

ESS Lighthouse: Magnetism and Quantum Materials (Q-MAT)

2024 Annual Report



The ESS Lighthouse Q-MAT is financed by the Danish Government through NUF1 and contains the Danish neutron- and ESS-related activities within the fields of Magnetism and Quantum Materials.

Q-MAT was officially opened December 1st, 2020.

This report contains all activities and budget status within Q-MAT for the year 2024.

1. Partners and Management

We here list the institutions and scientists in Q-MAT and emphasize the changes that has taken place since the inauguration of the Lighthouse.

1.1 Partners

Q-MAT is composed of six partner institutions.

- AAU (University of Aalborg), Department of Materials and Production
- AU (University of Aarhus), Department of Chemistry
- SDU (University of Southern Denmark), Department of Physics, Chemistry, and Pharmacy
- RUC (Roskilde University), Department of Science and Environment
- DTU (Technical University of Denmark), Department of Energy Conversion and Storage; Department of Chemistry; Department of Physics
- KU (University of Copenhagen), Department of Geosciences; Department of Chemistry; Niels Bohr Institute

and the additional partners (observers)

- ESS Science Division, Lund
- ESS Data Management Center, Copenhagen
- DTI (Danish Technological Institute)

1.2 Daily Management

The day-to-day management group (in Danish known as "Fyrmestre") consists of:

- Niels Bech Christensen (DTU Physics)
- Jesper Bendix (KU Chemistry)
- Henrik M. Rønnow (KU NBI and EPFL)
- Brian Møller Andersen (KU NBI)
- Kim Lefmann (KU NBI)

under the directorship of Kim Lefmann and Niels Bech Christensen as Vice-Director. Administrative support by Maria Batista (KU, NBI).

Ulla Gro Nielsen (SDU) withdrew from the management group and from Q-MAT due to a change in position.

This group has met, virtually, 3 times in 2024.

1.3 The Steering Group

Consolidated on 18th December 2020, the Steering Group includes most of the scientists active in Q-MAT. In addition to the *Fyrmestre* members, these are:

- Lars Diekhöner (AAU)
- Mogens Christensen, Dan Mannix, and Bo B. Iversen (AU)
- Hans Jørgen Aagaard Jensen (SDU) (since May 2023)
- Dorte Posselt (RUC)
- Thomas Olsen, Cathrine Frandsen and Rasmus Toft-Petersen (DTU, Physics)
- Kasper Steen Pedersen (DTU, Chemistry)
- Nini Pryds (DTU, Energy)
- Kirsten M. Ø. Jensen (KU, Chemistry)
- Kristoffer Szilas (KU, Geoscience)
- Andreas Kreisel, assistant professor (KU, NBI)
- Sara Lopez Paz, assistant professor (KU, Chemistry) (from April 2024)

Furthermore, as observers:

- Jacob Overgaard (DTI)
- Pascale P. Deen (ESS)
- Greg Tucker (ESS-DMSC)

Thomas G. Pedersen (AAU), Jens-Erik Jørgensen (AU), and Jonathan Taylor (ESS-DMSC) withdrew from Q-MAT in 2021, while Tonci Balic-Zunic (KU) and Hossein Alimadadi (DTI) withdrew in 2022, and Peter Krogstrup Jeppesen (NBI) withdrew in 2023. Jacob Overgaard moved from AU to DTI but continues in Q-MAT.

1.4 The Reference Group

This group represents the political level at the partners and ensures the anchoring of Q-MAT within the partner organizations:

- KU: Joachim Matthiesen (NBI)
- DTU: Jane H. Nielsen (Physics)
- RUC: Dorthe Posselt
- SDU: Lars P. Christensen
- AU: Mogens Christensen
- AAU: Kjeld Pedersen, to be replaced in 2025
- DI (Danish Industry): Richard Larsen, withdrew in 2024

This group has met twice; April 2021 and November 2022. Joachim Matthiesen has replaced Jan W. Thomsen (NBI). A meeting mid-2024 was unfortunately canceled and a meeting in spring 2025 has been scheduled.

1.5 The International Advisory Board

This Board gives independent scientific advice to Q-MAT and consists of international experts in the field:

- Sian Dutton (University of Cambridge)
- Helen Walker (ISIS neutron facility, UK)
- Colette Boskovic (Melbourne University)
- Michael Baker (University of Manchester)
- Olav Syljuåsen (University of Oslo)
- Johan Chang (University of Zürich)

The board was established after the inauguration of Q-MAT and met for the first time in February 2023. The group will provide an evaluation in relation to the 2025 (physical) annual meeting.

