Supporting centres of excellence in research for strengthening international competitiveness and top quality

MID-TERM EVALUATION REPORT OF PROJECT

PROJECT DATA

Name and registry code of beneficiary	National Institute of Chemical Physics and Biophysics, 74000257
Project title	Emerging orders in quantum and nanomaterials
Project number	2014-2020.4.01.15-0005
Leader of CER	Urmas Nagel
Partners	Tartu University Tallinn University of Technology Estonian University of Life Sciences
Reporting period of project (project start date until December 31, 2018)	01.08.2015 – 31.12.2018
Start and end date of project	01.08.2015 – 01.03.2023
Name and position of person responsible for report	Urmas Nagel, Leader of CER, Director of the National Institute of Chemical Physics and Biophysics
Telephone number of person responsible for report	+372 5690 1425
E-mail address of person responsible for report	urmas.nagel@kbfi.ee

1. RESEARCH RESULTS

1.1 Work and activities performed. *Describe the work and activities performed by the centre and provide an overview of the results of the research (3-5 most important results), highlighting their novelty and added value.*
The importance of the result is in the novelty of the investigated state of matter, a quantum spin liquid, and its excitations. The research method is terahertz spectroscopy of quantum spin dynamics in alpha-RuCl3, a system proximate to the Kitaev honeycomb model, as a function of temperature and

magnetic field. We follow the evolution of an extended magnetic continuum below the structural phase transition at T_s2 = 62 K. With the onset of a long-range magnetic order at T_N = 6.5 K, spectral weight is transferred to a well-defined magnetic excitation at 2.48 meV, which is accompanied by a higher-energy band at h_omega(2) = 6.48 meV. Both excitations soften in a magnetic field, signalling a quantum phase transition close to B-c = 7 T, where a broad continuum dominates the dynamical response. Above B-c, the long-range order is suppressed, and on top of the continuum, emergent magnetic excitations evolve. These excitations follow clear selection rules and exhibit distinct field dependencies, characterizing the dynamical properties of a possibly field-induced quantum spin liquid. [Z. Wang, S. Reschke, D. Hüvonen, S. H. Do, K. Y. Choi, M. Gensch, U. Nagel, T. Rõõm, and A. Loidl. Magnetic Excitations and Continuum of a Possibly Field-Induced Quantum Spin Liquid in alpha-RuCl3. **Phys. Rev. Lett., 119**(22), NOV 28 2017].

In the second result we show that the magnetoelectric domains can be controlled with applied electric and magnetic fields and once a single magnetoelectric domain state is achieved, it stays present at low temperature even if the external fields are switched off. Additionally, our new theoretical approach showed that this monodomain state in not a ferrotoroidal state as previously claimed [B. B. Van Aken, J-P. Rivera, H., Schmid, and M. Fiebig, Nature 449, 702-705 (2007); A. S. Zimmermann, D. Meier, and M. Fiebig, Nat. Commun. 5, 4796 (2014**)].** One of the goals of multiferroic research is the development of a new-generation non-volatile memory devices, where magnetic bits are controlled via electric fields with low energy consumption. Here, we demonstrate the optical identification of magnetoelectric (ME) antiferromagnetic (AFM) domains in the $LiCoPO_4$ exploiting the strong absorption difference between the domains. This unusual contrast, also present in zero magnetic field, is attributed to the dynamic ME effect of the spin-wave excitations, as confirmed by our microscopic model, which also captures the characteristics of the observed static ME effect. The control and the optical readout of AFM/ME domains, demonstrated here, will likely promote the development of ME and spintronic devices based on AFM insulators. [V. Kocsis, K. Penc, T. Room, U. Nagel, J. Vit, J. Romhanyi, Y. Tokunaga, Y. Taguchi, Y. Tokura, I. Kezsmarki, and S. Bordacs. Identification of Antiferromagnetic Domains Via the Optical Magnetoelectric Effect. **Phys. Rev. Lett., 121**(5), AUG 1 2018].

The most recent CER remarkable result (the paper is being written by I. Reile) is in the field of developing a novel NMR methodology for the detection of cancer metabolites that uses nuclear hyperpolarization to enhance NMR sensitivity by 2-3 orders of magnitude. The excitation energies of nuclear spins in magnetic field are very small, in the radio frequency range, or less than microKelvin if we consider the relevant temperature range. Therefore, due to the Boltzmann distribution, the energy levels of nuclear spins in external magnetic field are almost uniformly populated at room temperature. Since the signal intensity in spectroscopic measurements based on magnetic resonance (NMR, MRI) is proportional to this (very small) population difference, such techniques are (very) insensitive. Sensitivity can, however, be improved if the population difference of the nuclear spin levels is increased by various hyperpolarization techniques. In collaboration with the North Estonian Medical Centre and the Radboud University (the Netherlands), we designed, built, optimized and tested the first NMR hyperpolarization setup in Estonia. The setup chemoselectively enhances NMR sensitivity by 2-3 orders of magnitude for certain analytes and allows detection of cancer metabolites that cannot be seen otherwise in biofluids. Our technique is based on parahydrogen and transfers the energy difference of the singlet and triplet ground states of H_2 to the studied nuclear spins. This result is not yet published. Its excellence in science lies in the way the method of hyperpolarization is used and applied.

1.2 Comparison of research results with international excellence in relevant field.

Assess the research results of the centre of excellence in comparison with the results of international excellence in the field.

The most important research results of the CER EQUiTANT, described in the previous section 1.1, are on the cutting edge in the world and represent true excellence in science.

1.3 Achieving the objectives of the centre of excellence. *Evaluate achieving the objectives of the centre of excellence as they were described in the application.*

There were three primary scientific goals in the application:

Firstly, we had demonstrated a strong DD effect at room temperature in a single multiferroic crystal in high magnetic fields. The goal of showing the same in this films or nanoparticles is still to be achieved. However, we have learned much about the multiferroic single crystals and their spectroscopy. We have also learned that growing suitable thick multiferroic films for THz spectroscopy is a much more challenging than originally anticipated. **The method of studying nonreciprocal directional dichroism spectra has been established as means of investigating magnetoelectric interactions in the scientific community.**

Secondly, we planned to study spin excitations on either side of field induced quantum critical points in disordered quantum magnets with the emphasis on mode localization and in-gap states using THz, neutron and NMR spectroscopy. **We have several papers on the subject, and we are still working on the topic**.

