10]

- N. Kardjilov, I. Manke, A. Hilger, T. Arlt, R. Bradbury, H. Markötter, **R. Woracek**, **M. Strobl**, W. Treimer, J. Banhart
The Neutron Imaging Instrument CONRAD—Post-Operational Review
Journal of Imaging, 7(1), p.11. (2021) [11]
- A. Backis, A. Khaplanov, R. Al Jebali, R. Ammer, I. Apostolidis, J. Birch, ... **R. Woracek**, ..
Time-and energy-resolved effects in the boron-10 based Multi-Grid and helium-3 based thermal neutron detectors
Measurement Science and Technology, 32(3), p.035903. (2020) [12]
- O. Löhmann, L. Silvi, P.M. Kadletz, N. Vaytet, O. Arnold, M.D. Jones, J. Nilsson, M. Hart, T. Richter, R. von Klitzing, A.J. Jackson, T. Arnold, **R. Woracek**
Wavelength frame multiplication for reflectometry at long-pulse neutron sources
Review of Scientific Instruments, 91(12), p.125111. (2020) [13]
- S. Samothrakitis, C.B. Larsen, **R. Woracek**, L. Heller, J. Kopeček, G. Gerstein, H.J. Maier, M. Rameš, M. Tovar, P. Šittner, S. Schmidt, M. Strobl
A multiscale study of hot-extruded CoNiGa ferromagnetic shape-memory alloys
Materials & Design, 196, p.109118. (2020) [14]
- M. Morgano**, N. Kalentics, C. Carminati, J. Capek, M. Makowska, **R. Woracek**, T. Maimaitiyili, T. Shinohara, R. Loge, M. Strobl
Investigation of the effect of Laser Shock Peening in Additively Manufactured samples through Bragg Edge Neutron Imaging
Additive Manufacturing 101201 (2020) [15]
- V. Maulerova, V., K. Kanaki, P.M. Kadletz, **R. Woracek**, T. Wilpert, K. Fissum, A. Laloni, N. Mauritzson, F. Issa, R.H. Hall-Wilton,
Vanadium-based neutron Beam Monitor
Physical Review Accelerators and Beams, 23(7), p.072901 (2020) [16]
- V. Maulerova, J. Nilsson, M. Olsson, S. Alcock, A. Quintanilla, D. Zielinski, A. Mukai, F. Issa, S. Kolya, W. Smith, D. Broderick, K. Löki, J. Sparger, **R. Woracek**, J. Taylor, T. Richter, R. Hall-Wilton, O. Kirstein, N. Tsapatsaris
First neutron data recorded at the V20 Test Instrument utilizing prototype chopper systems and beam monitors planned for ESS
EPL (Europhysics Letters) 128, no. 5: 52001 (2020) [17]
- A. Addazi, K. Anderson, S. Ansell, K. Babu, J. Barrow, ... **R. Woracek**, ..
New high-sensitivity searches for neutrons converting into antineutrons and/or sterile neutrons at the European Spallation Source.
arXiv preprint arXiv:2006.04907. (2020) [18]
- M. Neikter, **R. Woracek**, C. Durniak, M. Persson, M.L. Antti, P. Åkerfeldt, R. Pederson, J. Zhang, S.C. Vogel, **M. Strobl**
Texture of electron beam melted Ti-6Al-4V measured with neutron diffraction
In MATEC Web of Conferences (Vol. 321, p. 03021). EDP Sciences. (2020)

General comments

- While all of the SFT members are very active scientifically, the activities within the SFT platform itself have just gained momentum, since there is currently still limited staff in this field employed at ESS itself.
- Very limited gain to be an SFT member leads to the lack of interest to participate or share the information. The membership should be revisited.

SFT members

Luca Zanini (ESS)

Phillip Bentley (ESS)

Richard Hall-Wilton (ESS)

Robin Woracek (ESS)

Jochen Fenske (HZG)

Markus Strobl (PSI)

Premysl Beran (NPI)

Stephen Hall (LTH)

Luise Theil Kuhn (DTU)

Rune E. Johnsen (DTU)

Monica-Elisabeta Lăcătușu (DTU)

Søren Schmidt (DTU)

Morten Sales (DTU)

Ralf F. Ziesche (UCL)

Magnus Neikter (LTU; not yet on the website)

Dmytro Orlov (LTH; not yet on the website)

Manuel Morgano (PSI; not yet on the website)

Should/will be invited to join the SFT:

Gregor Nowak (HZG)

Peter Hedström (KTH)

Magnus Hörnqvist Colliander (Chalmers University)

Ru Peng (LIU)

SFT Life Science & Soft Condensed Matter

(Coordinator: Esko Oksanen)

Selected Scientific Highlights

Wojciech Potrzebowski (instrument data scientists at DMSC) together with collaborators from [Lund University](#), [University of Copenhagen](#) & [ISIS](#) has developed a method that combines molecular modelling with time-resolved small-angle scattering to investigate the self-assembly process of hepatitis B virus (HBV) in the presence and absence of RNA. The understanding of such mechanisms is critical for the development of antiviral drugs, biotechnology, protein engineering and vaccine development. The method was applied to study the HBV virus, but it could be further extended to study other viruses. For this study, time-resolved small angle X-ray scattering data was collected at [ESRF](#), which provides sufficient time resolution and quality to observe intermediate structures. It doesn't, however, provide full insight into RNA/protein composition which can be obtained from experiments using neutrons. ESS's [LOKI](#) instrument, with its high flux, will open up for such possibilities in the future. The full article about Wojciech's research can be found here: <https://pubs.acs.org/doi/10.1021/acsnano.0c03569>

An international collaboration between the UK's UCL School of Pharmacy, Lund Protein Production Platform at Lund University, and ESS - through its DEMAX laboratory, have initiated bio-physical and structural studies of three non-structural proteins from the novel coronavirus, SARS CoV-2, the causative agent of COVID-19.

To be able to find an efficient drug, which prohibits the novel coronavirus from causing the disease COVID-19, one important aim is to understand how to block the virus from replicating its genomic material. By doing so, the virus will 'die out' over time as it fails to reproduce or make infectious particles. One way of obtaining this knowledge is to use X-rays to obtain an image of the structure of the proteins involved in this process. There are several proteins involved with proofreading of the viral RNA and its protection by RNA cap methylation, ensuring RNA replication. The research team's studies focus on three of these: Nsp10, Nsp14, and Nsp16. A key part of this work is to establish crystallisation conditions to enable high-throughput fragment-based screening in the search for novel small molecule inhibitors that can block the viral replication cycle.

Recently, the research team had success and were able to produce crystals of one of these proteins, Nsp10. The structure was determined to approx. 2.6 Å resolution and structural analysis is ongoing. The ultimate goal for this research project is to obtain high resolution X-ray crystal structures of these proteins alone or in complex with each other to enable the search for small molecule inhibitors that disrupt their activity. These structural studies will also be complemented with other biophysical characterisation experiments such as thermal stability, microscale thermophoresis and solution scattering studies using X-rays and neutrons.

Grants, Networks, Seminars and Committees

Vetenskapsrådet:

1. A New Method to Model the Dynamic Structure Factor by Molecular Dynamics Simulations, PI Jan Swenson, Chalmers University, Co-PIs: Heloisa N. Bordallo (NBI/KU), Thomas H. Rod (DMSC/ESS) and Anders Markvardsen (ISIS)
2. VR 2016-01164 Linking genes, membrane lipid composition, and antifungal drug resistance in pathogenic yeast. PI, Co-PI: Wolfgang Knecht (LU), Hanna Wacklin (ESS/LU).
3. VR Röntgen-Ångström grant 2015-06099 "Non-equilibrium thermodynamics of biology studied by time resolved small angle X-ray and neutron scattering", 9.6 MSEK, 2016-2019, PI: Gergely Katona, Gothenburg University. (979200 SEK ESS)
4. VR 2016-06963 "Organization of mitochondrial membranes under oxidative stress: Implications for their active role in regulation of apoptosis", 5.06 MSEK 2017-2020, PI: Gerhard Gröbner, Umeå University.
5. VR Neutron scattering project 2017-2020: Computational methods for analyzing self-assembly with time resolved SANS/SAXS, Thomas Holm Rod, Wojciech Potrzebowski (ESS/LU).

Human Frontier Science Program

1. Program grant RGP0031/2019 "Do hydrocarbons induce membrane curvature in photosynthetic organisms?" Main PI David Lea-Smith (University of East Anglia ,UK), co-PI's Melissa Sharp (ESS, Sweden), Oscar Ces (Imperial College, UK), Jane Allison (University of Auckland, NZ) (2019-2022, \$1.2M USD)

Sophie Ayscough is a postdoctoral fellow at ESS funded by the HFSP grant

RAMP-ITN (a Marie Curie training network)

1. Coordinator is Monika Budaoyova-Spano (UGA, France), co-PI Esko Oksanen (ESS/LU). Swati Aggarwal is a PhD student employed at ESS.

BrightnESS² WP2 sub-task: deuteration pilot. 'Deuteration for Soft Matter and Life Sciences'. Anna Leung, Oliver Bogojevic (ESS); Peixun Li, John Webster (STFC).

Crafoordska Stiftelsen

1. Grant Nr. 20190750 "Colloidal Nanoparticles in Deep Eutectic Solvents" PI: Andrew Jackson (ESS/LU), co-PI: Adrian Sanchez-Fernandez (LU)

LENS Pilot Action 3: Global health challenges - Role of cell membranes in health and disease
Coordinator Hanna Wacklin-Knecht (ESS); participants ESS, ILL, STFC, JCNS.

DEUNET international deuteration network

Coordinator Hanna Wacklin-Knecht (ESS); members ESS, ILL, STFC, JCNS, ANSTO, J-PARC MLF, HANARO, Gifu Pharmaceutical University, Kyoto Pharmaceutical university, NIST-UMB BL2, ORNL Biodeuteration facility.

