# ESS Lighthouse: Magnetism and Quantum Materials (Q-MAT) 2023 Annual Report

The ESS Lighthouse Q-MAT is financed by the Danish Government through NUFI 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 of 2023.



## **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, 5 times in 2023.

#### 1.3 The Steering Group

Consolidated on 18<sup>th</sup> 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)
- Dorthe 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.

In 2024, the group will be enriched by one additional hire, in Q-MAT:

• NN1, post doc (DTU, Physics)

#### 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 2024
- DI (Danish Industry): Richard Larsen, to be replaced in 2024

This group has met twice; April 2021 and November 2022. Joachim Matthiesen has replaced Jan W. Thomsen (NBI)

#### 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. We aim for the group to provide a mid-term evaluation in early 2024.

## 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, the activity (measured as budget spending) has reached close to the intended level.

#### 2.1 Meeting activity

#### 2.1.1 Annual Meeting and Steering Group Meeting, 1-2 November 2023, held at Rødvig

This meeting was held at Hotel Klitten in Rødvig, Stevns. Due to the pandemics, this was only the second Q-MAT outing, having 20 participants. 5 of the QMAT PhD students presented their projects which gave rise to long discussion. In addition, there were a handful of other presentations; in particular the coming Q-MAT tenure track professor Sara Lopez Paz presented her research and visions.

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.

The adjacent SG meeting confirmed the adjustment of SG members and discussed the formation of the International Advisory Committee.

#### 2.1.2 International Advisory Group Meeting, February 2023

In this first meeting of the international advisory group, the foundations were laid for the groups future meetings. The group were given relevant documents to prepare for a mid-term evaluation of the Lighthouse.

Unfortunately, the mid-term evaluation has been postponed, but will resume in Q2, 2024.

#### 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     | Торіс                       | <mark>Start date -End date</mark> |
|--------------------|-------------|-------------|-----------------------------|-----------------------------------|
| 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.       | PhD student | RUC         | Magnetic Polymers           | Jan. 2022 – Dec. 2024             |
| Kristensen         |             |             |                             |                                   |
| Lise G Hanson      | PhD student | DTU Physics | Magnetic Nanoparticles      | Oct. 2022 – Sept. 2025            |
| NN                 | PhD student | DTU Physics | Quantum Magnetism and       | 2024- 2027                        |
|                    |             |             | Superconductivity           |                                   |
| NN                 | Postdoc     | DTU Physics | Q-MAT experiments           | 2024- 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       | PhD student | KU NBI      | Superconducting and ESS     | Apr. 2022 – June 2026             |

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| Krighaar        |                           |          | instrumentation            |                        |
|-----------------|---------------------------|----------|----------------------------|------------------------|
| Emma Y Lenander | PhD student               | KU NBI   | Frustrated Magnetism       | Jun. 2022 – June 2026  |
| Andreas Kreisel | Assistant<br>Professor    | KU NBI   | Q-MAT Theory               | Sept. 2022 – Dec. 2025 |
| Sara Lopez Paz  | Tenure track<br>Professor | KU Chem. | Q-MAT material development | April 2024             |

The essential position at KU Chemistry within Materials Development was initially planned as an assistant professorship, but the department has upgraded the position to a tenure track assistant professorship. The position was filled in 2023. At the time of writing (April 2024), Sara Lopez Paz has started her contract.

#### 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 Budget and spending in Q-MAT

In the original Q-MAT budget, many hires were aimed to start in 2021, and the largest part of the 2 MDKK Chemistry lab was placed this year. The pandemic changed this, giving some delays in hiring, in particular the associate professor at KU Chemistry and two positions at DTU. This led to a 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 the spending is almost on level with the plans. The later start has meant that we have applied for an extension of the budget period. With an annual spending on par with the 2023 spending, the natural ending point of the project will be ultimo 2026, which is what we have applied for.