Thirdly, study of the role of frustration in ME magnets and its effect on the structure of 1/3 and 1/2 plateaus in SrCu2(BO3)2. This study is work in progress in collaboration with the high field laboratories both in Europe and USA but requires stronger magnets and new NMR probes and may take quite a while before new experiments can be done.

While working on the primary goals, our horizon has broadened, and we have found new collaborators from the world that bring up new challenges. This process itself is probably the most important of the general goals but was not stated explicitly in the proposal.

Applications of our research were not defined as goals in the proposal, but our researchers are working on them now. As developments in nanoparticle research E. Rauwel's group is working on the use of composite nanoparticles in water purification filters and L. Seinberg is studying the use of coated ferroic nanoparticles as contrast agents for MRI. I. Reile is working on novel NMR methodology to detect tiny amounts of molecules in biofluids.

1.4 Changes made to research activities and objectives compared to the initial plan. *What changes to the research have proven to be necessary? Provide an assessment of activities and any potential modifications planned until the end of the eligibility period.*

The initial research plan was built on the ongoing IUT and PUT projects that all had their research specific directions. General methods and goals of the CER have not been changed, but quite naturally the specific actions within the projects evolve with time. The IUT projects carry on until end of 2019 and people will write new grant applications in spring 2019, it will be their decision to choose a well-focused important topic that falls in line with the CER.

The groups of R. Stern from NICPB and A. Tamm from the University of Tartu, after their PUT projects had ended, came up with a joint grant proposal "Emerging Novel Phases in Strongly Frustrated Quantum Magnets" (PRG4). Their focus is in line with the original CER application. They study frustrated spin systems that exhibit a variety of behaviours ranging from exotic ground states and novel types of magnetic excitations, to the enhanced magnetocaloric effect and multiferroicity, relevant for applications. A corollary of the vibrant research in this field are new frustrated materials, both bulk and films, that hold promise for novel phases, interesting physics, and potentially useful properties. They proposed to perform comprehensive studies of these materials, from both experiment and theory, aiming to provide a realistic picture of their physics on both phenomenological and microscopic level. This combined approach gives them a rare opportunity to obtain novel experimental results, understand them within a suitable theoretical framework, and use this insight for the design of new materials. Their methods include low-temperature thermodynamic and microscopic(AFM-MFM)measurements, NMR and THz spectroscopy, neutron scattering, and DFT calculations combined with microscopic modelling.

Several young researchers have joined the CER with their own grants (section 1.5) and brought new ideas and directions. Most remarkably, I. Reile has launched a new experimental method for the detection of cancer metabolites that uses nuclear hyperpolarization to enhance NMR sensitivity by 2-3 orders of magnitude within two years after returning from post-doctoral research in Radboud University. He uses the method of hyperpolarization to enhance the spin order to detect tiny amounts of molecules and this work is one of our highlights (see section 1.1).

1.5 Changes in research teams compared to the initial plan.
Describe the changes made in research teams involved in the centre of excellence due to the needs for the research carried out in the centre of excellence. Describe the impact of the changes on the interdisciplinarity of the research carried out at the centre and on the efficiency of the centre's work.

The research groups are defined by their research method. The list of the members of each research team as at 31 December 2018 is provided as and additional document. The changes in the groups are listed below, and up to now all changes have had a positive impact on the efficiency of the centre's work.

National institute of Chemical Physics and Biophysics (NICPB) terahertz spectroscopy.
Dr. Anna Šugai was on maternity leave from summer 2017 to December 2018, PhD student Kirill Amelin started in 2017.

NICPB NMR spectroscopy.
Dr. J. Adamson joined in 2017 with his own post-doctoral grant MOBJD39 and supervises a PhD student Anna Peterson and Master's student Mari-Liis Ludvig. Dr. I. Reile joined the group in 2017 with his own returning scientist grant MOBTP51, and got a personal research grant PSG11 in 2018. He is supervising a Master's student Karl-Kristjan Kaup. Dr. Kerti Ausmees joined the group in 2018 and works on PSG11 as senior staff member.

NICPB nonlinear optical spectroscopy and quantum chemical computations.
A PhD student Sophie Maria Teresa Gronlier Marinucci De Reguardati Di Castelfranco graduated in 2017. Dr. Charles Stark joined the group in 2017 with his own post-doctoral reasarch grant MOBJD69 and got a personal research grant PSG317 that starts in 2019. Dr. Meelis-Mait Sildoja joined the group with his own returning scientist grant MOBTP128 in the fall of 2018. Dr. Aleksander Trummal and Dr. Merle Uudsemaa are doing quantum chemistry calculations that are needed for the nonlinear optical spectroscopy and are now less involved with the NMR group. Matt Rammo completed his Master's degree in 2017 and started as a PhD student. Batchelor degree student Katrin Petritsenko started in the fall of 2017.

NICPB PPMS and AFM
The group leader is Dr. Raivo Stern, who is also pursuing research in the field of NMR and is thus part of the NMR team of NICPB got a research grant PRG4 together with Dr. Aile Tamm from the University of Tartu (the ALD group of EQUiTANT). Dr. Oleg Janson, a post-doctoral researcher in his team left for his next position in TU Wien in end of 2016. Dr. Tanmoy Chakrabarty joined the group in 2017 with his own post-doctoral research grant MOBJD295. Dr. Valeriy Verchenko joined in the end of 2018 with his own post-doctoral research grant MOBJD449.

NICPB synthesis and study of nanoparticles, nanoecotoxicology
Dr. Angela Ivask left NICPB in 2018 and Dr. Kaja Kasemets from the Nanoecotoxicology lab of NICPB took over her role, supported by Dr. Anne Kahru and Dr. Olesja Bondarenko. Dr. Liis Seinberg joined in 2016 with her own research grant PUT1046. The PhD students in the group are Meeri Visnapuu since 2016 Maria Volokhova since 2017 and Merilin Rosenberg since 2018.