Tillväxtverket SREss3 programme at ESS:

1. "Managing and mining small-angle scattering and complementary spectroscopic data" Judith Houston (ESS), Wojciech Potrzebowski (ESS), Cedric Dicko (LU), Adrian Rennie (UU).
2. "A new method to model inelastic and quasielastic neutron scattering data by molecular dynamics simulations"
Thomas Holm Rod (ESS), Félix J. Villacorta(ESS), Pascale Deen(ESS), Daria Noferini (ESS), Jan Swenson (Chalmers), Heloisa Nunes Bordallo, (NBI), Anders Markvardsen (ISIS)

Seminars

1. Accelerate talk series: presentations by Judith Houston, Zöe Fisher, Andrew Jackson
2. The Light Stuff (online lecture series): The Path to LoKI and SANS at the ESS, 9th October
3. Northern Lights on Food Masterclass, Lund (Sweden), 1st Sept 2020

Publications

- 1 MTB Clabbers, SZ Fisher, M Coinçon, X Zou, H Xu "Visualizing drug binding interactions using microcrystal electron diffraction" (2020) *Communications biology* **3**, 417 <https://doi.org/10.1038/s42003-020-01155-1>
- 2 A Rogstam, M Nyblom, S Christensen, C Sele, VO Talibov, T Lindvall, A Andersson Rasmussen, I André, Z Fisher, W Knecht, F Kozielski "Crystal Structure of Non-Structural Protein 10 from Severe Acute Respiratory Syndrome Coronavirus-2" (2020) *Int. J. Mol. Sci.* **21**(19), 7375 <https://doi.org/10.3390/ijms21197375>
- 3 K Koruza, AB Murray, BP Mahon, JB Hopkins, W Knecht, R McKenna, SZ Fisher "Biophysical Characterization of Cancer-Related Carbonic Anhydrase IX" (2020) *Int. J. Mol. Sci.* **21**, 5277; doi:10.3390/ijms21155277
- 4 M Budayova-Spano, K Koruza, Z Fisher "Large crystal growth for neutron protein crystallography" (2020) *Methods in enzymology* **634**, 21-46 <https://doi.org/10.1016/bs.mie.2019.11.015>
- 5 C Dicko, A Engberg, JE Houston, AJ Jackson, A Pettersson, RM Dalglish, FA Akeroyd, D Alba Venero, SE Rogers, A Martel, L Porcar, AR Rennie "NURF—Optimization of in situ UV-vis and fluorescence and autonomous characterization techniques with small-angle neutron scattering instrumentation" (2020) *Rev. Sci. Inst.* **91**, 075111 <https://doi.org/10.1063/5.0011325>
- 6 A Sanchez-Fernandez, AE Leung, EG Kelley, AJ Jackson "Complex by design: Hydrotrope-induced micellar growth in deep eutectic solvents" (2020) *J. Colloid. Interface Sci.* **581**, 292-298 <https://doi.org/10.1016/j.jcis.2020.07.077>
- 7 A Eriksson, O Caldararu, U Ryde, E Oksanen "Automated orientation of water molecules in neutron crystallographic structures of proteins" (2020) *Acta Cryst. D* **76**, 1025-1032 <https://doi.org/10.1107/S2059798320011729>
- 8 N Junius, E Vahdatahar, E Oksanen, J-L Ferrer, M Budayova-Spano "Optimization of crystallization of biological macromolecules using dialysis combined with temperature control" (2020) *J. Appl. Cryst.* **53**, 686-698 <https://doi.org/10.1107/S1600576720003209>

- 9 J Bergmann, M Davidson, E Oksanen, U Ryde, D Jayatilaka "fragHAR: towards ab initio quantum-crystallographic X-ray structure refinement for polypeptides and proteins" (2020) *IUCrJ* **7**, 158-165 <https://doi.org/10.1107/S2052252519015975>
- 10 O Caldararu, M Misini Ignjatović, E Oksanen, U Ryde "Water structure in solution and crystal molecular dynamics simulations compared to protein crystal structures" (2020) *RSC Adv.* **10**, 8435-8443 <https://doi.org/10.1039/C9RA09601A>
- 11 M Markó, G Nagy, G Aprigliano, E Oksanen "Neutron macromolecular crystallography at the European spallation source" (2020) *Methods in enzymology* **634**, 125-151 <https://doi.org/10.1016/bs.mie.2020.01.005>
- 12 SJ Hjorth-Jensen, E Oksanen, P Nissen, T Lykke-Møller Sørensen "Prospects for membrane protein crystals in NMX" (2020) *Methods in enzymology* **634**, 47-68 <https://doi.org/10.1016/bs.mie.2019.11.019>
- 13 RC Oliver, W Potrzebowski, SM Najibi, M Nors Pedersen, L Arleth, N Mahmoudi, I André "Assembly of Capsids from Hepatitis B Virus Core Protein Progresses through Highly Populated Intermediates in the Presence and Absence of RNA" (2020) *ACS Nano* **14**, 10226–10238 <https://doi.org/10.1021/acsnano.0c03569>
- 14 C Blayo, EA Kelly, JE Houston, N Khunti ^d, NP Cowieson, RC Evans " Light-responsive self-assembly of a cationic azobenzene surfactant at high concentration" (2020) *Soft Matter* **16**, 9183-9187 <https://doi.org/10.1039/D0SM01512A>
- 15 D Noferini, O Holderer, H Frielinghaus "Effect of mild nanoscopic confinement on the dynamics of ionic liquids" (2020) *Phys. Chem. Chem. Phys.*, **22**, 9046-9052, <https://doi.org/10.1039/C9CP05200C>
- 16 SCL Hall, LA Clifton, C Tognoloni, KA Morrison, TJ Knowles, CJ Kinane, TR Dafforn, KJ Edler, T Arnold "Adsorption of a styrene maleic acid (SMA) copolymer-stabilized phospholipid nanodisc on a solid-supported planar lipid bilayer" (2020) *J. Colloid. Interface Sci.* **574**, 272-284 <https://doi.org/10.1016/j.jcis.2020.04.013>
- 17 M Chevrier, J Kesters, JE Houston, N Van den Brande, S Chambon, S Richeter, B Van Mele, T Arnold, A Mehdi, R Lazzaroni, P Dubois, RC Evans, W Maes, S Clément " Phosphonium-based polythiophene conjugated polyelectrolytes with different surfactant counterions: thermal properties, self-assembly and photovoltaic performances" (2020) *Polym. Int.* 6088 <https://doi.org/10.1002/pi.6088>
- 18 AR McCluskey, JFK Cooper, T Arnold, T Snow "A general approach to maximise information density in neutron reflectometry analysis" (2020) *Mach. Learn.: Sci. Technol.* **1** 035002 <https://doi.org/10.1088/2632-2153/ab94c4>
- 19 O Bogojevic, AE Leung, "Enzyme-assisted synthesis of high-purity, chain-deuterated 1-Palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine" (2020) *ACS Omega* **5**, 22395-22401 <https://doi.org/10.1021/acsomega.0c02823>
- 20 J Larsson, AE Leung, C Lang, B Wu, M Wahlgren, T Nylander, S Ulvenlund, A Sanchez-Fernandez "Tail unsaturation tailors the thermodynamics and rheology of a self-assembled sugar-based surfactant" (2021) *J. Colloid. Interface Sci.* **585**, 178-183 doi.org/10.1016/j.jcis.2020.11.063
- 21 T Cleveland IV, E Blick, S Krueger, A Leung, T Darwish, P Butler "Direct localization of detergents and bacteriorhodopsin in the lipidic cubic phase by small-angle neutron scattering" (2021) *IUCrJ* **8**, 22-32 <https://doi.org/10.1107/S2052252520013974>
- 22 J Larsson, A Sanchez-Fernandez, AE Leung, R Schweins, B Wu, T Nylander, S Ulvenlund, M Wahlgren "Molecular structure of maltoside surfactants controls micelle

formation and rheological behaviour" (2021) *J. Colloid. Interface Sci.* **581**, 895-904
<https://doi.org/10.1016/j.jcis.2020.08.116>

23 M Valero, PP Levin, NB Sultimova, JE Houston, "Photochemistry of nabumetone in aqueous solution of sodium dodecyl sulfate (SDS) micelles" (2020) *J. Mol. Liquids*, 2020, **319**, 114093 <https://doi.org/10.1016/j.molliq.2020.114093>

24 I Meazzini, S Comby, KD Richards, AM Withers, F-X Turquet, JE Houston, RRM Owens, RC Evans "Synthesis and Characterisation of Biocompatible Organic-Inorganic Core-Shell Nanocomposite Particles Based on Ureasils" (2020) *J. Mater. Chem. B*, 2020, <https://doi.org/10.1039/D0TB00100G>

25 EA Kelly, N Willis-Fox, JE Houston, C Blayo, G Divitini, N Cowieson, R Dal, RC Evans "A Single-Component Photorheological Fluid with Light-Responsive Viscosity" (2020) *Nanoscale*, 2020, **12**, 6300-6306 <https://doi.org/10.1039/C9NR10350C>

26 G Vitiello, V Venezia, M Verrillo, A Nuzzo, J Houston, S Cimino, G D'Errico, A Aronne, L Paduano, A Piccolo, G Luciani, "Hybrid humic acid/titanium dioxide nanomaterials as highly effective antimicrobial agents against gram(-) pathogens and antibiotic contaminants in wastewater" (2020) *Environ. Res.*, 2021, **193**, 110562
<https://doi.org/10.1016/j.envres.2020.110562>

27 J Puig-Rigall, C Fernández-Rubio, J González-Benito, JE Houston, A Radulescu, P Ngyewa, G González-Gaitano "Structural characterization by scattering and spectroscopic methods and biological evaluation of polymeric micelles of poloxamines and TPGS as nanocarriers for miltefosine delivery" (2020) *International J. Pharmaceutics*, 2020, **578**, 119057. <https://doi.org/10.1016/j.ijpharm.2020.119057>

28 R Delhom, A Nelson, V Laux, M Haertlein, W Knecht, G Fragneto, HP Wacklin-Knecht, "The Antifungal Mechanism of Amphotericin B Elucidated in Ergosterol and Cholesterol-Containing Membranes Using Neutron Reflectometry" (2020) *Nanomaterials* **10**, 2439. <https://doi.org/10.3390/nano10122439>

29 JMO Rodriguez, E Krupinska, H Wacklin-Knecht, W Knecht, "Preparation of human dihydroorotate dehydrogenase for interaction studies with lipid bilayers" (2020) *Nucleosides Nucleotides & Nucleic Acids* 1-14. <https://doi.org/10.1080/15257770.2019.1708100>

30 A Luchini, R Delhom, V Cristiglio, W Knecht, H Wacklin-Knecht, G Fragneto "Effect of ergosterol on the interlamellar spacing of deuterated yeast phospholipid multilayers" (2020) *Chemistry and Physics of Lipids*, **227** 104873.
<https://doi.org/10.1016/j.chemphyslip.2020.104873>

Members

ESS Members:

Andreas Schreyer
Andrew Jackson
Anna Leung
Esko Oksanen (SFT coordinator)
Hanna Wacklin-Knecht
Marie-Louise Ainalem
Melissa Sharp
Sophie Ayscough
Sindra Petersson Årsköld
Thomas Arnold
Wojciech Potrzebowski
Zoe Fisher
Judith Houston
Swati Aggarwal
Daria Noferini

Partner Members:

Adrian Sanchez Fernandez
Ann Terry
Claes von Wachenfeldt
Heloisa N. Bordallo
Katarina Koruza
Manuel Orozco
Marite Cardenas
Michael Monkenbusch
Peter Schurtenberger
Robin Delhom
Selma Maric
Uwe Müller
Vinardas Kelpsas
Wolfgang Knecht