2. Activities in Q-MAT, Organization and Budget

In the initial phase of the Lighthouse, the most important activities were recruitment, administration, and networking. Unfortunately, the pandemic limited the number of physical meetings.

In 2022 we expanded our activities, such as meetings and facility experiment and, as such, started the planned scientific program within Q-MAT. In 2023 and 2024, the activity (measured as annual budget spending) reached closer to the intended level.

2.1 Meeting activity

2.1.1 Annual Meeting and Steering Group Meeting, 9-10 October 2024, held at Rødvig

This meeting was held at Hotel Klitten in Rødvig, Stevns. Due to the pandemics, this was the third Q-MAT outing, having 32 participants. 5 of the Q-MAT PhD students presented their projects which gave rise to long discussions. In addition, there were 5 presentations from PhD students in related projects, not funded by Q-MAT. In addition, there was an update from ESS and from Nini Pryds, head of Functional Oxide Materials at DTU Energy. Together this shows that Q-MAT has been able to attract additional funding and connect the scientific community within magnetism and quantum material in Denmark.

The atmosphere was in general lively and collaborative. It was also discussed how we could approach private foundations as a group to obtain funding in the future; a preliminary plan targeting the Novo Nordisk Foundation was devised.

There was no adjacent SG meeting due to the lack of administrative points to discuss.

2.1.2 International Advisory Group Meeting

Due to scheduling issues, a planned IAG meeting was postponed to 2025.

2.2 Recruitment at Q-MAT

All planned positions in Q-MAT are now filled, except for two. Below we bring a total overview.

Name	Position	Partner	Topic	Start date -End date
Francesco Zamboni	PhD student	AAU	Single Molecule Magnets	Sept. 2021 - Aug. 2024
Jack Thomas-Hunt	PhD student	AU	Spin Seebeck effect	Mar. 2022 - Feb. 2025
Hannah H Nielsen	PhD student	AU	Single Molecule Magnets	Feb. 2021 - Jan. 2024

Mickey Pedersen	PhD student	SDU	Frustrated Magnetism	Apr. 2022 - Mar. 2025
Christian K. Kristensen	PhD student	RUC	Magnetic Polymers	Jan. 2022 – Dec. 2024
Lise G Hanson	PhD student	DTU Physics	Magnetic Nanoparticles	Oct. 2022 – Sept. 2025
NN	PhD student	DTU Physics	Quantum Magnetism and Superconductivity	2025- 2028
Sandip Guchait	Postdoc	DTU Physics	Q-MAT experiments	2025- 2026
Naoki Eguchi	PhD student	DTU Chem.	Frustrated Magnetism	Sept. 2022 – Aug. 2025
Clara Neerup Breiø	PhD student	KU NBI	Theory of superconductivity	Sept. 2020 – Aug. 2023
Kristine M L Krighaar	PhD student	KU NBI	Superconducting and ESS instrumentation	Apr. 2022 – June 2026
Emma Y Lenander	PhD student	KU NBI	Frustrated Magnetism	Jun. 2022 – June 2026
Andreas Kreisel	Assistant Professor	KU NBI	Q-MAT Theory	Sept. 2022 – Dec. 2025
Sara Lopez Paz	Tenure track Professor	KU Chem.	Q-MAT material development	April 2024

The essential position at KU Chemistry within Materials Development is an assistant professorship, which the department has upgraded to a tenure track professorship. Sara Lopez Paz started in this position April 2024.

2.3 Associated staff at Q-MAT

In addition to participants in the Steering Committee and mentioned observers, Q-MAT includes the following permanent employees.

- KU NBI: Jens Paaske
- KU Chemistry: Høgni Weihe, Stergios Piligkos
- DTU Energy: Jean-Claude Grivel

Around 30 young researchers in temporary positions are affiliated with Q-MAT but not financed by the grant. An overview of these positions is given in appendix A.1.

2.4 Q-MAT home page

A web page for Q-MAT has been established on the address <https://www.q-mat.nbi.ku.dk/> containing general information on Q-MAT; a list of related staff; Broad-brush description of the research areas; List of publications; News and Events; Job postings. It is maintained and updated by the Q-MAT admin.

