ERC Starting Grant 2020
Research proposal [Part B1][1]
(Part B1 is evaluated both in Step 1 and Step 2,
Part B2 is evaluated in Step 2 only)

Magnetoelastic Materials beyond Born-Oppenheimer Approximation

Cover Page:

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- 60 months

Nearly a century ago, the **Born–Oppenheimer approximation** simplified condensed matter physics by separating motion of nuclei and electrons. When this concept is violated, interactions between phonons and elementary excitations, such as plasmons, magnons or particle-hole pairs, lead to emergent functionalities such as multiferroic behaviour, polar order or superconductivity. These phenomena are usually rare and applicable to a limited number of compounds. In **our recent study**, we have demonstrated an abundance of magnetoelastic (ME) interactions in intermetallic cerium compound, revealing that the connection between electrons and one thousand times heavier atomic nuclei is far more common.

MaMBA aims to show that ME effects are a general property of solid-state physics and argues that the assumption of Born and Oppenheimer must be **thoroughly checked**. Due to the challenge of detecting ME modes, it was not realized before that the only direct method capable of doing so is through inelastic neutron scattering on a single crystal. My long-standing experience as an instrument scientist makes me **an ideal candidate** to carry out such a study.

I believe that hidden ME modes are responsible for many unresolved problems, and its proper description will lead to rapid progress in the area. MaMBA seeks to experimentally exploit ME modes in a) heavy fermion materials, where unconventional superconductivity was discovered; b) Uranium ruthenium silicide with still unresolved "hidden order", where ME correlations were proposed; and c) iron pnictides, where symmetry breaking is related to ME effects. A significant element of the project is the **development of a bespoke device, the Automatic Laue Sample Aligner (ALSA)**, for automatic single crystal alignment. **I will use my knowledge** of computer vision to drastically speed up the sample preparation process. The device will be truly revolutionary in the field of neutron spectroscopy and will have an immense impact **beyond the scope of MaMBA**.

[1] Instructions for completing Part B1 can be found in the '*Information for Applicants to the Starting and Consolidator Grant 2020 Calls*'.

Section a: Extended Synopsis of the scientific proposal

MaMBA project aims to show, that **magnetoelastic effects are a general property of condensed matter** and Born-Oppenheimer approximation [1] is surpassed far more often than generally thought. Here it is important to clarify to what extent I will use the term magnetoelastic. MaMBA doesn't plan to study response of the lattice dimensions to the application of the external magnetic field and is also not interested in interaction between magnons and phonons. Magnetoelastic properties within scope of this projects are general interaction between lattice vibrations and electron spins. This coupling is well known and studied in several compounds referred as materials with high magnetoelastic coupling [2, 3, 4]. Such interactions occur in any material, but their effects are usually neglected. MaMBA research will show, that even a small ME coupling can lead to a formation of the new states in matter and therefore be responsible for diverse ground states and exotic modes in materials.

It is fully new approach with a **strong impact to solid-state physics** (see Fig. 1): 1) a newly developed robotic sample coaligner will address a critical challenge of insufficient sample mass for neutron experiments, and 2) a new types of methodology will be established to include magnetoelastic coupling in phonon calculations and crystalline electric field models.

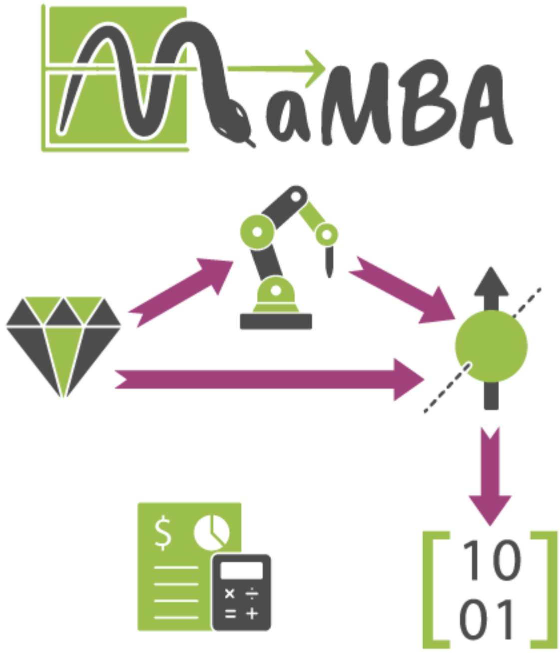


Fig. 1: MaMBA in a nutshell: We will grow the single crystals, small ones will be automatically coaligned by artificial intelligence robot, and analyze them using inelastic neutron spectroscopy giving valuable input for magnetoelastic theory development.