Students and PostDocs

Not directly supported, co-supervised by ESS staff, working on neutron projects:

- 1) Swati Aggarwal (UGA, FR & Lund University, SE) (Esko Oksanen) (Co-supervisor: Monika Budayova-Spano, UGA)
- 2) Samuel Hjort-Jensen (Aarhus University, DK) (Esko Oksanen, Main supervisor Poul Nissen)
- 3) Justin Bergmann (Lund University, SE) (Esko Oksanen) (Main supervisor: Ulf Ryde, LU)
- 4) Manuel Orozco-Rodriguez (Lund University, SE) (Hanna Wacklin-Knecht, Zoe Fisher) (Main supervisor: Wolfgang Knecht, LU)

SFT Magnetism and Chemistry

Members:

ESS Staff: Alexander Holmes, Arno Hiess, Jonathan Taylor, Malcolm Guthrie, Monika Hartl, Premek Beran

In-kind Staff: Artur Glavic, Dan Mannix, Félix Villacorta, Florence Porcher, Jochen Fenske, Mikhail Feygenson, Piotr Rozyczko, Rasmus Toft-Petersen

Mikhail Feygenson

1. Publications (with FZJ affiliation)

T Brückel, H Kleines, J Fenske, S Kleefisch, M Feygenson, PE Doege and et al.,
„Conceptual Design Report Jülich High Brilliance Neutron Source (HBS)“
<https://juser.fz-juelich.de/record/884799>

Benjamin A. Frandsen, Emil S. Bozin, Eleni Aza, Antonio Fernández Martínez, Mikhail Feygenson, Katharine Page, and Alexandros Lappas „Nanoscale degeneracy lifting in a geometrically frustrated antiferromagnet“ Phys. Rev. B 101, 02442 (2020)

2. Research grant applications / successful

The Röntgen-Ångström Cluster (RÅC) funding for the project : „*nPDFSAS: Simultaneous polarized SANS and NPDF methods to study novel electrode nanomaterials*“ (funds cold neutrons polarizer and SANS detector for DREAM)

SRESS3 funding for the project “*Development of electrochemical cell for in-situ neutron diffraction and small-angle scattering measurements*” (funds 2 postdocs at Uppsala University)

3. Invited talks

“*Scientific capabilities of DREAM diffractometer at ESS*”, South Africa-BrightnESS2 Mini-Symposium
“*Inorganic Crystallography*”, September 23, 2020

„*Using Neutron and X-ray Pair-Distribution Function Method for Structural Studies of Nanoparticles*“
Jülich Center for Neutron Science-2 Institute seminar, December 17, 2020.

M Guthrie:

(1) Publications

R. Edberg et al PRB 102 (18) 184408 (2020)

M. Capone et al Phys Stat Sol B 2000413 DOI: 10.1002/pssb.202000413 (2020)

B. Massanni et al Hi. Press. Res. 40 (3) 339-357 (2020)

(2) Research grant applications / successful none

(3) Workshops (title and number of invitees – any photos will be welcome) none

(4) Invited talks.

Invited plenary, European High Pressure Research Group annual meeting
(6-11 Sept 2020).

Félix J Villacorta

(1) Publications

- LENS Report. "Low Energy Accelerator-driven Neutron Sources" LENS Ad-hoc Working Group CANS Nov. 2020. Editors: Thomas Brückel, Eric Eliot, Thomas Gutberlet, Alain Menelle, Frederic Ott. Participants: Fernando Sordo, Felix Villacorta, Ibon Bustinduy, Pierfrancesco Mastinu, Gianfranco Prete, Luca Silvestrin, Jeffrey Wyss, Philip King, Robert McGreevy, Michael Jentschel, Yoann Calzavara, Knud Thomsen, Jerome Schwindling, Holger Podlech, Henrik Ronnow, Eric Mauerhofer, Ulrich Rücker, Jörg Voigt, Paul Zakalek.
- M. Pérez, F. Sordo, I. Bustinduy, J. L. Muñoz & F. J. Villacorta, "ARGITU compact accelerator neutron source: A unique infrastructure fostering R&D ecosystem in Euskadi", *Neutron News*, 31:2-4, 19-25 (2020).
- Masatoshi Arai, Luca Zanini, Ken H. Andersen, Esben Klinkby, Félix J. Villacorta, Kaoru Shibata, Kenji Nakajima and Masahide Harada, "The Performance of ESS Spectrometers in Comparison with Instruments at a Short-pulse Source", *J. Neutron Res.* **22**, 71-85 (2020).
- Sandra Cortijo-Campos; Rafael Ramírez-Jiménez; Esteban Climent-Pascual; Montserrat Aguilar-Pujol; Felix Jiménez-Villacorta; Lidia Martínez; Rafael Jiménez-Riobóo; Carlos Prieto; Alicia de Andrés, "Raman amplification in the ultra-small limit of Ag nanoparticles on SiO₂ and graphene: size and inter-particle distance effects", *Mater. Des.* **192**, 108702 (2020).
- K. H. Andersen, et al., "The instrument suite of the European Spallation Source" (**Review article**), *Nucl. Instrum. & Meth. A* **957**, 163402 (2020).

(2) Research grant applications / successful

- "A new method to model inelastic and quasielastic neutron scattering data by molecular dynamics simulations" granted under the Tillväxtverket SREss3 programme at ESS (Total: 1.500.000 SEK ~150.000 €)
PI: Jan Swenson
Co-proposer: H.N. Bordallo, F. J. Villacorta, P P Deen, D. Noferini, T. Holm Rod

(3) Workshops

- Program Committee member of the 65th Conference on Magnetism and Magnetic Materials (**MMM-2020**), Palm Beach, 2-6 November 2020.
- F. J. Villacorta, "Polarization Analysis in MIRACLES: first steps" Presentation in ESS Polarisation Workshop. (1.9.2020)

(4) Invited talks.

(QENS-WINS invited talk was postponed to 2022)

P. P. Deen

(1) Publications

- Effects of uniaxial pressure on the spin ice Ho₂Ti₂O₇

R. Edberg, I. M. B. Bakke, H. Kondo, L. Ørdu Sandberg, M. L. Haubro, M. Guthrie, A. T. Holmes, J. Engqvist, A. Wildes, K. Matsuhira, K. Lefmann, P. P. Deen, M. Mito, and P. Henelius
Phys. Rev. B 102, 184408 (2020)

- Magnetic ground state of the ordered double-perovskite Sr₂YbRuO₆: Two magnetic transitions

Shivani Sharma, D. T. Adroja, C. Ritter, D. Khalyavin, P. Manuel, Gavin B. G. Stenning, A. Sundaresan, A. D. Hillier, P. P. Deen, D. I. Khomskii, and S. Langridge
Phys. Rev. B 102, 134412 (2020)

- Classical spin liquid or extended critical range in h-YMnO?

Sofie Janas, Jakob Lass, Ana-Elena Tutueanu, Morten L. Haubro, Christof Niedermayer, Uwe Stuhr, Guangyong Xu, Dharmalingam Prabhakaran, Pascale P. Deen, Sonja Holm-Dahlin, Kim Lefmann
arXiv:2006.03396

- Emergent magnetic behaviour in the frustrated YbGaO garnet

Lise Ordu Sandberg, Richard Edberg, Kasper S. Pedersen, Monica Ciomaga Hatnean, Geetha Balakrishnan, Lucile Mangin-Thro, Andrew Wildes, B. Fak, Georg Ehlers, Gabriele Sala, Patrik Henelius, Kim Lefmann, Pascale P. Deen
arXiv preprint arXiv:2005.10605

- “The instrument suite of the European Spallation Source” (**Review article**), *Nucl. Instrum. & Meth. A* **957**, 163402 (2020). K. H. Andersen, et al.,
- Time- and energy-resolved effects in the boron-10 based multi-grid and helium-3 based thermal neutron detectors. A Backis^{1,2}, A Khaplanov², R Al Jebali^{1,2}, R Ammer², I Apostolidis², J Birch³, C C Lai^{2,3}, P P Deen^{2,4}, M Etxegarai², N de Ruette² Measurement Science and Technology, Volume 32, Number 3

(2) Research grant applications / successful

- “A new method to model inelastic and quasielastic neutron scattering data by molecular dynamics simulations” granted under the Tillväxtverket SREss3 programme at ESS (Total: 1.500.000 SEK ~150.000 €)
PI: Jan Swenson
Co-proposer: H.N. Bordallo, F. J. Villacorta, P P Deen, D. Noferini, T. Holm Rod

(3) Workshops

- ESS-ILL Topical Workshop on Chemistry and Magnetism

Magnetism

1. *Manila Songvilay (Institut Neel, CNRS, Grenoble)*
2. *Lingjia Shen (Lund University)*
3. *Matthew Coak (Warwick University)*
4. *Romain Sibille (PSI)*

Chemistry

1. *Matthew Rosseinsky (Liverpool University)*
2. *Eleonora Vottero (University of Turin)*
3. *Werner Paulus (Institut Charles Gerhardt Montpellier)*
4. *Pascale Launois (Laboratoire de Physique des Solides, CNRS/Université Paris Saclay)*

(4) Invited talks

- QENS-WINS invited talk. postponed to 2021
- Institut Neel March 2020: Quantum spins on a hyperkagome lattice: a neutron scattering study with a view to future neutron scattering possibilities at the European Spallation Source.
- SA Science and Innovation: An update of the European Spallation Source and the cold time of flight spectrometer, CSPEC, as a future tool for the study of magnetic excitations.
- African school of physics. Neutron scattering as a tool to understand quantum magnetism: Magnetism and the European Spallation Source.

(5) Extra:

Member of LINX New Materials Theme: 2020-2023.

Member of Quantum Magnetism Lighthouse project. Denmark Universities.

Thesis opponent: Catelin Vadim

Thesis entitled: Spin ice: magnetic monopoles, fluctuation dissipation and fragmentation.

9th March 2020.

Students and PostDocs

- L. Orduk Sandberg (Ph.D student, Copenhagen University), Frustration under pressure
- M. Haubro (Masters student, Copenhagen University), Frustration under pressure. Completed January 2021.
- I-M. Bakke. (Oslo University). Frustration under pressure

SFT Fundamental Physics

Three different experiments for particle and nuclear physics have been identified at ESS in the past years:

- The cold beam line: ANNI.

This beam line has several associated experiments that include: measurements of correlation coefficients in neutron beta decay, study of the hadronic weak interactions, electromagnetic properties of the neutrons and a dedicated mirror neutron searches experiment called HIBEAM “High Intensity Baryon extraction and measurement”

- The neutron-antineutron experiment: NNBAR

- A dedicated UCN source

In addition to the neutron project there are two neutrinos proposed experiments:

-the nuESS that will study the Coherent Elastic Neutrino-Nucleus Scattering (CEvNS) process at ESS

-the ESSnuSB project that has the ambitious goal of creating a sufficiently intense neutrino Super Beam to enable measurement of leptonic CP violation.