2.5 Budget and spending in Q-MAT

In the original Q-MAT budget, many hires were aimed at 2021, and most of the 2 MDKK Chemistry lab was placed here. The pandemic changed this, giving delays in hiring, in particular the associate professor at KU Chemistry and two positions at DTU. This led to significant underspending in the initial part of the project.

The financial flow of the project is listed below; all amounts include 44% overhead (and the small spending in the end of 2020 has been merged into 2021). As one will see, the project has caught up, and in 2023-2024 the spending is 15-20% lower than planned. The later start has meant that we have applied for and received an extension of the budget period to ultimo 2026.

2021-2022

The delays do not give rise to re-distribution of funds between partners.	Position	Planned start	Actual start	Budget 2021 kkr.	Spending 2021 kkr.	Budget 2022 kkr.	Spending 2022 kkr.
RUC	PhD	2021/3	2022/1	289	0	527	361
AAU	PhD	2021/3	2021/9	308	168	602	498
SDU	PhD	2022/3	2022/4	29	1	309	404
AU	PhD 1	2022/3	2022/3	337	188	910	746
	PhD 2	2021/3	2021/2				
DTU Phys	Post doc	2020/9	-	1309	62	1925	327
	PhD 1	2022/9	-				
	PhD 2	2021/3	2022/9				
DTU Chem	PhD	2022/3	2022/9	0	0	323	109
DTU Energy	-	-	-	58	0	58	0
KU Geosci	-	-	-	29	33	29	52
KU Chem	Ass. Prof	2020/9	2024/4	2239	137 + 33	1.109	10
KU NBI	PhD 1	2021/3	2020/9	1096	775 +23	1443	1182
	PhD 2	2022/3	2022/3				
	PhD 3	2022/3	2022/6				
	Ass. Prof	2022/9	2022/10				
Sum	-	-	-	5693	1365 +56	7233	3690

2022-2024

The delays do not give rise to re-distribution of funds between partners.	Position	Planned start	Actual start	Budget 2023 kkr.	Spending 2023 kkr.	Budget 2024 kkr.	Spending 2024 kkr.	Difference 2024 Budget - spend (kkr)	Unspent total (kkr)
RUC	PhD	2021/3	2022/1	498	485	529	338	191	447
AAU	PhD	2021/3	2021/9	573	625	489	483	6	17
SDU	PhD	2022/3	2022/4	602	520	624	380	244	486
AU	PhD 1	2022/3	2022/3	1175	1023	1281	1120	161	505
	PhD 2	2021/3	2021/2						
DTU Phys	Post doc	2020/9	-	2291	1000	2216	793	1423	5818
	PhD 1	2022/9	-						
	PhD 2	2021/3	2022/9						
DTU Chem	PhD	2022/3	2022/9	573	503	676	637	39	541
DTU Energy	-	-	-	58	24	43	109	-66	155
KU Geosci	-	-	-	29	71	-12	0	-12	-12
KU Chem	Ass. Prof	2020/9	2024/4	1130	768	1497	1549	-52	3876
KU NBI	PhD 1	2021/3	2020/9	2589	2255	2182	2557	-375	2615
	PhD 2	2022/3	2022/3						
	PhD 3	2022/3	2022/6						
	Ass. Prof	2022/9	2022/10						
Sum	-	-	-	9518	7274	9525	7966	1559	14448

2.6 Connection to ESS

Q-MAT maintains its strong connection to ESS:

- Mogens Christensen and Dan Mannix (AU) are PI and instrument scientist for HEIMDAL, respectively.
- Niels B. Christensen and Rasmus Toft-Petersen (DTU): PI and instrument scientist for BIFROST, respectively.
- Pascale P. Deen (adjoint to KU, NBI) is the ESS Spectroscopy Division Head and also designed C-SPEC. All 3 instruments will play an important role for future activities related to Q-MAT
- Gregory Tucker and Henrik Jacobsen, ESS-DMSC, participated in the 2024 annual meeting of Q-MAT.
- The ESS Director General Helmut Schober is adjoint professor at DTU, Physics and associated with Q-MAT.

3. Activities in Q-MAT, Scientific

3.1 Highlights 2024

Lars Diekhöner (AAU) and Jesper Bendix (KU Chemistry):

We have investigated magnetic molecules adsorbed on surfaces under Ultra High Vacuum conditions. Experiments have been done by combining Scanning Tunneling Microscopy to study adsorption and ordering of molecules on the surface and Scanning Tunneling Spectroscopy to investigate the electronic structure and correlated electron phenomena of the molecule-surface systems. In addition, magnetic studies have been undertaken by employing X-ray absorption techniques.