The delays do not give rise to re-distribution of funds between partners.

| Institution | Position  | Planned start | Actual start | Budget<br>2021 (kkr) | Spending 2021<br>(kkr) | Budget<br>2022 (kkr) | Spending 2022<br>(kkr) | Budget<br>2023 (kkr) | Spending 2023<br>(kkr) | Difference<br>Budget –<br>spend. (kkr) | Unspent (kkr) |
|-------------|-----------|---------------|--------------|----------------------|------------------------|----------------------|------------------------|----------------------|------------------------|--|---------------|
| RUC         | PhD       | 2021/3        | 2022/1       | 289                  | 0                      | 527                  | 361                    | 498                  | 485                    | 192                                    | 500           |
| AAU         | PhD       | 2021/3        | 2021/9       | 308                  | 168                    | 602                  | <b>498</b>             | 573                  | 625                    | 465                                    | 1625          |
| SDU         | PhD       | 2022/3        | 2022/4       | 29                   | 1                      | 309                  | 404                    | 602                  | 520                    | 14                                     | 866           |
| AU          | PhD 1     | 2022/3        | 2022/3       | 337                  | 188                    | 910                  | 746                    | 1175                 | 1023                   | 468                                    | 785           |
|             | PhD 2     | 2021/3        | 2021/2       |                      |                        |                      |                        |                      |                        |  |               |
| DTU Phys    | Post doc  | 2020/9        | -            | 1309                 | 62                     | 1925                 | 327                    | 2291                 | 1000                   | 4136                                   | 6612          |
|             | PhD 1     | 2022/9        | -            |                      |                        |                      |                        |                      |                        |  |               |
|             | PhD 2     | 2021/3        | 2022/9       |                      |                        |                      |                        |                      |                        |  |               |
| DTU Chem    | PhD       | 2022/3        | 2022/9       | 0                    | 0                      | 323                  | 109                    | 573                  | 503                    | 284                                    | 1179          |
| DTU Energy  | -         | -             | -            | 58                   | 0                      | 58                   | 0                      | 58                   | 24                     | 149                                    | 264           |
| KU Geosci   | -         | -             | -            | 29                   | 33                     | 29                   | 52                     | 29                   | 71                     | -70                                    | -12           |
| KU Chem     | Ass. Prof | 2020/9        | 2024/4       | 2239                 | 137+33                 | 1109                 | 10                     | 1130                 | 768                    | 3530                                   | 5424          |
| KU NBI      | PhD 1     | 2021/3        | 2020/9       | 1096                 | 775+23                 | 1443                 | 1182                   | 2589                 | 2255                   | 893                                    | 5173          |
|             | PhD 2     | 2022/3        | 2022/3       |                      |                        |                      |                        |                      |                        |  |               |
|             | PhD 3     | 2022/3        | 2022/6       |                      |                        |                      |                        |                      |                        |  |               |
|             | Ass. Prof | 2022/9        | 2022/10      |                      |                        |                      |                        |                      |                        |  |               |
| Sum         | -         | -             | -            | 5693                 | 1365+56                | 7233                 | 3690                   | 9518                 | 7274                   | 10062                                  | 22417         |

#### 2.5. Connection to ESS

Q-MAT maintains its strong connection to ESS:

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

#### 2.6 Q-MAT home page

A web page for Q-MAT has been established on the address <u>https://www.q-mat.nbi.ku.dk/</u> 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.

## 3. Activities in Q-MAT, Scientific

#### 3.1 Highlights 2023

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

We developed the ability to deposit large magnetic molecules into UHV by Installing an Electrospray Deposition System. By this, we are not limited to study magnetic molecules that survive standard sublimation deposition methods. Lanthanide-based molecules were investigated on metal single crystal surfaces with Scanning Tunneling Microscopy, and magnetic measurements (XAS and XMCD) were done at the SLS synchrotron, using the X-treme beamline.

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

Detection of the symmetry of the superconducting state in unconventional superconductors is a challenging scientific task which has in some variants been carried out by the use of disorder. We have contributed theoretical investigations on two distinct unconventional superconductive materials where scanning tunneling microscopy data is available. One is the elusive superconductor Sr2RuO4 where an analysis including the effect of the tunneling into the orbital states on the surface was taken into account to directly compare to already published experimental data. Another an iron based superconductor in its monolayer configuration where signatures of sign reversal scattering was found, underlining theoretical proposals on topological nature of this Fe(Se,Te). The work together with a leading experimental group in China was published in Nano Letters. A purely theoretical work dedicated to the same material in bulk form found that magnetic structures can be generated by potential impurities, thus allowing for a topological superconductor induced by non-magnetic impurities. That work in collaboration with a group at the University of Florida was published in PRB.

Further works on strongly inhomogeneous cuprate superconductors revealed properties on the low-temperature penetration depth that is commonly investigated experimentally with Muon-spin relaxation measurements. We found that unusual properties of the spectral gap and linear behavior of the superfluid density can be explained by standard BCS theory. Further projects on inhomogeneous cuprate superconductors are ongoing.