University of Tartu atomic layer deposition (ALD)
The group leader Dr. Aile Tamm since 2018 participates in the group research grant PSG4 of Dr. Raivo Stern (NICPB). PhD students Marko Part and Taivo Jõgiaas graduated in 2017, Taivo Jõgiaas stayed with the group. Master's students Peep Uudeküll graduated in 2017, Mats Mikkor started in 2017 and Mikk Kull started in 2018.

Estonian University of Life Sciences nanoparticle synthesis
In 2018 Dr. Erwan Rauwel moved his group from the Tartu College of TalTech to the Estonian University of Life Sciences as he found much better working conditions there.
Master's students Arnaud Behr was in the group in 2017 and Martin Malm started in 2018.

1.6 Popularisation and distribution of research results.
Give an overview of the research results' popularisation and dissemination activities.

We started with the kickoff seminar in April 2016, where most of the participants were from partnering institutions.
The web page was published in autumn 2016 https://kbfi.ee/chemical-physics/centre-of-excellence-134/?lang=en
Before the end of 2016 Archimedes produced a video clip what introduce the CER EQUiTANT and published it http://archimedes.ee/blog/urmas-nagel-see-mis-teeme-maailma-mastaabis-ebatavaline/

Members of the CER publish articles in newspapers that popularize the science and stress the need to have a scientific background of statements, we talk on radio and in TV. We participate in the campaign "Kust sa tead?", in English "Ask for evidence?" that targets the political discussions in Estonia with the aim of better science-based decision making. In 2018 there were two special seminars of the Estonian centres of excellence that targeted journalists and general public, one in May 2018 in Tartu and another in October in Tallinn, where each centre of excellence had the opportunity to give a half-hour presentation of general interest. We visit schools and talk at meetings of informal societies.

On professional level we present our research on national and international conferences and seminars. Each member of TK134 EUiTANT, including PhD students has had a presentation at least on one international meeting annually. We publish regular research papers, preferably in high impact journals whenever that is possible. To make our results more accessible, we have published also some open access papers: 8 in 2017 and 10 in 2018.

1.7 Most important publications.
Bring out up to 10 of the most important publications by researchers of the centre of excellence and describe the relevance of the publications from the point of view of achieving the aims of the centre of excellence .

Papers are ordered alphabetically by the family name of the first author. In addition to the relevance to the project, the selection criteria were number of citations and journal impact factor.

[1] R. S. Fishman, S. Borda´cs, V. Kocsis, I. K´ezsm´arki, J. Viirok, U. Nagel, T. Rõõm, A. Puri, U. Zeitler, Y. Tokunaga, Y. Taguchi, and Y. Tokura. Competing exchange interactions in multiferroic and ferrimagnetic CaBaCo4O7. **Phys. Rev. B**, 95(2), JAN 23 2017.

In the paper the mechanism of producing a large spin-induced electric polarization in CaBaCo4O7 is described. Competing exchange interactions can produce complex magnetic states together with spin-induced electric polarizations. With competing interactions on alternating triangular and kagome layers, the swedenborgite CaBaCo4O7 may have one of the largest measured spin-induced polarizations of similar to 1700 nC/cm2 below its ferrimagnetic transition temperature at 70 K. Upon rotating our sample about c = [0,0,1] while the magnetic field is fixed along [1,0,0], the threefold splitting of the spin-wave frequencies indicates that our sample is hexagonally twinned. Magnetization measurements then suggest that roughly 20% of the sample is in a domain with the a-axis along [1,0,0] and that 80% of the sample is in one of two other domains. Powder neutron-diffraction data, magnetization measurements, and terahertz (THz) absorption spectroscopy reveal that the complex spin order in each domain can be described as a triangular array of bitetrahedral c-axis chains ferrimagnetically coupled to each other in the ab-plane. The electric-field dependence of bonds coupling those chains produces the large spin-induced polarization of CaBaCo4O7.

[2] K. Juganson, M. Mortimer, A. Ivask, S. Pucciarelli, C. Miceli, K. Orupõld, and A. Kahru. Mechanisms of toxic action of silver nanoparticles in the protozoan Tetrahymena thermophila: From gene expression to phenotypic events. **Environ. Pollut.**, 225:481–489, JUN 2017.

Nanoparticles, including magnetic or multiferroic nanoparticles, have numerous applications and the mechanisms of toxicity of nanoparticles must be very well understood before using them in everyday life. Silver nanoparticles (AgNPs) are highly toxic to aquatic organisms, however, there is no consensus whether the toxicity is caused solely by released Ag-ions or also by reactive oxygen species (ROS). Here, the effects of protein-coated AgNPs (14.6 nm, Collargol) were studied on viability, oxidative stress and gene expression levels in wild type strains (CU427 and CU428) of ciliate Tetrahymena thermophila. Viability-based 24 h EC50 values of AgNPs were relatively high and significantly different for the two strains: similar to 100 mg/L and similar to 75 mg/L for CU427 and CU428, respectively. Similarly, the expression profiles of oxidative stress (OS) related genes in the two strains were different. However, even though some OS related genes were overexpressed in AgNP-exposed ciliates, intracellular ROS level was not elevated, possibly due to efficient cellular antioxidant defence mechanisms. Compared to OS related genes, metallothionein genes were upregulated at a considerably higher level (36 versus 5000-fold) suggesting that Ag-ion mediated toxicity mechanism prevailed over OS related pathway. Also, comparison between Agions released from AgNPs at EC50 concentration and the respective EC50 values of AgNO3 indicated that Ag-ions played a major role in the toxicity of AgNPs in T. thermophila. The study highlights the importance of combining physiological assays with gene expression analysis in elucidating the mechanisms of action of NPs to reveal subtle cellular responses that may not be detectable in bioassays. In addition, our data filled the gaps on the toxicity of AgNPs for environmentally relevant and abundant organisms. The parallel study of two wild type strains allowed us to draw conclusions on strain to strain variability in susceptibility to AgNPs.

[3] V. Kocsis, K. Penc, T. Room, U. Nagel, J. Vit, J. Romhanyi, Y. Tokunaga, Y. Taguchi, Y. Tokura, I. Kezsmarki, and S. Bordacs. Identification of Antiferromagnetic Domains Via the Optical Magnetoelectric Effect. **Phys. Rev. Lett.**, 121(5), AUG 1 2018.