Sara Lopez Paz (KU Chemistry):

Q-MAT has supported the establishment of a solid-state chemistry laboratory at KU Chemistry for advanced crystal growth of quantum materials. Facilities for crystal growth including a floating-zone mirror furnace and high-temperature modified atmosphere furnaces have been set up and tested. The research team lead by Sara Lopez involves currently 2 BSc, 2MSc and 1 PhD students, and is working in close collaboration with research groups at NBI. Preliminary neutron scattering studies of frustrated and quantum magnetic materials developed at the laboratory are in progress.

Brian M. Andersen and Andreas Kreisel (KU NBI):

Magnetism and unconventional superconductivity are tied together within investigations on correlated materials since it turns out that spin-fluctuations can explain a plethora of the experimental facts in the superconducting phase of cuprates, iron-based materials, heavy fermion systems and Sr_2RuO_2 . However, there is also a possibility that the superconductor becomes intrinsically “magnetic”, i.e. the time-reversal symmetry is broken in the superconducting phase. Several scenarios for this phenomenon have been proposed, a review article has been published on this topic and some of the proposals have been examined theoretically in the CMT group: One is the generation of spontaneous supercurrents close to non-magnetic disorder, another possibility is the condensation of two components of superconducting order parameters. On this topic was worked within two different projects: First, the possibility of unconventional superconductivity in kagome materials was examined and spectroscopic signatures calculated. Second, the example of a triplet superconducting state was considered where the presence of the so-called d-vector describing the order parameter allows for non-unitary states that also exhibit a non-zero magnetization and has unique properties in the specific heat. Finally, a project on multiband superconductivity revealed how ferromagnetic fluctuations can form a superposition of singlet and triplet superconductivity which exhibits an exotic state with Bogoliubov Fermi surfaces. Mixing between singlet and triplet superconductivity also occurs once spin-orbit coupling is included: Pairing in an so-called Ising-superconductor was examined in a work together with a group at IIT Madras, India, where members of the CMT group hold visiting professorships.

Two more projects were dedicated to the understanding of the superconducting state Sr_2RuO_2 where effects of nodal superconductivity on the magnetic penetration depth were theoretically calculated and explained experimental data that was published as joint articles on PRB.

The group has continued to work together with experimental colleagues on understanding local phenomena as measured with a tunneling microscope to reveal how unconventional superconductors behave if confined to small islands or if superconductivity is suppressed at the surface of a bulk material.

Finally, the group has participated in the exiting new development of unconventional magnets, called altermagnets where multiple joint projects with a group at the university of Milwaukee, USA were started and first results being published in a work on minimal models for this magnetic state.

Several projects are ongoing and close yield research output; some examples are about inhomogeneous cuprates, surface properties of triplet superconductors and unconventional magnets (altermagnets).

Emma Lenander, Kim Lefmann (KU NBI), Pascale Deen (ESS) and Andrea Kirsch (KU Chem):

We have investigated the magnetic excitations at low temperatures in a single crystal of the material $\text{Bi}_2\text{Fe}_4\text{O}_9$. This material is highly unusual, since the magnetic Fe^{3+} spins are antiferromagnetically coupled in five-spin rings of different orientations, leading to an unusual type of a 3D frustrated system. We have for the first time found the spin wave signal up to the top of the band. A detailed model of the magnetic interactions in the system is proposed and will soon be published. In addition, we find a continuum of scattering, reminiscent of fractionalized excitations known from low-dimensional quantum spin systems. The experiments took place at the neutron facilities SINQ, ILL, and J-PARC.

Kristine Krighaar, Jeppe Cederholm, Christine Lauritzen, Ellen Schriver, Kim Lefmann (KU NBI) and Machteld Kamminga (Q-MAT and Utrecht):

The cuprate superconductor $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_4$ (NCCO) is peculiar because O-annealing of the crystal is necessary for it to become superconducting, no matter the content of the chemical dopant, Ce. We have used neutron spectroscopy to study the magnetic excitation spectrum of two pieces of the same NCCO crystal, one annealed and one as-grown. For the as-grown sample we find a large pseudo spin gap, reminiscent of a finite-size effects of a diluted spin system. It is therefore likely that the absence of superconductivity in as-grown NCCO is caused by structural disorder and not doping levels. The experiments took place at the neutron facilities ANSTO and ILL.