Grants and other Funding Applications

- Nordforsk fellow “Design of a fundamental physics Capability for the ESS”
The major objective of this work is a full design proposal of the fundamental physics beamline, taking into account the most recent developments in ESS design and will expand the previous ANNI design to also include the HIBEAM experiment.
- An ESS-led European Commission INFRADEV proposal of 3 MEUROS has been awarded and funded as Research and Innovation Action with the EU Horizon 2020 program. The project acronym is HighNESS (High Intensity Neutron source for ESS), and its main scientific object is to develop the CDR for the ESS upgrade. In the context of this project a full workpackage is dedicated to Fundamental Physics searches for future instrument at ESS. The project started in October 2020.
- VR Grant has been awarded by David Milstead for the project “The HIBEAM Experiment to Search for Baryon Number violation at the ESS” for 3MSEK that will be spent largely on a PhD student. The grant is basically a design study of HIBEAM for ANNI including detector studies for nnbar (at HIBEAM). The aim is the design and quantification of the potential of HIBEAM.

Seminars, Conferences and Outreach

ASP Online Seminars: <https://indico.cern.ch/event/983217/>

Fundamental physics possibilities with neutrons at the European Spallation Source
Valentina Santoro, 2 February 2021

Partikeldagarna 2020: <https://indico.cern.ch/event/933206/>

-HighNESS and future free neutron oscillation searches @ ESS, Valentina Santoro, 24 November 2020

-A neutron antineutron annihilation detector for the NNBAR experiment Katherine Dunne, 24 November 2020

-Cosmic ray background at the NNBAR experiment Sze Chung Yiu, 24 November 2020

ESS-ILL User meeting: <https://indico.esss.lu.se/event/1507/>

A Topical Workshop about Fundamental Physics has been held digitally on the 14th of October 2020. Total of 66 registrants have attended the workshop with many participants from non-Europeans countries. As a follow-up to this meeting the fundamental physics community is working towards a combined paper about “Fundamental physics possibilities at ESS”.

Theoretical Innovations for Future Experiments Regarding Baryon number Violation:
<https://indico.fnal.gov/event/44472/>

The European Spallation Source and Future Free Neutron Oscillations Searches
Valentina Santoro, 3 August, 2020

Mini-workshop on neutron scattering and the phase shift
[:https://indico.esss.lu.se/event/1477/](https://indico.esss.lu.se/event/1477/)

22 June 2020, organized by Valentina Santoro, David Milstead and Albert Young

Seminar with the title “Future upgrade possibilities of the ESS linac for the ESSnuSB project” by Björn Gålnander ESS March 5, 2020

Publications

New high-sensitivity searches for neutrons converting into antineutrons and/or sterile neutrons at the European Spallation Source, Addazi *et al*

<https://arxiv.org/abs/2006.04907> (submitted to Journal of Physics G: Nuclear and Particle Physics)

$|\Delta B|=2$: A State of the Field, and Looking Forward--A brief status report of theoretical and experimental physics opportunities, [Kaladi Babu](#) *et al*

<https://arxiv.org/abs/2010.02299>

Coherent Elastic Neutrino-Nucleus Scattering at the European Spallation Source, **D. Baxter** *et al* Journal of High Energy Physics volume 2020, Article number: 123 (2020)

Members

Alan Takibayev , Arno Hiess , Beate Linnenberg , Douglas Di Julio , Esben Bryndt Klinkby, Günter Muhrer , Linda Coney, Luca Zanini , Mats Lindroos, Nataliia Cherkashyna, Phillip Bentley, Richard Hall-Wilton, Thomas Kittelmann, Valentina Santoro, Yong Joong Lee

Students and PostDocs (co-supervised by ESS staff)

- 1) by Valentina Santoro: Blahoslav Rataj " Design of a fundamental Physics Capability for the ESS : the HIBEAM/NNBAR program"
- 2) by Valentina Santoro: Vijay Sharm Nordforsk fellow "Design of a fundamental physics Capability for the ESS"
- 3) by Douglas Di Julio: Jesper Karlsson Gumprecht

Annual Analysis of Published Research Arising from ESS

Introduction

Scientific publications are one of the most significant outputs from ESS. In addition to recording the total number of publications in a year, it is important to make an estimate of the overall scientific impact being made by those publications. This report will be produced each year to present data for the previous year, and to update the scientific impact figures for the previous five years.

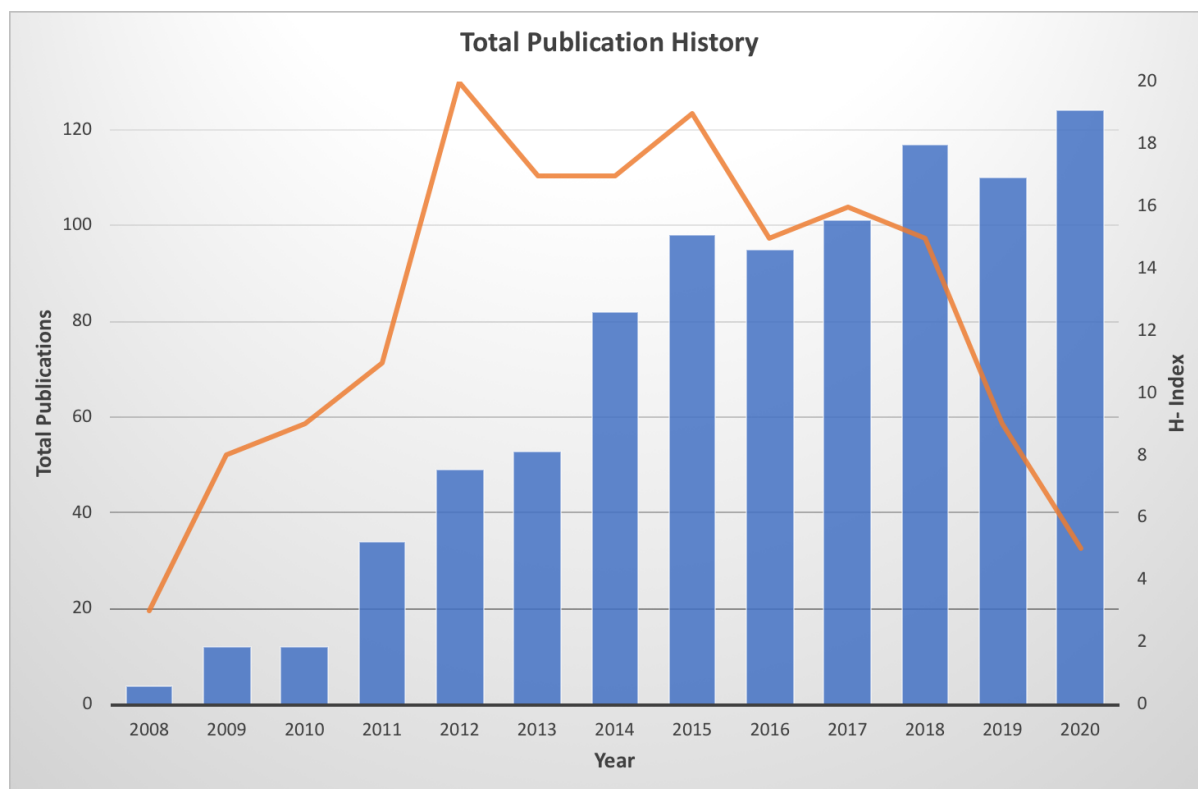
Total Publications

The method used to trace publications involving ESS is to search the Web of Science database for author addresses that include ESS, Lund, SE or ESS, DMSC, Copenhagen, DK. This search is flexible to include 24 potential ways of presenting the address (see Appendix 1). The list is manually audited to remove the false positives. This provides the total publications figure for the year.

The total number of publications for the most recent year is subject to change while databases update to reflect the actual status of that year. ***As of January 16th 2021, ESS has 124 publications in the Core Collection of Web of Science.***

H-index

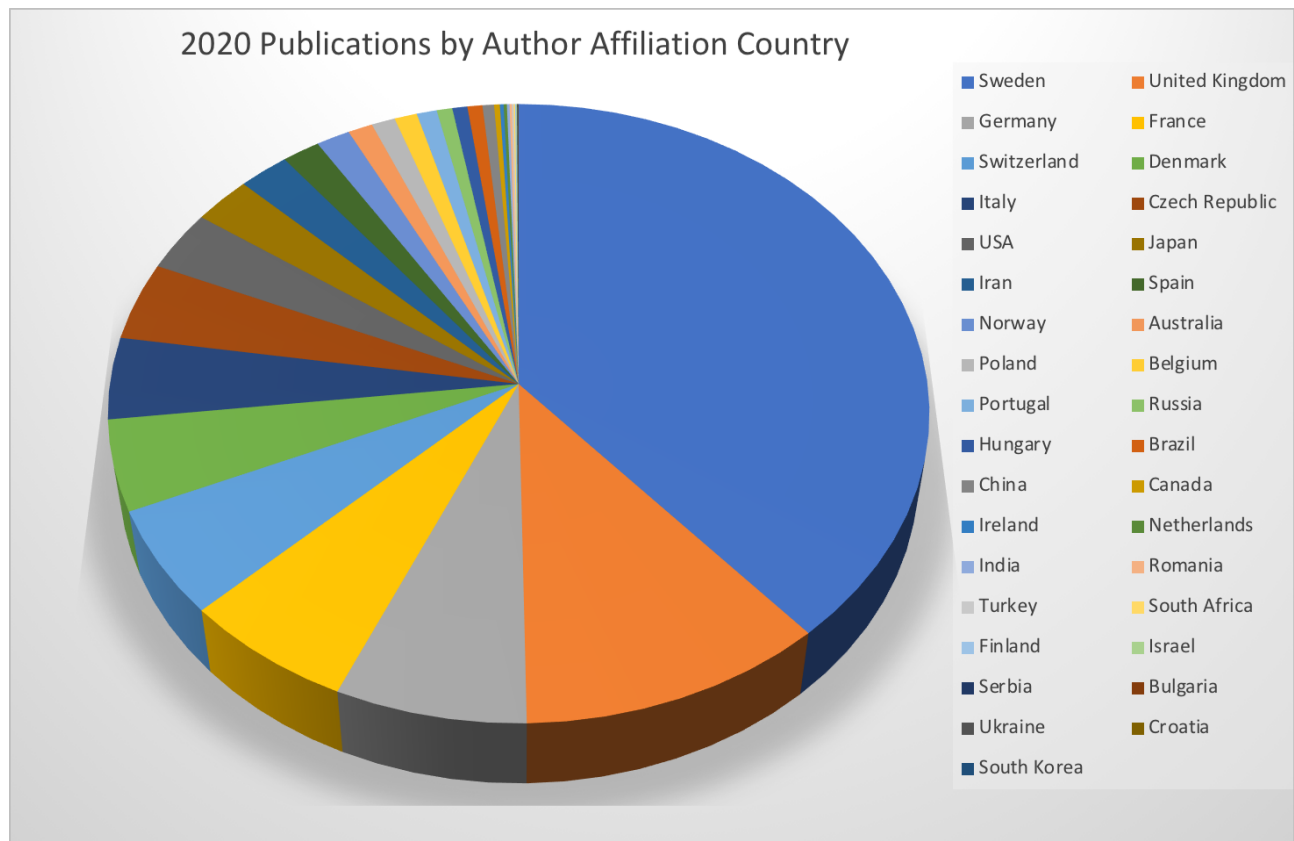
Having identified all the publications for a given year the H-index has been taken from the data included in Web of Science. The H-index means that there are h papers that have been cited at least h times and therefore gives an indication of the scientific impact of the publications. This is determined for the institute using the *annual* publication list, in the same way as an individual would determine their H-index over their total publications. Example: Today 17 out of 53 publications from 2013 have been cited 17 times or more. Since the H-index requires publications to be cited, there is typically a lag phase in the H-index settling.