#### 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 Bi2Fe4O9. This material is highly unusual, since the magnetic Fe3+ spins are antiferromagnetically coupled in five-spin rings of different orientations, leading to an unusual type of a 3D frustrated system. We find a very clear spin wave signal, much more detailed than published by other groups. In addition, we find a continuum of scattering, reminescent of fractionalized excitations known from low-dimensional quantum spin systems. The experiments took place at the neutron facilities SINQ and ILL.

#### Kristine Krighaar, Emma Lenander, Kim Lefmann (KU NBI) and Machteld Kamminga (Q-MAT and Utrecht):

By high-resolution neutron spectroscopy at J-PARC and ILL, we found the ordering temperature of the magnetic stripes in a cuprate superconductor (La,Sr)2CuO4 to have a much lower value than found by earlier neutron studies. Our results compare favourably with muon spin rotation experiments performed on PSI. The

reason for the difference is that quasielastic magnetic scattering appear from the stripes at temperatures below the superconducting transition, and that earlier measurements interpreted this signal as elastic scattering. The implications of the quasielastic spectral component will be discussed with the Q-MAT theory group.

#### Kasper S. Pedersen (DTU Chemistry)

Materials based on periodic tessellations involving more than a single type of 'tile', the so-called Archimedean tessellations (ATs), are theoretically predicted to harbor novel, frustrated magnetic phases, but their exploration remains absent due to a severe scarcity of materials candidates. Furthermore, slightly increasing the triangle-to-square ratio would lead to the disappearance of translational symmetry, and the formation of quasi-periodic structures, 'quasicrystals'. We have developed a general synthetic strategy to tailor the structure and electronic structure of ATs, which has now led to the development of frustrated metal-organic magnets and ensuing large magneto-caloric effects, and the discovery of tunable valence change transitions in rare earth materials.

#### Bo B. Iversen (AU Chemistry):

We have investigated the magnetic anisotropy, present in single molecule magnets. Both lanthanide and transition metal complexes have been studied with synchrotron X-ray diffraction on single crystals to investigate the electron density and magneto-structural correlations. Furthermore, powder polarized neutron diffraction has been used to study the local susceptibility tensor for both a Co-complex, and for multiple lanthanide complexes. The project that started with an experiment at ILL and will continue in 2024, with planned beam time at HFIR.

#### Mogens Christensen and Jacob Valentin (AU Chemistry):

We are establishing a procedure to extract information on materials texture from neutron powder diffraction data from 2D area detector at SINQ.

#### Niels Bech Christensen and Rasmus Toft-Petersen (DTU Physics)

We have a strong focus on the complex impact of magnetic structure on magnetoelectric properties in Liorthophosphates LiMPO<sub>4</sub> (M=Mn, Fe, Co, Ni) and TbPO<sub>4</sub>. A highlight was a detailed neutron diffraction and bulk characterization study of LiNi<sub>1-x</sub>Fe<sub>x</sub>PO<sub>4</sub> where the addition of Fe on the transition metal site causes unforeseen magnetic phase transitions that have direct and dramatic implications for the electric polarisation induced by an applied magnetic field.

#### Nini Pryds (DTU Energy)

In recent years, we have achieved significant progress by mastering the controlled growth and transfer of singlecrystalline freestanding oxide membranes. Correlated oxide materials, including the notably efficient La0.7Sr0.3MnO3 (LSMO), have received widespread attention. LSMO is known for its high Curie temperature (about 369 K), significant spin polarization, and its colossal magnetoresistance, making it a focal point of research in its freestanding membrane form. Freestanding LSMO membranes exhibiting ferromagnetism varied in thickness ranging from 20 to 60 nanometers (nm), prepared by growing the LSMO epitaxially on a sacrificial layer, followed by release and transfer. Our latest work advances this research, showing that enhanced ferromagnetism and conductivity can be induced in even ultrathin LSMO membranes, specifically those less than 4 unit cells thick. Furthermore, we have discovered that by applying strain to these thin, freestanding membranes, we can adjust their transition temperature, opening new avenues in strain engineering.

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

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 that we aim to follow up by neutron spectroscopy measurements.