Sofie Holm-Janass, Paola Catarina Forino, Niels Bech Christensen (DTU Physics), Adheena Painganoor (DTU Physics and ILL), Rasmus Toft-Petersen (DTU Physics and ESS)

The magnetization of magnetoelectric LiFePO_4 for magnetic fields along b reveals the presence of a phase transition at 32T conjectured to be associated with a re-orientation of the electronic magnetic moments. We performed a pulsed-field neutron diffraction experiment in fields up to 35T at NOBORU, J-PARC and were able to directly verify the existence of a spin-flop transition. Supporting measurements of the electric polarization induced by the magnetic field revealed that while the magnetoelectric tensor α in the spin-flop phase has a finite diagonal component, α_{bb} ,

as expected from symmetry analysis, the off-diagonal component, a_{ab} , characteristic of the zero-field phase remains finite in the high field phase. In turn, this observation suggests that the high-field spin structure, while predominantly of the spin-flop type, has sub-dominant components that allow finite values of a_{ab} , but could not be determined unambiguously in the backscattering geometry used in our diffraction experiment.

Mickey Pedersen, Ulla Gro Nielsen and Hans Jørgen Aagaard Jensen (SDU), Emma Lenander, Thomas Sahl Christensen, and Kim Lefmann (KU NBI), Pascale Deen (ESS)

The magnetically frustrated mineral herbertsmithite has long been considered an ideal quantum spin liquid candidate. However, disorder within the material causes ambiguity regarding the true magnetic ground state. Using a combination of several techniques including synthesis, NMR, low-temperature susceptibility and Neutron diffraction, we have obtained new insight of the amount of disorder has been obtained. Importantly, one synthesis aiming to obtain “pure” herbertsmithite showed unusual anomalies in the low-temperature susceptibility. High-resolution neutron spectroscopy measurements at ILL (IN16b) showed too low intensity and we will continue our search in 2025 at OSIRIS (ISIS).

3.2 Publications within Q-MAT, 2024

Q-MAT had in 2024 in total 38 publications, of which 14 were directly related to the Lighthouse funding. This shows that the publication rate of the Q-MAT PhD students and post docs is building up. The full list can be seen in the appendix B.

3.3 Patents

No patent applications were filed within the Q-MAT topic in 2024.

3.4 Student degrees

During the Q-MAT faculty has supervised theses corresponding to 13 B.Sc. 13 M.Sc. degrees and 4 Ph.D. degrees. See list in appendix D.

In 2022, the corresponding number was 12 B.Sc. degrees, 7 M.Sc. degrees and 4 Ph.D. degrees, and in 2023 the numbers were 8, 11, and 2. Hence, the amount of students in Q-MAT is slightly increasing.

3.5 New funding 2024

Revealing the physics behind the apparent hot-spot effect of induction heated nanoparticles

PI: Cathrine Frandsen, DFF, 3.2 MDDK

The project is based in part on an idea developed in the Q-MAT PhD project with Lise G. Hanson.

Novel magnets through interdisciplinarity and nanocomposites (NOMAGIC)

PI's: Mogens Christensen, Aarhus University, Cathrine Frandsen, DTU Physics, and Rasmus Bjørk, DTU Energy, Carlsberg Foundation Semper Ardens Advance grant, 25 MDKK

The project aims to develop a new magnetic material, a nanocomposite permanent magnet. The material formation process will be studied with a palette of techniques including neutron scattering.

NNF Starting Package for Sara Lopex Paz, 4 MDKK

DFF-Research Project 1 (Inge Lehmann): Sara Lopez Paz 2 MDKK

4. Summary

In its first three years, the Lighthouse Q-MAT focused on recruitment, networking and start-up of scientific projects; in particular the PhD projects. In 2024 the speed has increased, and a number of the PhD projects are showing results. This is not yet reflected in the publication list, due to the typical 2-3 years turn-around time for publications, but we expect this to show in 2025.

The important position as tenure-track professor in Chemistry at KU has been filled, while a post doc and a PhD position at DTU are in recruitment.

The spending for the first 4 years has been 11.6 MDKK below budget. With a 2024 spending of 8.0 MDKK, the unspent amount corresponds to just over one year of full budget spending. Since the project has been extended by 13 months to ultimo 2026, we will be able to spend the full budget and carry out the expected activities.