One of the goals of multiferroic research is the development of a new-generation non-volatile memory devices, where magnetic bits are controlled via electric fields with low energy consumption. Here, we demonstrate the optical identification of magnetoelectric (ME) antiferromagnetic (AFM) domains in the $LiCoPO_4$ exploiting the strong absorption difference between the domains. This unusual contrast, also present in zero magnetic field, is attributed to the dynamic ME effect of the spin-wave excitations, as confirmed by our microscopic model, which also captures the characteristics of the observed static ME effect. The control and the optical readout of AFM/ME domains, demonstrated here, will likely promote the development of ME and spintronic devices based on AFM insulators.

[4] A. Krachmalnicoff, R. Bounds, S. Mamone, S. Alom, M. Concistre, B. Meier, K. Kouril, M. E. Light, M. R. Johnson, S. Rols, A. J. Horsewill, A. Shugai, U. Nagel, T. Rõõm, M. Carravetta, M. H. Levitt, and R. J. Whitby. The dipolar endofullerene HF@C60. **Nat. Chem.**, 8(10):953–957, OCT 2016.

One of the aims of studying endofullerenes is their potential use in applications of NMR spectroscopy as contrast agents, where they can fasten the relaxation or enhance contrast, especially in medical applications like MRI. The cavity inside fullerenes provides a unique environment for the study of isolated atoms and molecules. We report the encapsulation of hydrogen fluoride inside C-60 using molecular surgery to give the endohedral fullerene HF@C-60. The key synthetic step is the closure of the open fullerene cage with the escape of HF minimized. The encapsulated HF molecule moves freely inside the cage and exhibits quantization of its translational and rotational degrees of freedom, as revealed by inelastic neutron scattering and infrared spectroscopy. The rotational and vibrational constants of the encapsulated HF molecules were found to be redshifted relative to free HF. The NMR spectra display a large H-1-F-19 J coupling typical of an isolated species. The dipole moment of HF@C-60 was estimated from the temperature dependence of the dielectric constant at cryogenic temperatures and showed that the cage shields around 75\% of the HF dipole.

[5] L. G. Lukasiewicz, H. G. Ryu, A. Mikhaylov, C. Azarias, M. Banasiewicz, B. Kozankiewicz, K. H. Ahn, D. Jacquemin, A. Rebane, and D. T. Gryko. Symmetry Breaking in Pyrrolo[3,2-b]pyrroles: Synthesis, Solvatofluorochromism and Two-photon Absorption. **Chem.-Asian J.**, 12(14):1736– 1748, JUL 18 2017.

In this paper the effect of the symmetry of molecules on the two-photon absorption cross section is studied, the importance of the work lies in classifying the molecules for use in the calibrated measurements. Five centrosymmetric and one dipolar pyrrolo{[}3,2-b]pyrroles, possessing either two or one strongly electron-withdrawing nitro group have been synthesized in a straightforward manner from simple building blocks. **For the symmetric compounds, the nitroaryl groups induce spontaneous breaking of inversion symmetry in the excited state, thereby leading to large solvatofluorochromism. To study the origin of this effect, the series employed peripheral structural motifs that control the degree of conjugation via altering of dihedral angle between the 4-nitrophenyl moiety and the electron-rich core.** We observed that for compounds with a larger dihedral angle, the fluorescence quantum yield decreased quickly when exposed to even moderately polar solvents. Reducing the dihedral angle (i.e., placing the nitrobenzene moiety in the same plane as the rest of the molecule) moderated the dependence on solvent polarity so that the dye exhibited significant emission, even in THF. To investigate at what stage the symmetry breaking occurs, we measured two-photon absorption (2PA) spectra and 2PA cross-sections (sigma(2PA)) for all six compounds. The 2PA transition profile of the dipolar pyrrolo{[}3,2-b]pyrrole, followed the corresponding one-photon absorption (1PA) spectrum, which provided an estimate of the change of the permanent electric dipole upon transition, approximate to 18D. The nominally symmetric compounds displayed an allowed 2PA transition in the wavelength range of 700-900nm. The expansion via a triple bond resulted in the largest peak value, sigma(2PA)=770GM, whereas altering the dihedral angle had no effect other than reducing the peak value two- or even three-fold. In the S0S1 transition region, the symmetric structures also showed a partial overlap between 2PA and 1PA transitions in the long-wavelength wing of the band, from which a tentative, relatively small dipole moment change, 2-7D, was deduced, thus suggesting that some small symmetry breaking may be possible in the ground state, even before major symmetry breaking occurs in the excited state.

[6] A. Mannig, J. S. Moller, M. Thede, D. Huvonen, T. Lancaster, F. Xiao, R. C. Williams, Z. Guguchia, R. Khasanov, E. Morenzoni, and A. Zheludev. Effect of disorder on a pressure-induced z=1 magnetic quantum phase transition. **Phys. Rev. B**, 94(14), OCT 14 2016.

Quantum phase transitions occur at 0K at the quantum critical point where the Hamiltonian of the system changes, in other words, the relations of movement and ordering in the system change. Understanding the effect of disorder in this process is important for any real-world use of these materials. Pressure-induced ordering close to a z = 1 quantum-critical point is studied in the presence of bond disorder in the quantum spin system (C4H12N2)Cu-2(Cl1-xBrx)(6) (PHCX) by means of muon-spin rotation and relaxation. As for the pure system (C4H12N2)Cu2Cl6, pressure allows PHCX with small levels of disorder (x <= 7.5\%) to be driven through a quantum-critical point separating a low-pressure quantum paramagnetic phase from magnetic order at high pressures. However, the pressure-induced ordered state is highly inhomogeneous for disorder concentrations x > 1\%. This behavior might be related to the formation of a quantum Griffiths phase above a critical disorder concentration 7.5\% < x(c) < 15\%. Br substitution increases the critical pressure and suppresses critical temperatures and ordered moment sizes.

[7] P. Rauwel, M. Salumaa, A. Aasna, A. Galeckas, and E. Rauwel. A Review of the Synthesis and Photoluminescence Properties of Hybrid ZnO and Carbon Nanomaterials. **J. Nanomater.**, 2016.