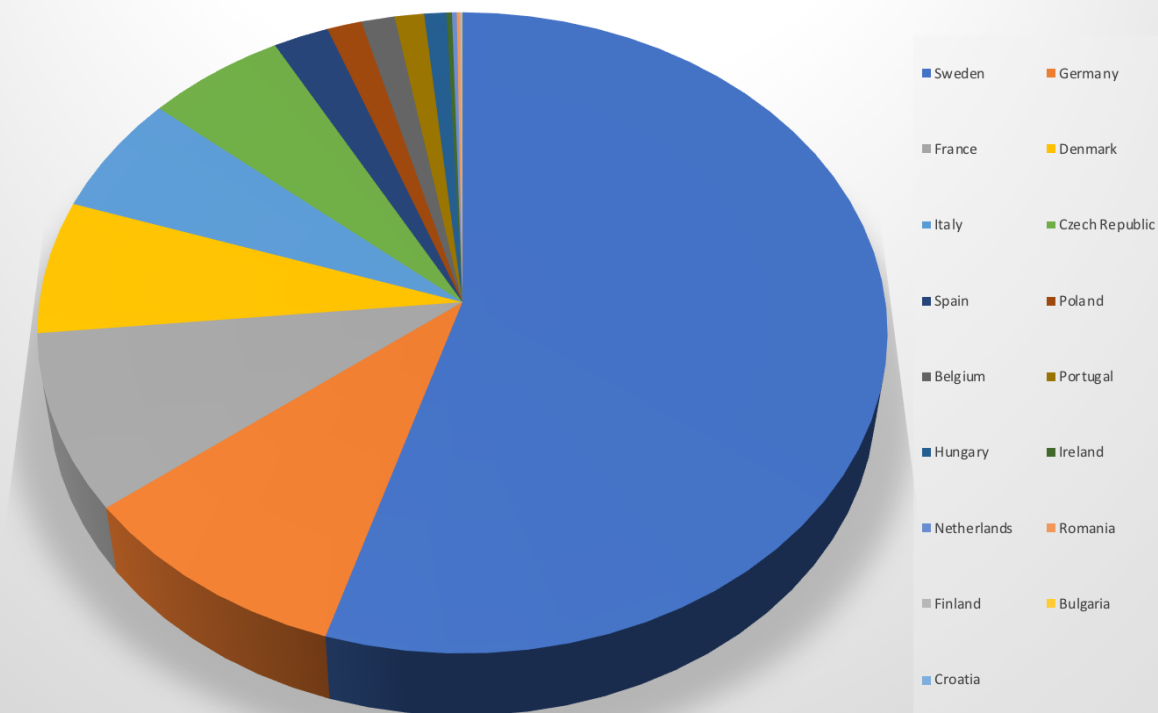
Share of Publication Authors by Country

This is determined according to the advice from ESFRI in the 2019 Working Group Report 'Monitoring of Research Infrastructure Performance'. Each publication is given a country unit of 1 that is divided equally among the countries given in the author affiliation. Where an author gives more than one affiliation, each is assumed to be equal.

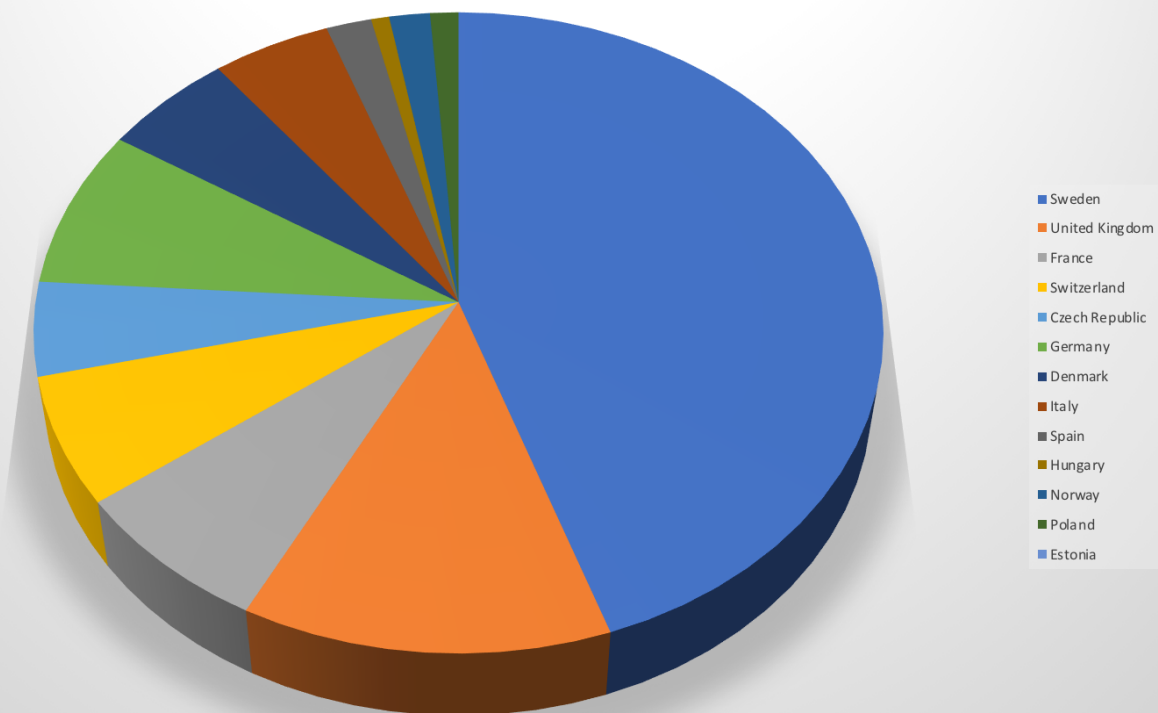
Data are shown for all countries, for ESFRI member countries and for ESS member countries. ***It should be noted that 70.5% of the publications are from ESFRI member countries and 86.3% of the publications come from ESS member countries.***



2020 Publications: Author affiliation by ESFRI member country



2020 Publications: Author affiliation by ESS member country



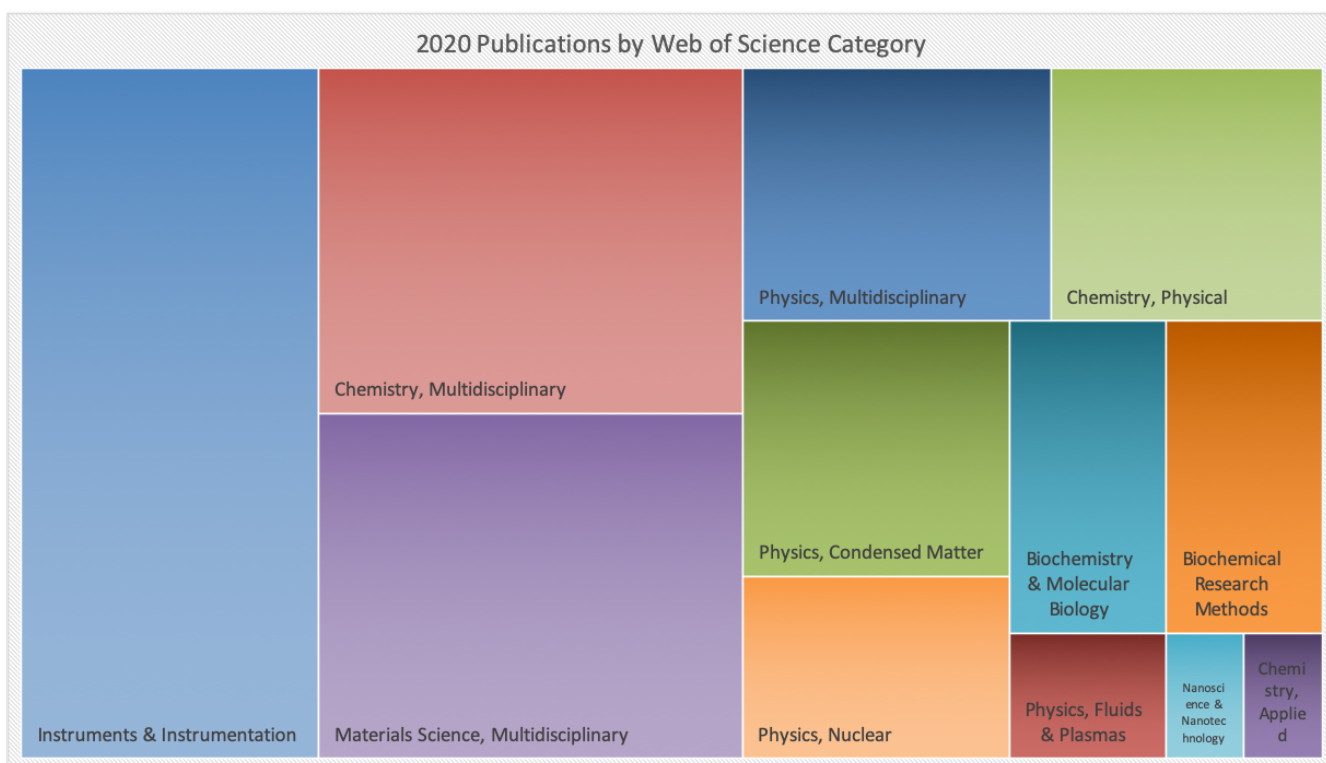
Share of Publications in Science Directorate

A list of members of the ESS science directorate and those matrixed to the ESS science directorate has been produced based on the organogram available on the ESS intranet. Using a search of last name and institute, the full publication list has been searched for publications from the ESS science directorate and affiliates.