The partners published 38 Q-MAT relevant publications in 2023, with 14 publications directly related to the Q-MAT funding. For comparison, in 2023, 14 Q-MAT funded publications appeared of a total of 35 publications. The 2024 number is satisfying, witnessing a significant activity. It is evident that the Q-MAT funded activities are resulting in publications, and this number is expected to increase in 2025 as the Q-MAT PhD projects are maturing.

Q-MAT maintains close connections to ESS in general, and in particular to the DK-led instruments BIFROST and HEIMDAL, but also to C-SPEC. Importantly, strong links with the ESS-DMSC have been established and the ESS CEO Helmut Schober has been affiliated with the Lighthouse.

Appendix

A. List of staff affiliated with Q-MAT, ultimo 2024

AAU

Staff: Lars Diekhöner
Post docs etc.: None
Ph.D. students: Francesco Zamboni

AU, Chemistry

Staff: Mogens Christensen, Bo B. Iversen, Dan Mannix
Post docs etc.: Mathias Mørch, Vijay Singh Parmar
Ph.D. students: Jack Thomas Hunt, Jacob Løwe Valentin, Amalie Povlsen, Jens Plum Frandsen, Hannah Hedegaard Nielsen, Sofie Stampe Leiszner

KU, NBI

Staff: Kim Lefmann, Brian Møller Andersen, Jens Paaske
Post docs etc.: Andreas Kreisel, Morten Holm Christensen, Henrik Jacobsen, Sonja Holm-Dahlin
Ph.D. students: Kristine Krighaar, Emma Lenander, Kamaldeep Dalal, Pia Jensen Ray

KU, Chem

Staff: Jesper Bendix, Høgni Weihe, Stergios Piligkos, Kirsten Ø. Jensen, Sara Lopez Paz
Post docs etc.: None
Ph.D. students: Sabina Svava Mortensen

KU, IGN

Staff: Kristoffer Szilas
Post docs etc.: None
Ph.D. students: None

DTU, Chem

Staff: Kasper Steen Pedersen
Post docs etc.: Maja A. Dunstan, Frédéric Aribot, James N. McPherson
Ph.D. students: Naoki Eguchi, Evgeniia Luneva, Anton Viborg, Anna S. Manvell

DTU, Physics

Staff: Niels Bech Christensen, Cathrine Frandsen, Thomas Olsen, Rasmus Toft-Petersen
Post docs etc.: Sandip Guchait (from January 2025), Miriam Varón, Sofie Holm Janas, John Michael Mangeri, Paola Forino
Ph.D. students: Lise Grüner Hanson, NN (2025), Adheena Painganoor, Mathias Zambach, Frederik Laust Durhuus, Thomas Veile, Martin Ovesen, Varun R Pavizhakumari

DTU, Energy

Staff: Nini Pryds, Jean-Claude Grivel
Post docs etc.: None
Ph.D. students: None

SDU

Staff: Hans Jørgen Aagaard Nielsen
Post docs etc.: None
Ph.D. students: Mickey Pedersen

RUC

Staff: Dorte Posselt
Post docs etc.: None
Ph.D. students: Christian Kristensen

B. Publications related to Q-MAT topics, 2024

The groups in Q-MAT published 38 peer-reviewed articles related to Q-MAT in 2024.

Publications marked with "*" are co-authored by staff funded by Q-MAT. 14 articles are in this category.

Publications with more than one Q-MAT partner are grouped after the first Q-MAT author.

AU, Chemistry (2; 2*)

* Hannah H. Nielsen, Pol Vilariño, Gemma Rodríguez, Florian Trepard, Olivier Roubeau, Guillem Aromí, David Aguilà

Self-assembly of a supramolecular spin-crossover tetrahedron

Dalton Transactions, **53**, 9792-9797 (2024)

* Morch, Mathias I., Thomas-Hunt, Jack, Laursen, Amalie P., Simonsen, Jesper, Frandsen, Jens Plum, Vijayan, Harikrishnan, Christensen, Mogens

Oriented Nanomagnets Originating from Topotactic and Pseudomorphic Reactions

Chemistry of Materials, **36**, 1919-1927 (2024)

AAU (2; 0*)

S. Jensen, I.A. Løge, J. Bendix and L. Diekhöner

An approach for patterned molecular adsorption on ferromagnets, achieved via Moiré superstructures