# Christian K. Kristensen and Dorthe Posselt (RUC), Kim Lefmann (KU) and Miriam Varón and Cathrine Frandsen (DTU):

We are using diblock copolymers to tailor magnetic structure, either by embedding magnetic nanoparticles in one type of domain in structured block copolymer thin films or by using block copolymers with an iron containing block. The thin films prepared are solvent vapor annealed in a magnetic field and this process is followed by in-situ Grazing Incidence Small-Angle X-ray Scattering. The resulting thin films are characterized with Atomic Force Microscopy, Magnetic Force Microscopy (in collaboration with Nanosurf AG) and with Scanning Nitrogen Vacancy Microscopy (in collaboration with QZabre AG).

#### 3.2 Publications within Q-MAT, 2023

Q-MAT had in 2023 in total 35 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 2023.

#### 3.4 Student degrees

During the Q-MAT faculty has supervised theses corresponding to 8 B.Sc. 11 M.Sc. degrees and 2 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.

## 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. The important position as tenure-track professor in Chemistry at KU has been filled, while a post doc and a PhD position at DTU remains unfilled. The recruitment process is ongoing and we expect both positions to be filled in 2024.

The spending for the first 3 years has been 10 MDKK below budget. With a 2023 spending of 7.3 MDKK, the unspent amount corresponds to just over one year of full budget spending. With an extension of the project to ultimo 2026, we will be able to spend the full budget and carry out the expected activities.

Two virtual meetings and two physical meetings have been held for all partners in Q-MAT.

The partners published 35 Q-MAT relevant publications in 2023, with 14 publications directly related to the Q-MAT funding. For comparison, in 2022, 4 Q-MAT funded publications appeared of a total of 28 publications. The 2023 number is satisfying, witnessing a significant activity. In particular, it is evident that the Q-MAT funded activities now are starting to result in publications. We expect a further increase in Q-MAT funded publications in 2024.

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, links with the ESS-DMSC has been established and the ESS CEO Helmut Schober has been affiliated with the Lighthouse.

## Appendix

## A. List of staff affiliated with Q-MAT, ultimo 2023

| <u>AAU</u><br>Staff:<br>Post docs etc.:                              | Lars Diekhöner   |
|--|--|
| Ph.D. students:  | Francesco Zamboni  |
| <u>AU, Chemistry</u><br>Staff:<br>Post docs etc.:<br>Ph.D. students: | Mogens Christensen, Bo B. Iversen, Dan Mannix<br>Mathias Mørch, Vijay Singh Parmar<br>Jack Thomas Hunt, Jacob Løwe Valentin, Amalie Povlsen, Jens Plum Frandsen,<br>Hannah Hedegaard Nielsen, Sofie Stampe Leiszner  |
| <u>KU, NBI</u><br>Staff:<br>Post docs etc.:<br>Ph.D. students:       | Kim Lefmann, Brian Møller Andersen, Jens Paaske<br>Andreas Kreisel, Morten Holm Christensen, Henrik Jacobsen, Sonja Holm-Dahlin<br>Kristine Krighaar, Emma Lenander, Kamaldeep Dalal   |
| <u>KU, Chem</u><br>Staff:<br>Post docs etc.:<br>Ph.D. students:      | Jesper Bendix, Høgni Weihe, Stergios Piligkos, Kirsten Ø. Jensen, Sara Lopez Paz (2024)  |
| <u>KU, IGN</u><br>Staff:<br>Post docs etc.:<br>Ph.D. students:       | Kristoffer Szilas  |
| DTU, Chem<br>Staff:<br>Post docs etc.:<br>Ph.D. students:            | Kasper Steen Pedersen<br>Maja A. Dunstan, Frédéric Aribot, James N. McPherson<br>Naoki Eguchi, Evgeniia Luneva, Anton Viborg, Anna S. Manvell  |
| DTU, Physics<br>Staff:<br>Post docs etc.:<br>Ph.D. students:         | Niels Bech Christensen, Cathrine Frandsen, Thomas Olsen, Rasmus Toft-Petersen<br>NN (2024), Miriam Varón, Sofie Holm Janas, John Michael Mangeri<br>Lise Grüner Hanson, NN (2024), Paola Forino, Adheena Painganoor, Mathias Zambach,<br>Frederik Laust Durhuus, Thomas Veile, Joachim Sødequist, Varun Rajeev Pavizhakumari,<br>Martin Ovesen, Mads Kruse |
| DTU, Energy<br>Staff:<br>Post docs etc.:<br>Ph.D. students:          | Nini Pryds, Jean-Claude Grivel   |
| <u>SDU</u><br>Staff:   | Hans Jørgen Aagaard Nielsen (Ulla Gro Nielsen, now at the Novo Nordisk Foundation)   |
| Q-MAT  | Universitetsparken 5, 2100 Copenhagen www.q-mat.nbi.ku.dk  |

Post docs etc.: Ph.D. students: Mickey Pedersen

RUCStaff:Dorthe PosseltPost docs etc.:Ph.D. students:Christian K. Kristensen

## **B.** Publications related to Q-MAT topics, 2023

The groups in Q-MAT published 35 peer-reviewed articles related to Q-MAT in 2023.