General background

Rapid enhancement of the instrumentation in the last decades allows us to analyse samples by several orders of magnitude faster than before. Combined with increasing pressure from funding agencies to publish, these developments have led to the fragmentation of research. There are more than 500 papers about the pronounced unclarified anomaly in specific heat of URu_2Si_2 (so-called "hidden order"), but the compound is still not fully understood. Unconventional superconductivity has been known about for more than 30 years [5], but it has still not been fully explained. It seems that we are missing a crucial part of the puzzle.
The MaMBA project takes a novel approach on these strongly correlated systems. I will not focus on discovering new materials or measuring existing compounds under more extreme conditions. The time has come **for new perspectives on old theories**. I am certain that there is a hidden general property of the matter that has been overlooked because of the techniques used. In order to convince you of it, we need to look into the history…

Back to roots

At the very beginning of the 20th century, German physicist Max Planck laid down the foundations of quantum physics, a fundamental theory that has shaped the technology we use in our everyday life. His work was so radical that its implications are still at the frontier of present-day research. From the earliest days of quantum theory, Nobel prize winner Max Born and his colleague Robert Oppenheimer suggested as an important approximation that the motion of atomic nuclei and electrons in condensed systems of atoms may be separated because of their very different masses and speeds [1]. The so-called **Born–Oppenheimer (B–O) approximation** simplifies the complexities of the quantum mechanical equations and has become the foundation for much of current solid-state physics.

It is a very important approach because the most complex system we can analytically solve without the B–O approximation is the atom of hydrogen. Nowadays, we are able to simulate plenty of physical properties using a normal computer or laptop, like the entire vibration spectrum of the single crystal [6], but we neglect electron–nuclei interaction. It is amazing that such a cornerstone of condensed matter research has **never been comprehensively questioned**, and it is not clear whether there are hidden consequences of overusing the B–O approximation. The polemic is already taking place in chemistry [7], where the world beyond the B–O approximation has important consequences [8, 9]. Recently, theoretical physicists have joined the discussion [10], and their theories are waiting for experimental verification [11, 12]. Through their ongoing ERC grant, very promising research is coming out of Mikhail Lemeshko's group [4] dealing with ME coupling using a novel approach of the angulon quasiparticle. See the *Detailed proposal section* for details. Surprisingly, experimental data for the verification of mentioned theories are missing and adopting a precise approach with **cutting-edge techniques** is needed to face the challenge.

The ordinary compound

I was the driving force of our novel research on an intermetallic material, $CeAuAl_3$ [13]. The most special property of this compound is that it is **fully ordinary**. It started purely by chance as a part of regular student Labcourse. We put sample to the beam just for training and next day we were extremely excited with our results – PANDA spectrometer revealed a **new unexpected mode**!

It is an archetypal Kondo lattice compound with a transition temperature T_N = 1.32 K [14]. It was studied before in detail by Adroja et al.; its magnetic structure was determined, and they claimed: "This study also indicates the absence of any CEF-phonon coupling unlike that observed in isostructural $CeCuAl_3$" [15]. Until 2015, it was one of many heavy fermion compounds. Our findings were surprisingly contradictory, and we were able to detect an abundance of magnetoelastic effects in the material [13]. **The reason is the technique used for measurement**. Unlike other researchers, we used three axis spectrometers [16] on high-quality single crystals of $CeAuAl_3$ [17]. This method is much more time-consuming and challenging, but it is worth doing it because it can reveal detailed changes in the spectra of lattice vibrations (phonons) as well as in the spectra of electronic excitations (crystalline electric field [CEF], in our case). Our outcomes pointed to two important conclusions. First, magnetoelastic coupling is **much more generic** than hitherto assumed; and second, even weak coupling can lead to the **creation of new states** in the matter.