Physical Chemistry Chemical Physics, **26**, 13710 (2024)

I.A. Løge, S. Jensen, J. Bendix and L. Diekhöner

Skabeloner til fremtidens elektronik

Dansk Kemi, **105**, 15 2024

(popular article in Danish)

KU, NBI (15; 11*)

* J. Lass, E. Y. Lenander, K. M. L. Krihaar, T. N. Totic, D. Prabhakaran, P. P. Deen, S. Holm-Janass, K. Lefmann

Characterizing the diffuse continuum excitations in the classical spin liquid $h\text{-YMnO}_3$

Physical Review B, **110**, 144429 (2024)

S. Holm-Dahlin, J. Larsen, H. Jacobsen, A. T. Rømer, A.-E. Tutueanu, M. Ahmad, J.-C. Grivel, R. Scheuermann, M. v. Zimmermann, M. Boehm, P. Steffens, Ch. Niedermayer, K. S. Pedersen, N. B. Christensen, B. O. Wells, K. Lefmann, L. Udby

Field-induced electronic phase separation in the high-temperature superconductor

$\text{La}_{1.94}\text{Sr}_{0.06}\text{CuO}_{4+y}$

Physical Review B, **109**, 174517 (2024)

Jacobsen, Henrik, Barthkowiak, Marek, Weber, Tobias, Stühr, Uwe, Roessli, Bertrand, Niedermayer, Christof, Staub, Urs

Phonon dispersion of quantum paraelectric SrTiO_3 in electric fields

Physical Review B, **110**, 054302 (2024)

Totic, Tara N., Deen, Pascale P., Simonov, Arkadiy, Spaldin, Nicola A.

Origin of correlated diffuse scattering in the hexagonal manganites

Physical Review Research, **6**, L042037 (2024)

* Clara N. Breiø, Andreas Kreisel, Mercè Roig, P. J. Hirschfeld, Brian M. Andersen

Time-reversal symmetry breaking from lattice dislocations in superconductors

Physical Review B, **109**, 014505 (2024)

* Henrik S. Røising, Max Geier, Andreas Kreisel, Brian M. Andersen

Thermodynamic transitions and topology of spin-triplet superconductivity: Application to UTe_2

Physical Review B, **109**, 054521 (2024)

* Brian M. Andersen, Andreas Kreisel, P. J. Hirschfeld

Spontaneous time-reversal symmetry breaking by disorder in superconductors

Front. Phys. **12**, 1353425 (2024)

* Guanyang He, Yu Li, Yuxuan Lei, Andreas Kreisel, Brian M. Andersen, Jian Wang

Lateral quantum confinement effect on monolayer high- T_c superconductors

Nano Letters, **24**, 7654-7661 (2024)

* Yifu Cao, Chandan Setty, Andreas Kreisel, Laura Fanfarillo, P.J. Hirschfeld

Spin fluctuations in the ultranodal superconducting state of $\text{Fe}(\text{Se},\text{S})$

Physical Review B, **110**, L020503 (2024)

* Mercè Roig, Andreas Kreisel, Yue Yu, Brian M. Andersen, Daniel F. Agterberg

Minimal Models for Altermagnetism

Physical Review B, **110**, 144412 (2024)

* Yi Dai, Andreas Kreisel, Brian M. Andersen

Existence of Hebel-Slichter peak in unconventional kagome superconductors

Physical Review B, **110**, 144516 (2024)

* Henrik S. Røising, Andreas Kreisel, Brian M. Andersen

Nonlocal electrodynamics and the penetration depth of superconducting Sr₂RuO₄

Physical Review B, **110**, 094511 (2024)

* Subhojit Roy, Andreas Kreisel, Brian M. Andersen, Shantanu Mukherjee

Unconventional pairing in Ising superconductors: Application to monolayer NbSe₂

2D Mater. **12**, 015004 (2024)

* Adrian Valadkhani, Jonas B. Profe, Andreas Kreisel, P. J. Hirschfeld, Roser Valentí

Why Scanning Tunneling Microscopy on Sr₂RuO₄ sometimes doesn't see the superconducting gap

npj Quantum Materials, **9**, 78 (2024)

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KU, Chem (3; 1*)

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DTU, Physics (15; 0*)

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Conservation laws for interacting magnetic nanoparticles at finite temperature
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Minority magnons and mode branching in monolayer Fe₃GeTe₂
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Magnetic order in the computational 2D materials database (C2DB) from high throughput spin spiral calculations
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Evidence for electron-hole crystals in a Mott insulator
Nature Materials, **23**, 1055

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Two-dimensional altermagnets from high throughput computational screening: Symmetry requirements, chiral magnons, and spin-orbit effects

Applied Physics Letters, **124**, 182409

SK Chaluvadi, SP Chalil, A Jana, D Dagur, G Vinai, F Motti, J Fujii, et al.