Photoluminescent ZnO carbon nanomaterials are an emerging class of nanomaterials with unique optical properties. They each, ZnO and carbon nanomaterials, have an advantage of being nontoxic and environmentally friendly. Their cost-effective production methods along with simple synthesis routes are also of interest. Moreover, ZnO presents photoluminescence emission in the UV and visible region depending on the synthesis routes, shape, size, deep level, and surface defects. When combined with carbon nanomaterials, modification of surface defects in ZnO allows tuning of these photoluminescence properties to produce, for example, white light. Moreover, efficient energy transfer from the ZnO to carbon nanostructures makes them suitable candidates not only in energy harvesting applications but also in biosensors, photodetectors, and low temperature thermal imaging. This work reviews the synthesis an photoluminescence properties of 3 carbon allotropes: carbon quantum or nanodots, graphene, and carbon nanotubes when hybridized with ZnO nanostructures. Various synthesis routes for the hybrid materials with different morphologies of ZnO are presented. Moreover, differences in photoluminescence emission when combining ZnO with each of the three different allotropes are analysed.

[8] H. J. Silverstein, R. Sinclair, A. Sharma, Y. Qiu, I. Heinmaa, A. Leitmae, C. R. Wiebe, R. Stern, and H. Zhou. Naturally tuned quantum critical point in the S=1 kagome YCa3(VO)(3)(BO3)(4). **Phys. Rev. Mat.,** 2(4), APR 26 2018.

Quantum phase transitions occur at 0K at the quantum critical point where the Hamiltonian of the system changes, in other words, the relations of movement and ordering in the system change. Search continues to find model systems where new theories can be tested that help to predict novel features and materials. Although S = 1/2 kagome systems have been intensely studied theoretically, and within the past decade been realized experimentally, much less is known about the S = 1 analogs. While the theoretical ground state is still under debate, it has been found experimentally that S = kagome systems either order at low temperatures or enter a spin glass state. In this work, YCa3(VO)(3)(BO3)(4) (YCVBO) is presented, with trivalent vanadium. Owing to its unusual crystal structure, the metal-metal bonding is highly connected along all three crystallographic directions, atypical of other kagome materials. Using neutron scattering it is shown that YCVBO fails to order down to at least 50 mK and exhibits broad and dispersionless excitations. B-11 NMR provides evidence of fluctuating spins at low temperatures while dc magnetization shows critical scaling that is also observed in systems near a quantum critical point such as Herbertsmithite, despite its insulating nature and S = 1 magnetism. The evidence shown indicates that YCVBO in naturally tuned to be a quantum disordered magnet in the limit of T = 0 K.

[9] Z. Wang, S. Reschke, D. Hüvonen, S. H. Do, K. Y. Choi, M. Gensch, U. Nagel, T. Rõõm, and A. Loidl. Magnetic Excitations and Continuum of a Possibly Field-Induced Quantum Spin Liquid in alpha-RuCl3. **Phys. Rev. Lett.,** 119(22), NOV 28 2017.

The importance of the paper is in the novelty the state of matter, a quantum spin liquid, and its excitations. We report on terahertz spectroscopy of quantum spin dynamics in alpha-RuCl3, a system proximate to the Kitaev honeycomb model, as a function of temperature and magnetic field. We follow the evolution of an extended magnetic continuum below the structural phase transition at T_s2 = 62 K. With the onset of a long-range magnetic order at T_N = 6.5 K, spectral weight is transferred to a well-defined magnetic excitation at 2.48 meV, which is accompanied by a higher-energy band at h_omega(2) = 6.48 meV. Both excitations soften in a magnetic field, signalling a quantum phase transition close to B-c = 7 T, where a broad continuum dominates the dynamical response. Above B-c, the long-range order is suppressed, and on top of the continuum, emergent magnetic excitations evolve. These excitations follow clear selection rules and exhibit distinct field dependencies, characterizing the dynamical properties of a possibly field-induced quantum spin liquid.

[10] F. Weickert, N. Harrison, B. L. Scott, M. Jaime, A. Leitmae, I. Heinmaa, R. Stern, O. Janson, H. Berger, H. Rosner, and A. A. Tsirlin. Magnetic anisotropy in the frustrated spin-chain compound beta-TeVO4. **Phys. Rev. B**, 94(6), AUG 1 2016.

Frustration in physics is a state when a system is unable to simultaneously achieve a minimum energy for each entity involved. For example, in the antiferromagnetic Heisenberg model on a triangular lattice, the ground state cannot be the Néel state, since there will always be one "unhappy" bond. The system must come to a compromise, and the ground state is some canted antiferromagnetic arrangement. The paper is about isotropic and anisotropic magnetic behaviour of the frustrated spin-chain compound beta-TeVO4, that is more complicated than a simple antiferromagnet and has three magnetic transitions in zero magnetic field. The transitions are tracked in fields applied along different crystallographic directions using magnetization, heat capacity, and magnetostriction measurements. Qualitatively different temperature-field diagrams are obtained below 10 T for the field applied along a or b and along c-axis, respectively. In contrast, a nearly isotropic high-field phase emerges above 18 T and persists up to the saturation that occurs around 22.5 T. Upon cooling in low fields, the transitions at T-N1 and T-N2 toward the spin-density-wave and stripe phases are of the second order whereas the transition at T-N3 toward the helical state is of the first order and entails a lattice component. Our microscopic analysis identifies frustrated J(1)-J(2) spin chains with a sizable antiferromagnetic interchain coupling in the bc-plane and ferromagnetic couplings along the a-direction. The competition between these ferromagnetic interchain couplings and the helical order within the chain underlies the incommensurate order along the a-direction, a observed experimentally. While a helical state is triggered by the competition between J(1) and J(2) within the chain, the plane of the helix is not uniquely defined because of competing magnetic anisotropies. Using high-resolution synchrotron diffraction and Te-12 nuclear magnetic resonance, we also demonstrate that the crystal structure of beta-TeVO4 does not change down to 10 K, and the orbital state of V4+ is preserved.

1.8 Research teams.

*A list of the members of each research team as at 31 December 2018 should be provided and the data presented as an **annex to the report**.*

2. ASSESSMENT OF BENEFICIARY OF EFFECTIVENESS AND IMPLEMENTATION OF PROJECT

2.1 Launch of research centre of excellence.

Provide an assessment of the launch of the centre and of consequent opportunities and effectiveness of work.