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 (8)

B. Muzzi, M. Albino, M. Petrecca, C. Innocenti, C. de Julián Fernández, G. Bertoni, M. R. Ibarra, M. Christensen, M. Avdeev, C. Marquina, & C. Sangregorio *Defect-Engineering by Solvent Mediated Mild Oxidation as a Tool to Induce Exchange Bias in Metal Doped Ferrites* Small Methods 7, 11, 2300647 (2023)

P. Shyam, F.H. Gjørup, M. I. Mørch, A.P. Laursen, A. Z. Eikeland, I. Kantor, M. R. V. Jørgensen, & M. Christensen *Sintering in seconds, elucidated by millisecond in situ diffraction.* Applied Materials Today 35, 101960 (2023)

H. Vijayan, A. P. Laursen, M. Stingaciu, P. Shyam, F. H. Gjørup, M. Christensen High Performance Hexaferrite Ceramic Magnets made from Nanoplatelets of Ferrihydrite by High Temperature Calcination for Permanent Magnet Applications ACS Appl. Nano Mater. 10, 8156–8167 (2023)

M. Mørch, M. Christensen *Controlling the magnetic structure in W-type hexaferrites* J. Appl. Cryst. 56, 597–602 (2023)

C. G. Knudsen, M. Mørch and M. Christensen *Texture formation in W-type hexaferrite by cold compaction of non-magnetic interacting anisotropic shaped precursor crystallites* Dalton Trans. 52, 281-289 (2023)

V. S. Parmar, A. M. Thiel, R. Nabi, G. K. Gransbury, M. S. Norre, P. Evans, S. C. Corner, J. M. Skelton, N. F. Chilton, D. P. Mills, and J. Overgaard *Influence of pressure on a dysprosocenium single-molecule magnet*, Chemical Communications 59(18), 2656–2659 (2023)

V. S. Parmar, A. M. Thiel, M. S. Norre, J. Overgaard *High-Pressure Investigation of a Five-Coordinate Dy Single-Molecule Magnet* Crystal Growth & Design, 23(9), 6410–6417 (2023) S. K. Gupta, H. H. Nielsen, A. M. Thiel, E. A. Klahn, E. Feng, H. B. Cao, T. C. Hansen, E. Lelièvre-Berna, A. Gukasov, I. Kibalin, S. Dechert, S. Demeshko, J. Overgaard, F. Meyer *Multi-Technique Experimental Benchmarking of the Local Magnetic Anisotropy of a Cobalt(II) Single-Ion Magnet* JACS Au, 3(2), 429–440 (2023)

#### AAU (2)

A. Ørsted, S.V. Salling and L. Diekhöner Unraveling the electronic structure of cobalt oxide nanoislands on Au(111) Physical Review B, **108**, 165424 (2023)

L. Diekhöner, C. S. Meyer and S. Eiskjær The magnetic field strength and the force distance dependency of the magnetically controlled growing rods used for early onset scoliosis Scientific Reports, **13**, 3045 (2023)

#### KU, NBI (16; 13\*)

\* Shinibali Bhattacharyya, Andreas Kreisel, X. Kong, T. Berlijn, Astrid T. Rømer, Brian M. Andersen, P. J. Hirschfeld *Superconducting gap symmetry from Bogoliubov quasiparticle interference analysis on Sr*<sub>2</sub>*RuO*<sub>4</sub> Phys. Rev. B **107**, 144505 (2023)

\* Yu Li, Dingyu Shen, Andreas Kreisel, Cheng Chen, Tianheng Wei, Xiaotong Xu, Jian Wang *Anisotropic gap structure and sign reversal symmetry in monolayer Fe(Se,Te)* Nano Lett. **23**, 140 (2023)