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Nano Letters, **24**, 7601

DTU, Chemistry (1; 0*)

Dunstan, Maja A., Manvell, Anna S., Yutronkie, Nathan J., Aribot, Frederic, Bendix, Jesper, Rogalev, Andrei, Pedersen, Kasper S.

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Nature Chemistry, **16**, 735 (2024)

RUC and SDU had no Q-MAT related publications in 2024.

C. Patents related to Q-MAT topics.

(none)

D. Student degrees 2024

Ph.D. degrees (4)

DTU, Physics (2)

- Paola Catarina Forino, *Magnetoelastic phase diagrams in magnetoelectric TbPO₄: a neutron and X-ray scattering study*
- Joachim Sødequist, *Chiral Magnetism in 2D Crystals from First Principles*

KU, NBI (2)

- Mercè Roig, *Unconventional Superconductivity and Altermagnetism*
- Clara N. Breiø, *Interaction- and Disorder-Induced Phases in Electronically Correlated Materials*

MSc degrees (13)

AAU (2)

- Metin Ahmed and Lucas Ebenau, *Characterization of MgO and NaCl as Decoupling Layers and Investigation of the Structural and Electronic Properties of C60*

DTU, Physics (1)

- Maciej Andrzej Glód, *Simulations of magnetic dynamics in nanoparticle clusters*

KU, NBI (10)

- Nicklas Leon Knudsen *Simulating neutron scattering results on frustrated spin systems by Langevin dynamics*
 - Peter J. S. Beck, *Quantum Simulations of Crystal Spectra Sample components for McStas from 2D RLexact simulations*
 - Jeppe J. Cederholm, *Magnetic structure of Mn₃Sn*
 - Peiyuan Liu, *Interdependence Between the Lattice Structure and the Magnetic Structure of the Mineral Jarosite*
 - Mads F. Engholm, *Implementation of dipole calculations in the Copenhagen Langevin Simulation Code for spin systems*
 - Xiaoyu (Dorothy) Wang, *Analyzing Neutron Scattering Data on the Excitations in the Spin 1 Haldane System NENP*
 - Kristine Marie Løfgren Krihhaar, *A Digital Twin of the BIFROST Neutron Spectrometer at ESS*
 - Emma Ynill Lenander, *Magnetically frustrated dynamics on the Cairo pentagonal lattice; Bi₂Fe₄O₉*
 - Yi Dai, *Unconventional superconductivity and the Hebel-Slichter peak of the kagome lattice*
-
- Hans Christensen, *Vortex States and Boundary Theories in Topological Spin-Triplet Superconductors*

Bsc. Degrees (13)

DTU, Physics (4)

- Mikkel Christian Larsen & Mikkel Ravn-Feld, *Monte Carlo Simulations of Lithium Orthophosphates*, June 2024
- Ruby Wimmelmann & Malene Ræbild Hamburger, *Implementation of an image-recognition based neutron data quality monitor*

KU, NBI (9)

- Benjamin Nordahl Wang, *Adjustments of the digital twin of the ESS spectrometer BIFROST*
- Ellen Skafte Schriver, *Investigation of the effects of reductive annealing on spin fluctuations of Nd_{1.85}Ce_{0.15}CuO₄-delta*
- Amalie Tanja Clausen, *Investigation of the Superconductor CsV₃Sb₅*
- Henrik Jacobsen, *Approximations of quantum solutions to describe internal magnetic interactions in azurite*
- Simon Kjær, *Optimization of the CAMEA Triple Axis Spectrometer based on MC-simulation*
- Carlos P. E. Gomez, *High-Entropy Spinel Oxides, Structural and magnetic characterization through neutron diffraction*
- Daniel Lomholt Christensen, *SALSA Virtual - A virtual neutron scattering instrument*
- Inga Pauline Gruning, *Altermagnetism in real-space*
- Rune C. Ekman, *Spin-orbit coupling induced weak ferromagnetism in altermagnets*