The CER TK134 EQUiTANT proposal was written in august 2015. All groups continued their everyday work and informal collaboration until the decision to fund the CER was made in spring 2016.
Only after that we started to use the project funds and learn to manage with the administrative burden. From then on, the launch of the CER has been quite smooth and there were no setbacks in the work of the groups during the launch. In April 2016 we had a workshop in NICPB where all groups made a presentation about their current work and plans, followed by a discussion of further actions.

The CER created a wave of enthusiasm in the research groups. Since 2016 several young researches have started in NICPB with their own grants and joined the CER: L. Seinberg, PUT1048 in 2016, C. Stark, MOBJB69 in 2017, J. Adamson, MOBJD39 in 2017, I. Reile MOBTP51 in 2017 and PSG11 in 2018, M.M. Sildoja, MOBTP128, 2018. This is a real success of the CER as the new people brought in new ideas.

2.2 Effectiveness and implementation of project.
Provide an assessment of the effectiveness and implementation of the project.

As a project, the CER has been implemented efficiently both at the administrative level and within research groups. The number of publications has been increasing faster than we predicted. We have attracted new researchers who have obtained their own research grants and started new directions. We have more graduate students. Collaborations are evolving both within NICPB and with groups from several universities, encouraged by the CER leadership. The number of collaborative research projects has increased.

To conclude, the CER functions in an effective way producing positive impact on the research performed by the groups as well as increase the visibility of the CER.

2.3 Achievement of results of project.
Provide an assessment of the results to be achieved by the end of the project.

It is quite realistic to hope that we achieve the results that were proposed in the CER project. We work efficiently, there have been no mayor problems. The number of papers that we publish each year is growing faster than we thought that we can do. We have more researches in the project and there have been more guest PhD students working in our labs than was written in the proposal.

3. COORDINATION AND MANAGEMENT OF WORK OF CENTRE OF EXCELLENCE AND COOPERATION WITH OTHER PARTIES

3.1 Functioning of structure of centre.
Describe and evaluate the structure of the centre of excellence and its functioning.

The CER consists of seven interacting and collaborating research groups that cover terahertz spectroscopy, nuclear magnetic resonance spectroscopy, nonlinear optical spectroscopy, atomic force microscopy and physical properties measurements complemented by nanoparticle synthesis and nonecotoxicology studies plus atomic layer deposition. Two out of the seven groups are in Tartu while the others are in Tallinn.

Different experimental methods are used to study common problems and the groups share their networks of international collaborators. As a result, the CER has led to an increased communication between the research teams mostly through informal communication, joint seminars and conferences as well as exchanging ideas and complementary viewpoints.

Since in our fields of research the working culture is based on international collaboration, we believe that the present structure of the CER and its functioning is optimal for our field. On the one hand, there are regular CER activities. The responsibility for achieving research results is at the hands of the CER researchers. This allows us to develop new research projects between us and international collaborators, and we consider it to be optimal for achieving our research goals.

3.2 Cooperation.
Describe and evaluate how the functioning of the centre of excellence has contributed to cooperation with other national and international research teams and the business sector.

The greatest added value that is created by the CER is the increased cooperation both on national and international level. The cooperation on international level is usually informal and results in research projects of various lengths and they produce new knowledge in the form of publications.

On national level the cooperation has taken the form of writing joint grant applications, successful examples are **a)** R. Stern, PI from NICPB and A. Tamm from University of Tartu and **b)** J. Adamson from NICPB and PI R. Aav from Tallinn University of Technology.

Cooperation with the business sector is quite difficult to work out for hard-core solid state physics, but we are working on it.

The most important long-term business contract of NICPB is with an Estonian company Elcogen (www.elcogen.com), who is developing solid oxide fuel cells (SOFC), responsible person is J. Subbi (NMR group). Today Elcogen has industry-leading SOFC technology positioned to achieve market-enabling targets in the 3 most critical fuel cell performance parameters: efficiency, lifetime and cost. This collaboration currently does not produce scientific papers as the target is optimizing an industrial process. The goals are high, the SOFC can be used in two ways, 1st to generate heat and electricity and 2nd to generate H_2 by electrolyzing water vapor when a small voltage is applied to the cell. Thus, the SOFC can be a cornerstone of a future green hydrogen power plant, generating H_2 for storage when wind or solar energy is abundant and using stored H_2 to generate heat and electricity at other times.

The Estonian high-tech chemistry companies, who synthesize organic substances frequently use our 800 MHz NMR facility and especially the expertise of our researchers (T. Pehk, J. Adamson, I. Reile), because they really need to find out what molecules did they create in their processes.

The atomic layer deposition (ALD) group of A. Tamm at the Institute of Physics in the University of Tartu has contacts with companies who need specialized thin film coatings. For example they created a process to coat the inner surfaces of high pressure gas cylinders with a chemically stable layer for a company who is selling gases of very high purity.

We are working with the hospitals on applying nanotechnologies in medicine (L. Seinberg) trying to show that the use of ferroic nanoparticles as contrast agents for MRI is a better alternative to current gadolinium-based MRI contrast agents which have side effects due to their toxicity. Another medical application that we work on together with the hospitals is the use of advanced NMR methods for studying biofluids (I. Reile).

3.3 Assessment of research groups.
Which advantages the functioning as a centre of excellence has helped to bring out between different research teams and which disadvantages this has helped to reduce.

The clear advantage of the CER has been increased communication between groups in general. The research groups are doing well, the CER has improved our visibility and we have been able to recruit young people who have been able to secure their own research grants. That is especially important for the NMR group of NICPB where several members are not so far from retirement, and now they likely have vibrant future ahead, but it applies to all groups. Second, the CER has helped a lot to move the nanoparticle synthesis group of E. Rauwel to the Estonian University of Life Sciences. The CER has covered the salaries of several PhD students who work with the groups and that is very important, because we need the students to carry out the research.

4. SOCIOECONOMIC IMPACT OF CENTRE OF EXCELLENCE

4.1 Technological, economic and cultural impact.
Provide an assessment of the key aspects of the technological, economic and cultural impact of the results of the research and activities of the centre at the Estonian and European Union levels.