If the list of science directorate staff is made available, this can be back-dated to 2008 when ESS publications began to appear in the database. Otherwise this indicator will be presented moving forward from 2019 when 56 publications include ESS science directorate staff or affiliates in the author list.

In 2020, the list of science directorate staff and affiliates has not been updated. It was created in the last quarter of 2019. ***In 2020 67 publications include ESS science directorate staff or affiliates in the author list.***

Web of Science gives each publication at least one science category. The tree map below has been produced by totalling the number of publications in 2020 with each primary science category. Only the first 12 categories are included, representing 75% of the publications from 2020.



Percentage of Top Cited Publications

The number of citations of a publication can give an indication of the quality of the publication. Since citations accrue over time this value will be carried out for a four-year period ending two years previously i.e. for 2020 it will look at publications from 2015 – 2018.

The methodology is somewhat complex but once established can simply be repeated. From the total paper search each publication has a total number of citations and a Web of Science category. The Web of Science category is converted to an InCites category. InCites is a database running alongside Web of Science and they provide the number of citations expected in each category for a top10% article for each year. A simple comparison between the number of citations each publication has and the top 10% figure gives the number of top 10% cited publications from ESS per year.

- 2015: 7 top 10% cited publications
- 2016: 3 top 10% cited publications
- 2017: 8 top 10% cited publications
- 2018: 11 top 10% cited publications

From the papers published in 2020, the most highly cited paper, with 22 citations, is:

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).

From all the papers published by ESS, the most highly cited paper, with 355 lifetime citations is:

Weller, M. T., Weber, O. J., Henry, P. F., Di Pumpo, A. M. & Hansen, T. C. Complete structure and cation orientation in the perovskite photovoltaic methylammonium lead iodide between 100 and 352 K. *Chemical Communications* **51**, 4180-4183, doi:10.1039/c4cc09944c (2015).

Appendix 1

Web of Science Search:

AD=(ESS OR ESS AB OR ESS ERIC OR ESS European Spallat Source OR ESS European Spallat Source ERIC OR ESS European Spallation OR Source ESS European Spallation Source AB OR ESS European Spallation Source ERIC OR ESS Scandinavia OR European Spallat Source OR European Spallat Source AB OR European Spallat Source ERIC OR European Spallat Source ERIC ESS OR European Spallat Source ESS OR European Spallat Source ESS AB OR European Spallat Source ESS ERIC OR European Spallation Source OR European Spallation Source AB OR European Spallation Source ERIC OR European Spallation Source ESS OR European Spallation Source ESS AB OR European Spallation Source ESS ERIC OR DMSC OR Data Management and software center) AND AD=(Lund OR Copenhagen) AND PY=2020

Appendix 2

References for the 2020 publications are given below.

- 1 Aden, J. *et al.* Mitochondrial Membranes Involved in Apoptosis - the Bcl-2 Proteins. *Biophysical Journal* **118**, 394A-394A (2020).
- 2 Ahmadiannamin, S. *et al.* Design of 100 MHz RF cavity for the storage ring of the Iranian Light Source Facility (ILSF). *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **981**, doi:10.1016/j.nima.2020.164529 (2020).
- 3 Albani, G. *et al.* High-rate measurements of the novel BAND-GEM technology for thermal neutron detection at spallation sources. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **957**, doi:10.1016/j.nima.2020.163389 (2020).
- 4 Alef, S. *et al.* The BGOOD experimental setup at ELSA. *European Physical Journal A* **56**, doi:10.1140/epja/s10050-020-00107-x (2020).
- 5 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**, doi:10.1016/j.nima.2020.163402 (2020).
- 6 Arai, M. *et al.* The performance of ESS spectrometers in comparison with instruments at a short-pulse source. *Journal of Neutron Research* **22**, 71-85, doi:10.3233/jnr-190119 (2020).
- 7 Arnold, P. *et al.* in *Advances in Cryogenic Engineering* Vol. 755 IOP Conference Series-Materials Science and Engineering (2020).
- 8 Balossino, I. *et al.* u-RANIA: a neutron detector based on mu-RWELL technology. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/09/c09029 (2020).
- 9 Belloni, F. *et al.* Five transversal beam profile monitors for the ESS Cold Linac. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/05/c05070 (2020).
- 10 Bentley, P. M. & Filges, U. Metaheuristic layout design of a 2 billion euro science facility. *Journal of Physics Communications* **4**, doi:10.1088/2399-6528/ab8782 (2020).
- 11 Bentley, P. Accurate Simulation of Neutrons in Less Than One Minute Pt. 2: Sandman-GPU-Accelerated Adjoint Monte-Carlo Sampled Acceptance Diagrams. *Quantum Beam Science* **4**, doi:10.3390/qubs4020024 (2020).
- 12 Bentley, P. M. Instrument suite cost optimisation in a science megaproject. *Journal of Physics Communications* **4**, doi:10.1088/2399-6528/ab8a06 (2020).

- 13 Beran, P. *et al.* In Situ Neutron Diffraction Study of Ni Addition in Co-Re-Cr High-Temperature Alloys and Influence on Phase Transformations. *Journal of Surface Investigation* **14**, S179-S184, doi:10.1134/s1027451020070071 (2020).
- 14 Bergmann, J., Davidson, M., Oksanen, E., Ryde, U. & Jayatilaka, D. fragHAR: towards ab initio quantum-crystallographic X-ray structure refinement for polypeptides and proteins. *Iucrj* **7**, 158-165, doi:10.1107/s2052252519015975 (2020).
- 15 Billington, D. *et al.* Bulk and element-specific magnetism of medium-entropy and high-entropy Cantor-Wu alloys. *Physical Review B* **102**, doi:10.1103/PhysRevB.102.174405 (2020).
- 16 Blayo, C. *et al.* Light-responsive self-assembly of a cationic azobenzene surfactant at high concentration. *Soft Matter* **16**, 9183-9187, doi:10.1039/d0sm01512a (2020).
- 17 Bogojevic, O. & Leung, A. E. Enzyme-Assisted Synthesis of High-Purity, Chain-Deuterated 1-Palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine. *Acs Omega* **5**, 22395-22401, doi:10.1021/acsomega.0c02823 (2020).
- 18 Bogomilov, M. *et al.* Demonstration of cooling by the Muon Ionization Cooling Experiment. *Nature* **578**, 53-+, doi:10.1038/s41586-020-1958-9 (2020).
- 19 Bordallo, H. N., Lioma, C., Taylor, J. & Argyriou, D. N. Is artificial intelligence magic dust for big-science facilities? *Iucrj* **7**, 1-2, doi:10.1107/s2052252519016476 (2020).
- 20 Budayova-Spano, M., Koruza, K. & Fisher, Z. in *Neutron Crystallography in Structural Biology* Vol. 634 *Methods in Enzymology* (ed P. C. E. Moody) 21-46 (2020).
- 21 Cai, X. X. & Kittelmann, T. NCrystal: A library for thermal neutron transport. *Computer Physics Communications* **246**, doi:10.1016/j.cpc.2019.07.015 (2020).
- 22 Caldararu, O., Ignjatovic, M. M., Oksanen, E. & Ryde, U. Water structure in solution and crystal molecular dynamics simulations compared to protein crystal structures. *Rsc Advances* **10**, 8435-8443, doi:10.1039/c9ra09601a (2020).
- 23 Caldararu, O., Manzoni, F., Oksanen, E., Logan, D. T. & Ryde, U. Refinement of protein structures using a combination of quantum-mechanical calculations with neutron and X-ray crystallographic data (vol D75, pg 368, 2019). *Acta Crystallographica Section D-Structural Biology* **76**, 85-86, doi:10.1107/s2059798319016383 (2020).
- 24 Capone, M., Ridley, C. J., Funnell, N. P., Guthrie, M. & Bull, C. L. Subtle Structural Changes in LaFeO(3) at High Pressure. *Physica Status Solidi B-Basic Solid State Physics* **258**, doi:10.1002/pssb.202000413 (2021).
- 25 Carminati, C. *et al.* Bragg-edge attenuation spectra at voxel level from 4D wavelength-resolved neutron tomography. *Journal of Applied Crystallography* **53**, 188-196, doi:10.1107/s1600576720000151 (2020).
- 26 Chambon, A., Klinkby, E., Emas, L. & Lauritzen, B. Assessment of shutdown dose rates at the ESS target cooling system using SCALE6.2. *Journal of Neutron Research* **22**, 309-318, doi:10.3233/jnr-190136 (2020).
- 27 Chevrier, M. *et al.* Phosphonium-based polythiophene conjugated polyelectrolytes with different surfactant counterions: thermal properties, self-assembly and photovoltaic performances. *Polymer International*, doi:10.1002/pi.6088 (2020).
- 28 Choi, J. *et al.* Spatially inhomogeneous competition between superconductivity and the charge density wave in YBa₂Cu₃O_{6.67}. *Nature Communications* **11**, doi:10.1038/s41467-020-14536-1 (2020).
- 29 Christensen, M. J. & Richter, T. Achieving reliable UDP transmission at 10 Gb/s using BSD socket for data acquisition systems. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/09/t09005

(2020).