\* Weijiong Chen, Clara Neerup Breiø, Freek Massee, M.P. Allan, C. Petrovic, J.C. Séamus Davis, P.J. Hirschfeld, Brian M. Andersen, Andreas Kreisel *Interplay of Hidden Orbital Order and Superconductivity in CeCoIn5* Nature Communications **14**, 2984 (2023)

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*Type II multiferroic order in two-dimensional transition metal halides from first principles spin-spiral calculations* 2D Materials, **10**, 035016 (2023)

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*Plane wave implementation of the magnetic force theorem for magnetic exchange constants: application to bulk Fe, Co and Ni* 

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Lise Grüner Hanson\*, Bianca Laura Hansen, Thomas Veile, Mathias Zambach, Niels Bech Christensen, Cathrine Frandsen *The Impact of Sample Insulation on Estimating the Heating Power of Magnetic Nanoparticles by AC Calorimetry* IEEE Magnetics Letters, vol. 14, pp. 1-5, 2023, Art no. 6100505

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H. Chen, A. S. Manvell, M. Kubus, M. A Dunstan, G. Lorusso, D. Gracia, M. S. B. Jørgensen, S. Kegnæs, F. Wilhelm, A. Rogalev, M. Evangelisti, K. S. Pedersen *Towards frustration in Eu(II) Archimedean tessellations Chem. Commun.* **2023**, 59, 1609 ("HOT Article")

#### SDU (1)

A. B. A. Andersen, R. Tang Christiansen, S. Holm-Janas, A. S. Manvell, K. S. Pedersen, D. Sheptyakov, J. P. Embs, H. Jacobsen, E. Dachs, J. Vaara, K. Lefmann, U. G. Nielsen Understanding the Magnetic Properties of  $MAl_4(OH)_{12}SO_4 \cdot 3H_2O$  with M = Co2+, Ni2+, and Cu2+ by a Combined Experimental and Computational Approach PCCP **25**, 3309-3322 (2023)

RUC and KU Chemistry had no Q-MAT related publications in 2023.

## C. Patents related to Q-MAT topics.

(none)

## D. Student degrees 2023

Ph.D. degrees (2)

Q-MAT

AU, Chemistry (1)

• Mathias Mørch: Topotactic texture transformations & Magnetostructural Modifications

DTU, Physics (1)

• Mads Kruse, Theory of Charged Domain Walls in Multiferroics

#### MSc degrees (11)

AAU (3)

- Martin Vigh: Investigation of complex molecules deposited in UHV by electrospray ionization
- Lars Nørskov Nielsen: (title as above)
- Simon Ragner Sørensen: (title as above)

AU, Chemistry (2)

- Amalie Povlsen Laursen: Understanding the effect of shape-controlled iron oxide precursors in the synthesis of strontium hexaferrite magnets
- Jacob Løwe Valentin: *Nanocrystallite texture in hexaferrite permanent magnets*

KU, NBI (6)

- Sofie Castro Holbæk: Superconductivity in Kagome Materials
- Eva Lopez Rojoi: *Charge bond order in kagome metals*
- Luca Buiarelli: *Structural properties of kagome-layered crystals*
- Petroula Karakosta: Using McStas Union components to simulate a magnet sample environment and predicting background with machine learning
- Søren Birkemose: Polarized Neutron Reflectometry investigation of SC-FMI-SM Heterostructures
- Thomas Sahl Christensen: Low Temperature AC Susceptibility of the Frustrated Spin-1/2 Antiferromagnetic Kagomé System Herbertsmithite

#### Bsc. Degrees (8)

AU, Chemistry (2)

- Johannes Aagaard Andersen: *Synthesis and study of d-FeOOH*
- Rasmus Ringsborg Nielsen: Hard-hard synthesis and analysis of M-type SrFe12O19 with commercial precursors

DTU, Fysik (1)

• Theis Harbers van Bijlevelt Rix: *Simulation of magnetic nanoparticles* 

#### KU, NBI (5)

- Asbjørn F. L. Preuss: *Extended critical range in Bi2Fe4O9*
- Christine P. Lauritzen: *High Entropy LSCO Synthesis & Testing, Introducing High Entropy to the LSCO superconductor*
- Niels Anders L. Bærentzen: (title as above)

- Karen R. Ovesen: Magnetic frustration in rare earth garnets; Modelling magnetic interactions in *Gd3Ga5O12 and Yb3Ga5O12 using Spinteract*
- Jeppe B. Jacobsen: (title as above)