While assessing the technological impact of basic research we need to consider that the research produces new knowledge that can be applied anywhere, where there are companies ready to use it and markets where to sell the product. Even the level of European Union is not enough, we need to consider the whole world. And then there is the time factor. We study and create new materials, of course we mostly study them, creating is much more difficult and requires more resources. When we use different spectroscopies to study new crystals, we rely on our friends, chemists, who constantly synthesize new materials and only very few of them are interesting enough to be grown into large crystals, that are suitable for spectroscopies. While we study these samples, we usually need to find theorists, who can understand end explain the results, because they have the required theoretical tools. Materials are different, experimental and theoretical tools also, so we constantly need to find new collaborations to advance to new fields. If we are good enough, we can collaborate with the top groups in the world.

Once we have understood one class of materials, it might happen, that they can be used to build something, but it still takes many years until some material gets truly widespread use like silicon today. In the process, we have offered an opportunity for quite several PhD students to do their research and graduate, become members of the science-based society. And that is probably the largest economic and cultural impact of our work.

4.2 Cooperation with interest groups.
List the centre's most important interest groups and describe their cooperation.

Our most important interest groups are from the scientific community. The CER has attracted several visiting scientists, PhD and master students to perform research projects at participating groups. All groups have established their own visitor programs. For several years we have used a bilateral collaboration agreement between the Estonian and Hungarian academies to enhance the joint projects. On one occasion in 2016 a PhD student Yuto Kinoshita from Tokyo University Institute of Solid State Physics (ISSP) spent 2 months with the THz group in Tallinn for training purpose, not research.

Another interest group is the community of local high-tech companies.

5. FINANCIAL REPORT

5.1 Use of project budget
The required information ***(Annex 1)*** *is provided about the use of the project budget, including explanations regarding over- or underuse compared to the estimates and targets set in the application. Changes to the budget made during the reporting period are also shown.*

5.2 Financial corrections and recoveries.
Information is provided on the financial corrections made and recoveries related to the project.

Due to human error on one occasion (MT nr 46077) the working hours and vacation time of Dr. L. Seinberg were accounted for incorrectly. This resulted in a financial correction of 1 607.94 €. Since MT nr 46077 has been paid out it was decided by Archimedes that the funds will be recovered by reducing the next payment.

5.3 Procurements conducted.
The procurements conducted as part of the project are reported: costs related to purchasing and updating the equipment necessary for research and development, costs related to information technology solutions,etc.
The data are presented as ***an annex*** *to the report.*

5.4 Potential changes to the budget.
Planned/potential changes to the project budget up to the end of the eligibility period are reported.

We have not planned any changes to the budget up to now, but we may need to review the budget in 2020, because the large institutional grants (IUT) that NICPB currently has, end with 2019, and depending on the outcome of the new grant applications, we may need to change something. Ending of IUTs is a problem because the system of science funding in Estonia has changed, calls for new IUTs have not been opened in last years and IUTs will be deprecated by the new law. The new personal grants are smaller and shorter in duration than the IUTs. Budget fluctuations in 2020 that are inevitable, considering the 20% average success rate on applying for new grants – even if we are doing twice as good (like in the 2018 round), some of us still get rejected and we probably need to increase the amount of personnel costs and reduce others, like costs for maintenance and repair.

6. LIST OF ADDITIONAL DOCUMENTS

The following additional documents have been annexed to the report (please note):	
☒	Financial statement of the project (as of the month preceding the submission of the interim report) (ANNEX 1)
☒	Centre of excellence result and effect indicators (ANNEX 2)
☒	List of publications of the centre of excellence (as at 31 December 2018)
☒	A list of the members of each research team (as at 31 December 2018)
☒	List of the procurements conducted
☐	Additional information

I confirm that all the data presented in this report are correct and that the assistance has been used in compliance with the obligations laid down in the Structural Assistance Act and in legislation issued on the basis thereof, in the decision of satisfying the assistance and in the regulation of the measure “Supporting research centres of excellence for strengthening international competitiveness and top quality”	
Name and position of the person with the right to represent the beneficiary	**Date**
Urmas Nagel	15.01.2019

ANNEX 1

FINANCIAL REPORT OF PROJECT BY COST TYPE

Cost objective	Project budget	Implementation of the project's budget		
		Implementation of the budget as of the date of submitting the most recent financial statement (cumulatively as from the beginning of the project)	Budget fulfilment, % Percent of budget implementation	Explanations about the implementation of the budget compared to the valid budget (incl. describe the content of the changes in the budget made until today)
Expenses and travel costs related to organizing trainings and participating in such trainings, and related to researcher mobility	112 000.00	20 673.30	18.46	As we have had other resources, mainly the institutional grants (IUT) and the administrative burden of using the CER funds is large, we have used less travel money. The last year of IUT-s is 2019 and it may happen that we need to use more CER funds to cover travel costs in the next years. Currently we do not plan to change the budget.
Rental costs related to equipment, machinery and vehicles needed for research	0			-
Purchase or leasing of a road vehicle specially adjusted for research	0			-
Costs related to acquisition, improvement, installation and configuration of equipment and machinery, lab furnishings and field study outfit and work equipment; also the costs related to the acquisition, improvement, installation and configuration of equipment, machinery and lab furnishings which are an integral part to work	200 000.00	136 609.40	68.30	The largest single item acquired was a femtosecond laser system that covers 112.3 k€, the next largest item was the glovebox (16.648 k€). We expected to invest mostly in the beginning of the project.
Maintenance and repair costs related to equipment and machinery to be purchased or already existing; also maintenance and repair	168 000.00	0.00	0.00	We have not had mayor breakdowns of main scientific instruments and we have had other resources to cover the smaller maintenance costs, we have not used CER funds for maintenance and repair up to now. We will decide latest in the beginning 2021 if we need to change the budget and allocate