- 30 Clabbers, M. T. B., Fisher, S. Z., Coincon, M., Zou, X. & Xu, H. Visualizing drug binding interactions using microcrystal electron diffraction. *Communications Biology* **3**, doi:10.1038/s42003-020-01155-1 (2020).
- 31 Collins, M. & Martins, C. A. Optimal Design of a High-Voltage DC/DC Converter for the 11.5-MW/115-kV ESS Long-Pulse Modulator. *Ieee Transactions on Plasma Science* **48**, 3332-3341, doi:10.1109/tps.2020.2991451 (2020).
- 32 Damay, F. *et al.* Magnetic phase diagram for Fe₃-xMnxBO₅. *Physical Review B* **101**, doi:10.1103/PhysRevB.101.094418 (2020).
- 33 Delhom, R. *et al.* The Antifungal Mechanism of Amphotericin B Elucidated in Ergosterol and Cholesterol-Containing Membranes Using Neutron Reflectometry. *Nanomaterials* **10**, doi:10.3390/nano10122439 (2020).
- 34 Dicko, C. *et al.* NUrF-Optimization of in situ UV-vis and fluorescence and autonomous characterization techniques with small-angle neutron scattering instrumentation. *Review of Scientific Instruments* **91**, doi:10.1063/5.0011325 (2020).
- 35 DiJulio, D. D., Lee, Y. J. & Muhrer, G. Impact of crystallite size on the performance of a beryllium reflector. *Journal of Neutron Research* **22**, 275-279, doi:10.3233/jnr-190135 (2020).
- 36 DiJulio, D. D., Svensson, I., Cai, X. X., Cederkall, J. & Bentley, P. M. Simulating neutron transport in long beamlines at a spallation neutron source using Geant4. *Journal of Neutron Research* **22**, 183-189, doi:10.3233/jnr-190134 (2020).
- 37 Edberg, R. *et al.* Effects of uniaxial pressure on the spin ice Ho₂Ti₂O₇. *Physical Review B* **102**, doi:10.1103/PhysRevB.102.184408 (2020).
- 38 Eriksson, A., Caldararu, O., Ryde, U. & Oksanen, E. Automated orientation of water molecules in neutron crystallographic structures of proteins. *Acta Crystallographica Section D-Structural Biology* **76**, 1025-1032, doi:10.1107/s2059798320011729 (2020).
- 39 Eshraqi, M. *et al.* First Protons in the ESS LINAC. *Journal of Surface Investigation* **14**, S42-S49, doi:10.1134/s1027451020070137 (2020).
- 40 Eshraqi, M. & Lagniel, J. M. Choice of Linac parameters to minimize the space-charge effects. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/07/p07024 (2020).
- 41 Evans, P. G. *et al.* Resonant nanodiffraction x-ray imaging reveals role of magnetic domains in complex oxide spin caloritronics. *Science Advances* **6**, doi:10.1126/sciadv.aba9351 (2020).
- 42 Farmer, T. O., Markvardsen, A. J., Rod, T. H., Bordallo, H. N. & Swenson, J. Dynamical Accuracy of Water Models on Supercooling. *Journal of Physical Chemistry Letters* **11**, 7469-7475, doi:10.1021/acs.jpclett.0c02158 (2020).
- 43 Fydrych, J., Pietrowicz, S. & Iop. in *Advances in Cryogenic Engineering* Vol. 755 IOP Conference Series-Materials Science and Engineering (2020).
- 44 Garcia, J. C. & Osorio, R. R. Comparison of Hardwired and Microprogrammed Statechart Implementations. *Electronics* **9**, doi:10.3390/electronics9071139 (2020).
- 45 Geprags, S. *et al.* Precise control of J(eff)=1/2 magnetic properties in Sr₂IrO₄ epitaxial thin films by variation of strain and thin film thickness. *Physical Review B* **102**, doi:10.1103/PhysRevB.102.214402 (2020).
- 46 Gohil, C. *et al.* Luminosity performance of the Compact Linear Collider at 380 GeV with static and dynamic imperfections. *Physical Review Accelerators and Beams* **23**, doi:10.1103/PhysRevAccelBeams.23.101001 (2020).

- 47 Guarini, E. *et al.* Neutron Brillouin scattering and ab initio simulation study of the collective dynamics of liquid silver. *Physical Review B* **102**, doi:10.1103/PhysRevB.102.054210 (2020).
- 48 Hall, S. C. L. *et al.* Adsorption of a styrene maleic acid (SMA) copolymer-stabilized phospholipid nanodisc on a solid-supported planar lipid bilayer. *Journal of Colloid and Interface Science* **574**, 272-284, doi:10.1016/j.jcis.2020.04.013 (2020).
- 49 Heybrock, S., Arnold, O., Gudich, I., Nixon, D. & Vaytet, N. Scipp: Scientific data handling with labeled multi-dimensional arrays for C++ and Python. *Journal of Neutron Research* **22**, 169-181, doi:10.3233/jnr-190131 (2020).
- 50 Hillenbrand, P.-M. *et al.* Experimental study of the proton-transfer reaction $C + H_2(+) \rightarrow CH^+ + H$ and its isotopic variant ($D_2(+) \rightarrow CD^+ + H$). *Physical Chemistry Chemical Physics* **22**, 27364-27384, doi:10.1039/d0cp04810k (2020).
- 51 Hjorth-Jensen, S. J., Oksanen, E., Nissen, P. & Sorensen, T. L.-M. in *Neutron Crystallography in Structural Biology* Vol. 634 *Methods in Enzymology* (ed P. C. E. Moody) 47-68 (2020).
- 52 Hogberg, H. *et al.* Reactive sputtering of CS_x thin solid films using CS₂ as precursor. *Vacuum* **182**, doi:10.1016/j.vacuum.2020.109775 (2020).
- 53 Ibison, M. G. *et al.* Development of a beam imaging system for the European spallation source tuning dump. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **950**, doi:10.1016/j.nima.2019.162790 (2020).
- 54 Jamalipour, M., Zanini, L. & Gorini, G. Implementation of Neutron Reflection with Nano-Dispersed Media in Geant4. *Journal of Surface Investigation* **14**, S75-S78, doi:10.1134/s1027451020070174 (2020).
- 55 Jellyman, E. *et al.* Unconventional superconductivity in the nickel chalcogenide superconductor TiNi₂Se₂. *Physical Review B* **101**, doi:10.1103/PhysRevB.101.134523 (2020).
- 56 Junius, N., Vahdatahar, E., Oksanen, E., Ferrer, J.-L. & Budayova-Spano, M. Optimization of crystallization of biological macromolecules using dialysis combined with temperature control. *Journal of Applied Crystallography* **53**, 686-698, doi:10.1107/s1600576720003209 (2020).
- 57 Kelly, E. A. A. *et al.* A single-component photorheological fluid with light-responsive viscosity. *Nanoscale* **12**, 6300-6306, doi:10.1039/c9nr10350c (2020).
- 58 Keyvani, A., Mostafavi, N., Bahamirian, M., Sina, H. & Rabieizadeh, A. Synthesis and phase stability of zirconia-lanthania-ytterbia-yttria nanoparticles; a promising advanced TBC material. *Journal of Asian Ceramic Societies* **8**, 336-344, doi:10.1080/21870764.2020.1743419 (2020).
- 59 Khodaei, M. *et al.* Magnesium/Nano-hydroxyapatite Composite for Bone Reconstruction: The Effect of Processing Method. *Journal of Bionic Engineering* **17**, 92-99, doi:10.1007/s42235-020-0007-6 (2020).
- 60 Kimber, S. A. J., Wildes, A. R., Mutka, H., Bos, J.-W. G. & Argyriou, D. N. Spin-chain correlations in the frustrated triangular lattice material CuMnO₂. *Journal of Physics-Condensed Matter* **32**, doi:10.1088/1361-648X/ab9d4b (2020).
- 61 Koller, M. *et al.* An ultrasonic study of relaxation processes in pure and mechanically alloyed tungsten. *International Journal of Refractory Metals & Hard Materials* **90**, doi:10.1016/j.ijrmhm.2020.105233 (2020).
- 62 Koruza, K. *et al.* Biophysical Characterization of Cancer-Related Carbonic Anhydrase IX. *International Journal of Molecular Sciences* **21**, doi:10.3390/ijms21155277 (2020).
- 63 Krauss, I. R. *et al.* Interaction with Human Serum Proteins Reveals Biocompatibility of Phosphocholine-Functionalized SPIONs and Formation of Albumin-Decorated Nanoparticles. *Langmuir* **36**, 8777-8791, doi:10.1021/acs.langmuir.0c01083 (2020).

- 64 Laface, E. & Folsom, B. T. Covariant Hamiltonian approach for time-dependent potentials applied to a pill-box cavity. *Physical Review Accelerators and Beams* **23**, doi:10.1103/PhysRevAccelBeams.23.104001 (2020).
- 65 Larsen, S. R. *et al.* Physicochemical characterisation of fluorohectorite: Water dynamics and nanocarrier properties. *Microporous and Mesoporous Materials* **306**, doi:10.1016/j.micromeso.2020.110512 (2020).
- 66 Lee, Y. Lifetime assessment of functional components in the ESS target environment during beam energy ramp up. *Journal of Neutron Research* **22**, 299-308, doi:10.3233/jnr-200151 (2020).
- 67 Lima, C. R. R. C. *et al.* Human hair: subtle change in the thioester groups dynamics observed by combining neutron scattering, X-ray diffraction and thermal analysis. *European Physical Journal-Special Topics* **229**, 2825-2832, doi:10.1140/epjst/e2020-900217-4 (2020).
- 68 Liu, T. *et al.* Vibrational Behavior of Water Adsorbed on Forsterite (Mg₂SiO₄) Surfaces. *Acs Earth and Space Chemistry* **4**, 1050-1063, doi:10.1021/acsearthspacechem.0c00084 (2020).
- 69 Loch, P. *et al.* Spontaneous formation of an ordered interstratification upon Ni-exchange of Na-fluorohectorite. *Applied Clay Science* **198**, doi:10.1016/j.clay.2020.105831 (2020).
- 70 Luchini, A. *et al.* Effect of ergosterol on the interlamellar spacing of deuterated yeast phospholipid multilayers. *Chemistry and Physics of Lipids* **227**, doi:10.1016/j.chemphyslip.2020.104873 (2020).
- 71 Luzin, V., Kirstein, O., Zahiri, S. H. & Fraser, D. Residual Stress Buildup in Ti Components Produced by Cold Spray Additive Manufacturing (CSAM). *Journal of Thermal Spray Technology* **29**, 1498-1507, doi:10.1007/s11666-020-01048-z (2020).
- 72 Lyngh, D. *et al.* Engineering and prototyping of ESS neutron beam extraction system. *Journal of Neutron Research* **22**, 109-118, doi:10.3233/jnr-200155 (2020).
- 73 Marattukalam, J. J. *et al.* The effect of laser scanning strategies on texture, mechanical properties, and site-specific grain orientation in selective laser melted 316L SS. *Materials & Design* **193**, doi:10.1016/j.matdes.2020.108852 (2020).
- 74 Margato, L. M. S. *et al.* Multilayer B-10-RPC neutron imaging detector. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/06/p06007 (2020).
- 75 Marko, M., Nagy, G., Aprigliano, G. & Oksanen, E. in *Neutron Crystallography in Structural Biology* Vol. 634 *Methods in Enzymology* (ed P. C. E. Moody) 125-151 (2020).
- 76 Marques, A. P. *et al.* Minimizing distortions with sectored GEM electrodes. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **961**, doi:10.1016/j.nima.2020.163673 (2020).
- 77 Martins, M. L., Bordallo, H. N., Arrese-Igor, S., Alegria, A. & de Leon, J. C. Effect of Paclitaxel in the Water Dynamics of MCF-7 Breast Cancer Cells Revealed by Dielectric Spectroscopy. *Acs Omega* **5**, 18602-18607, doi:10.1021/acsomega.0c00897 (2020).
- 78 Massani, B. *et al.* On single-crystal neutron-diffraction in DACs: quantitative structure refinement of light elements on SNAP and TOPAZ. *High Pressure Research* **40**, 339-357, doi:10.1080/08957959.2020.1767100 (2020).
- 79 Mauri, G. *et al.* The Multi-Blade Boron-10-based neutron detector performance using a focusing reflectometer. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/03/p03010 (2020).
- 80 Maxim, F. *et al.* Thermodynamics and Dynamics of Supercritical Water Pseudo-Boiling. *Advanced Science* **8**, doi:10.1002/advs.202002312 (2021).
- 81 Meazzini, I. *et al.* Synthesis and characterisation of biocompatible organic-inorganic core-shell nanocomposite particles based on ureasils. *Journal of Materials Chemistry B* **8**, 4908-4916, doi:10.1039/d0tb00100g (2020).