costs for technology that is integral part to equipment and machinery to be purchased or already existing				some of the maintenance and repair costs to direct staff expenses.
Costs for subcontracting in order to carry out the project	0			-
Costs for IT solutions, including the expenses related to creating data entry and analysis environment, database development, hardware and software; except for the IT solution costs described in the Joint Order Article 9 SubSection 5 Item 3 (IT expenses considered to be a project's overhead costs)	50 000.00	6 782.43	13.56	We have spent less than originally planned on IT solutions. We will decide latest in the beginning 2021 if we need to change the budget and allocate some of the costs of IT solutions to direct staff expenses.
Costs related to dissemination, publication and popularization of research results; including costs related to event organization (at least 2% of the allocation)	74 000.00	9 289.61	12.55	Clearly dissemination, publication and popularization of research results and costs related to event organization has not been implemented well enough and we need to act. We plan to make a dissemination campaign in the second part of the CER period that focuses on the obtained results and new prospectives.
Other costs directly related to supported activities and necessary for the said activities (e.g. materials, accessories, etc.)	95 666.32	41 979.66	43.88	This section of the budget has been used almost proportionally with the time span of the CER.
Direct staff expenses (except for staff expenses related to project administration)	2 738 601.79	864 962.26	31.58	We have been slightly conservative in using the budget for direct staff expenses, because we are probably facing fluctuations in the budget when the IUTs in NICPB end with 2019 and we need to secure several new grants.
Indirect expenses, 15% of direct staff expenses (Joint Order Article 9 SubSections 46)	410 790.27	129 744.67	31.58	No comments.
Total eligible costs	3 849 058.38	1 210 041.33	31.44	No comments

ANNEX 2

The output indicator of the centre of excellence

Number of publications published by CER scientists in a calendar year in the Thomson Reuters Web of Science database (databases SCIEXPANDED, SSCI and A&HCI) and in journals indexed in European Reference Index for the Humanities and the Social Sciences (ERIH PLUS).	2016	2017	2018
The output indicator in the application	21	23	25
Actual results of the centre of excellence	15	36	32

Add explanations if the planned results are not achieved

2016	The centre of excellence started after the application turned out to be a success in 1st quarter of 2016 and the grant number was not added to papers that were submitted in the beginning of the year 2016. Therefore, the actual number reached in 2016 is less than projected in 2015. In the 2016 annual report the number of published papers was 14, but now it appears that the actual number was 15. The reason for the difference is a paper published close to the end of the year. See the list of publications that is split between the years.
2017	The original target indicator from the proposal 28 was reduced to 23 in February 2016 after the project was approved with reduced budget. However, we did much better than we expected! The number of published papers that was reported in the 2017 annual report was 37, now it appears that the correct number was 36. The reason for the difference is a paper published close to the end of the year. See the list of publications that is split between the years.
2018	The original target indicator from the proposal 29 was reduced to 25 in February 2016 after the project was approved with reduced budget. However, we did much better than we expected also in 2018!

2016 list of publications as of 31.12.2018

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A list of the members of each research team (as at 31 December 2018)

- **National institute of Chemical Physics and Biophysics (NICPB)** terahertz spectroscopy

  Toomas Rõõm (IUT23-3 principal investigator), **Urmas Nagel** (leader of CER TK134), **Dan Hüvonen**, **Girsh Blumberg**, PhD students **Laur Peedu, Johan Viirok, Kirill Amelin**

- **NICPB** NMR spectroscopy

  Ivo Heinmaa (IUT23-7 principal investigator), **Indrek Reile** (MOBTP51 and PSG11 principal investigator), **Jasper Adamson** (MOBJD39 principal investigator), **Tõnis Pehk**, **Juhan Subbi**, **Kerti Ausmnees**, PhD student **Anna Peterson**, Master's students **Mari-Liis Ludvig** and **Karl Kristjan Kaup**

- **NICPB** nonlinear optical spectroscopy and quantum chemical computations

  Aleksander Rebane (IUT23-9 principal investigator), **Charles Stark** (MOBJD69 principal investigator), **Meelis-Mait Sildoja** (MOBTP128 principal investigator) **Aleksander Trummal**, **Merle Uudsemaa**, **Sirje Vija**, PhD student **Matt Rammo**, batchelor student **Katrin Petritsenko**

- **NICPB** PPMS and AFM

  Raivo Stern (PRG4 principal investigator), **Tanmoy Chakrabarty** (MOBJD295 principal investigator), **Valeriy Verchenko** (MOBJD449 principal investigator), PhD student **Joosep Link**

- **NICPB** synthesis and study of nanoparticles, nanoecotoxicology

  Anne Kahru (IUT23-5 principal investigator), **Kaja Kasemets** (NAMUR+ principal investigator), **Liis Seinberg** (PUT1046 principal investigator), **Olesja Bondarenko** (PUT1015 principal investigator), PhD students **Merilin Rosenberg, Meeri Visnapuu, Maria Volokhova**

- **University of Tartu** atomic layer deposition

  Aile Tamm, **Taivo Jõgiaas**, PhD students **Kristian Kalam**, **Helina Seemen**, **Andreas Nõlvak**, Master's students **Peep Uudeküll** (graduated), **Mats Mikkor**, **Mikk Kull**

- **Estonian University of Life Sciences** nanoparticle sythesis

  Erwan Rauwel, **Protima Rauwel**, PhD student **Siim Küünal**, Master's student **Martin Malm**

List of the procurements conducted

Costs related to acquisition, improvement, installation and configuration of equipment (indicating only the part that was payed by the CER):

- 10.03.2016, 669.90 EUR, Magnetic stirrer MR Hei-Tec, Biotecha Eesti OÜ (12459554), H-168790
- 27.02.2018, 900.00 EUR, Osone generator and analyzer, BMT Messtechnik GmbH (DE86146265)
- 20.11.2017, 112 300.00 EUR, Femtosecond laser system, UAB MGF Šviesos Konversija (Light Conversion) (222598890), H-188194
- 07.07.2017, 16 648.00 EUR, Glovebox, Faneks Eesti (12235010), H-180321
- 25.10.2018, 1 091.50 EUR, Analytical balance MA1803163, HNK Analüüsitehnika (10360403)

Costs for IT solutions:

- 18.04.2016, 84.99 EUR, Virus protection software Avast viirusetõrje
- 20.04.2016, 6 260.98 EUR, Software OriginPro 9.1-2016, DoubleClick AB (556766-3678)
- 23.11.2016, 412.50 EUR, Software Mnova NMR,Mestrelab Research S.L. (ESB15964521)
- 05.07.2017 3, 23.96 EUR, Software, Advanced System Optimizer