- 82 Mehendale, S. *et al.* Characterization of boron-coated silicon sensors for thermal neutron detection. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **972**, doi:10.1016/j.nima.2020.164124 (2020).
- 83 Michalcova, A. *et al.* Structure and Properties of High-Strength Ti Grade 4 Prepared by Severe Plastic Deformation and Subsequent Heat Treatment. *Materials* **13**, doi:10.3390/ma13051116 (2020).
- 84 Michels, L. *et al.* The Impact of Thermal History on Water Adsorption in a Synthetic Nanolayered Silicate with Intercalated Li⁺ or Na⁺. *Journal of Physical Chemistry C* **124**, 24690-24703, doi:10.1021/acs.jpcc.0c05847 (2020).
- 85 Milas, N., Plostinar, C., Miyamoto, R., Eshraqi, M. & Liu, Y. Position-based cavity tuning. *Physical Review Accelerators and Beams* **23**, doi:10.1103/PhysRevAccelBeams.23.114002 (2020).
- 86 Miller, T. M., DiJulio, D. D. & Santoro, V. Application of ADVANTG variance reduction parameters with MCNP6 at ESS. *Journal of Neutron Research* **22**, 199-208, doi:10.3233/jnr-200158 (2020).
- 87 Mirfayzi, S. R. *et al.* A miniature thermal neutron source using high power lasers. *Applied Physics Letters* **116**, doi:10.1063/5.0003170 (2020).
- 88 Miyamoto, R. *et al.* Highlights from the first beam commissioning stage at ESS for its ion source and low energy beam transport. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/07/p07027 (2020).
- 89 Morgano, M. *et al.* Investigation of the effect of Laser Shock Peening in Additively Manufactured samples through Bragg Edge Neutron Imaging. *Additive Manufacturing* **34**, doi:10.1016/j.addma.2020.101201 (2020).
- 90 Morozov, A., Margato, L. M. S. & Stefanescu, I. Simulation-based optimization of a multilayer B-10-RPC thermal neutron detector. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/03/p03019 (2020).
- 91 Nafradi, G. *et al.* Shielding considerations for ESS LoKI. *Journal of Neutron Research* **22**, 119-129, doi:10.3233/jnr-200152 (2020).
- 92 Oliver, R. C. *et al.* Assembly of Capsids from Hepatitis B Virus Core Protein Progresses through Highly Populated Intermediates in the Presence and Absence of RNA. *Acs Nano* **14**, 10226-10238, doi:10.1021/acsnano.0c03569 (2020).
- 93 Pietropaolo, A. *et al.* Neutron detection techniques from mu eV to GeV. *Physics Reports-Review Section of Physics Letters* **875**, 1-65, doi:10.1016/j.physrep.2020.06.003 (2020).
- 94 Piscitelli, F., Mauri, G., Laloni, A. & Hall-Wilton, R. Verification of He-3 proportional counters' fast neutron sensitivity through a comparison with He-4 detectors: He-3 and He-4 proportional counters' fast neutron sensitivity and evaluation of the cosmic neutron fluxes at ESS. *European Physical Journal Plus* **135**, doi:10.1140/epjp/s13360-020-00600-8 (2020).
- 95 Pospelov, G. *et al.* BornAgain: software for simulating and fitting grazing-incidence small-angle scattering. *Journal of Applied Crystallography* **53**, 262-276, doi:10.1107/s1600576719016789 (2020).
- 96 Robarts, H. C. *et al.* Extreme Fermi Surface Smearing in a Maximally Disordered Concentrated Solid Solution. *Physical Review Letters* **124**, doi:10.1103/PhysRevLett.124.046402 (2020).
- 97 Rodriguez, J. M. O., Krupinska, E., Wacklin-Knecht, H. & Knecht, W. Preparation of human dihydroorotate dehydrogenase for interaction studies with lipid bilayers. *Nucleosides Nucleotides & Nucleic Acids* **39**, 1306-1319, doi:10.1080/15257770.2019.1708100 (2020).
- 98 Rofors, E. *et al.* Response of a Li-glass/multi-anode photomultiplier detector to focused proton and deuteron beams. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators*

- Spectrometers Detectors and Associated Equipment* **984**, doi:10.1016/j.nima.2020.164604 (2020).
- 99 Rogstam, A. *et al.* Crystal Structure of Non-Structural Protein 10 from Severe Acute Respiratory Syndrome Coronavirus-2. *International Journal of Molecular Sciences* **21**, doi:10.3390/ijms21197375 (2020).
 - 100 Samothrakitis, S. *et al.* A multiscale study of hot-extruded CoNiGa ferromagnetic shape-memory alloys. *Materials & Design* **196**, doi:10.1016/j.matdes.2020.109118 (2020).
 - 101 Sanchez-Fernandez, A. *et al.* An integrative toolbox to unlock the structure and dynamics of protein-surfactant complexes. *Nanoscale Advances* **2**, 4011-4023, doi:10.1039/d0na00194e (2020).
 - 102 Santoro, V. *et al.* Development of high intensity neutron source at the European Spallation Source. *Journal of Neutron Research* **22**, 209-219, doi:10.3233/jnr-200159 (2020).
 - 103 Sato, K. *et al.* Coexistence of Two Components in Magnetic Excitations of La₂-xSr_xCuO₄ (x=0.10 and 0.16). *Journal of the Physical Society of Japan* **89**, doi:10.7566/jpsj.89.114703 (2020).
 - 104 Scharenberg, L. *et al.* Gaseous detector studies with the VMM3a ASIC and the Scalable Readout System. *Journal of Instrumentation* **15**, doi:10.1088/1748-0221/15/08/c08026 (2020).
 - 105 Scharenberg, L. *et al.* Resolving soft X-ray absorption in energy, space and time in gaseous detectors using the VMM3a ASIC and the SRS. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **977**, doi:10.1016/j.nima.2020.164310 (2020).
 - 106 Schmakat, P. *et al.* Wavelength frame multiplication chopper system for the multi-purpose neutron-imaging instrument ODIN at the European Spallation Source. *Nuclear Instruments & Methods in Physics Research Section a-Accelerators Spectrometers Detectors and Associated Equipment* **979**, doi:10.1016/j.nima.2020.164467 (2020).
 - 107 Scionti, G. *et al.* Neutronic Calculations for the Shielding Design of the VESPA Instrument at the European Spallation Source. *Journal of Surface Investigation* **14**, S190-S194, doi:10.1134/s1027451020070411 (2020).
 - 108 Scotti, A. *et al.* Phase behavior of ultrasoft spheres show stable bcc lattices. *Physical Review E* **102**, doi:10.1103/PhysRevE.102.052602 (2020).
 - 109 Sharma, S. *et al.* Magnetic ground state of the ordered double-perovskite Sr₂YbRuO₆: Two magnetic transitions. *Physical Review B* **102**, doi:10.1103/PhysRevB.102.134412 (2020).
 - 110 Simpson, A. *et al.* Muon tomography for the analysis of in-container vitrified products. *Applied Radiation and Isotopes* **157**, doi:10.1016/j.apradiso.2019.109033 (2020).
 - 111 Stoltzfus, D. M. *et al.* Perdeuteration of poly 2-methoxy-5-(2'-ethylhexyloxy)-1,4-phenylenevinylene (d-MEH-PPV): control of microscopic charge-carrier spin-spin coupling and of magnetic-field effects in optoelectronic devices. *Journal of Materials Chemistry C* **8**, 2764-2771, doi:10.1039/c9tc05322k (2020).
 - 112 Strunz, P. *et al.* Texture and Differential Stress Development in W/Ni-Co Composite after Rotary Swaging. *Materials* **13**, doi:10.3390/ma13122869 (2020).
 - 113 Strunz, P., Kuncicka, L., Beran, P., Kocich, R. & Hervoches, C. Correlating Microstrain and Activated Slip Systems with Mechanical Properties within Rotary Swaged WNiCo Pseudoalloy. *Materials* **13**, doi:10.3390/ma13010208 (2020).
 - 114 Su, X. T. *et al.* in *Advances in Cryogenic Engineering* Vol. 755 IOP Conference Series-Materials Science and Engineering (2020).
 - 115 Tatsumoto, H. *et al.* in *Advances in Cryogenic Engineering* Vol. 755 IOP Conference Series-Materials Science and Engineering (2020).

- 116 Toft-Petersen, R., Georgii, R., Schneider, M., Nishiki, N. & Boeni, P. Characterization of pyrolytic graphite with cold neutrons. *Nuclear Instruments & Methods in Physics Research Section a- Accelerators Spectrometers Detectors and Associated Equipment* **977**, doi:10.1016/j.nima.2020.164341 (2020).
- 117 Uhlig, M. *et al.* New structural approach to rationalize the foam film stability of oppositely charged polyelectrolyte/surfactant mixtures. *Chemical Communications* **56**, 952-955, doi:10.1039/c9cc08470c (2020).
- 118 Unnep, R. *et al.* Thylakoid membrane reorganizations revealed by small-angle neutron scattering of *Monstera deliciosa* leaves associated with non-photochemical quenching. *Open Biology* **10**, doi:10.1098/rsob.200144 (2020).
- 119 Urbain, X. *et al.* in *31st International Conference on Photonic, Electronic and Atomic Collisions* Vol. 1412 *Journal of Physics Conference Series* (eds L. U. Ancarani *et al.*) (2020).
- 120 Valero, M., Levin, P. P., Sultimova, N. B. & Houston, J. E. Photochemistry of nabumetone in aqueous solution of sodium dodecyl sulfate (SDS) micelles. *Journal of Molecular Liquids* **319**, doi:10.1016/j.molliq.2020.114093 (2020).
- 121 Wang, X. L. *et al.* in *Advances in Cryogenic Engineering* Vol. 755 *IOP Conference Series-Materials Science and Engineering* (2020).
- 122 Willendrup, P. K. & Lefmann, K. McStas (i): Introduction, use, and basic principles for ray-tracing simulations. *Journal of Neutron Research* **22**, 1-16, doi:10.3233/jnr-190108 (2020).
- 123 Zanini, L., DiJulio, D., Kennedy, S., Klinkby, E. & Santoro, V. Neutronic Design of the Bunker Shielding for the European Spallation Source. *Journal of Surface Investigation* **14**, S251-S253, doi:10.1134/s1027451020070538 (2020).
- 124 Zhang, C., Podlech, H. & Tanke, E. Realizing long radio-frequency quadrupole accelerators with multiple shorter and independent cavities. *Physical Review Accelerators and Beams* **23**, doi:10.1103/PhysRevAccelBeams.23.042003 (2020).