Magnetoelastic zoo

Our research was done on one intermetallic heavy fermion compound, but we believe that magnetoelastic coupling is key and a general property in condensed matter physics. There is a diverse portfolio of materials that have exhibited unique properties with different potential applications in which magnetoelastic effects have turned out to **be crucial systems properties**, like cerium Kondo systems [2, 18, 19], pyrochlores [20, 21, 22], neptunium oxides [23] or multiferroics [24, 25]. Also Aksenov's prediction about coupled quadrupole-phonon excitation should also be mentioned, since he theoretically described the existence of crosstalk between electrons and acoustic lattice vibrations in the year 1983 [26]. He was unable to observe the effect directly, and the **theory waited 35 years** before we calculated [27] and observed same effect in $CeAuAl_3$ [13].

However, unifying theories are still missing, and scientists from different fields of research have very often been unaware of each other. In general, the creation of new ME hybridized modes is still considered an exceptional case, and no one is treating it from a broader perspective. There is a general need for advanced theories and complex computational approach to simulate magnetoelastic effects, and more compounds need to be investigated in detail to verify the theoretical predictions.

Detailed proposal

We have opened up a new field in condensed matter physics where the Born–Oppenheimer approximation is no longer valid. **The goal of the MaMBA** project is to show that magnetoelastic coupling is a general property of matter, and even if it is weak, it can have immense consequences. We have identified three areas of research where magnetoelastic coupling will shed new light on the problematics:

1) **Coexistence of magnetism and superconductivity in correlated systems**
   Unconventional superconductivity was first observed in heavy fermion material $CeCu_2Si_2$ [28] in 1979 and is still an unresolved topic [29]. Although many groups of unconventional superconductors exist with high critical temperatures [30], a proper understanding of the mechanism of the creation of superconducting condensate in heavy fermions is a key step in understanding all other materials. Heavy fermion compounds belong to the group of strongly correlated systems, where dominant driving force is the **enhanced electron-electron interaction**. We have revealed that new concepts should be applied, while even in the presence of strong interelectron interactions, weak electron-phonon coupling can lead to significant changes in the density of electronic and phononic states [13]. In addition, a common property of heavy fermions is the existence of *f*-electron magnetism, which is always accompanied by a crystalline electric field (CEF). We already know that CEF hybridization with phonons can lead to the creation of new states in materials [31], but **complex magnetoelastic studies** on heavy fermion superconductors are missing.

2) **Hidden order in URu_2Si_2**

Heavy-fermion superconductor URu_2Si_2 exhibits a second-order phase transition at $T_0 = 17.5\,\mathrm{K}$ manifested as a large anomaly in specific heat. The nature of the transition and the whole ordered phase below it remains unclear and is referenced as a hidden order (HO) phase. Currently there are two different possible theories: either the compound is an itinerant band metal or Uranium electrons are localized in $5f^2$ configuration and HO phase is originating from its crystal-field ground state (or dual nature scenario) [32]. Localized option was often neglected, because no CEF levels were detected by inelastic neutron scattering on powder [33]. This was changed with recent **quantum oscillation measurements** supporting localized scenario [34] or novel anisotropic itinerant system [35]. The CEF excitations were recently observed by X-Rays [36] and not yet confirmed by neutrons.

Despite an incredible amount of published research, comprehensive study of phonon spectra in the material is still missing [32]. We have already learned, that even a weak coupling can lead to the creation of emerging states in matter. These states can be undetectable on the powder measurement [13] and detailed inelastic neutron study on single crystal is needed. In addition a recent study by Wartenbe et al. has revealed **the importance of coupling** [37], making URu_2Si_2 an ideal candidate for our investigation.

3) **Mechanisms behind structural distortion in iron pnictides**

Unlike other unconventional superconductors, superconducting transition in pnictides is accompanied by a structural transition connected with symmetry breaking. We have learned [13] that symmetry is a key point for the creation of hybridized states in matter. Despite iron pnictides being a very hot topic, their magnetoelastic effects are rarely studied. There are **emerging new theories** based on angulon quasiparticles, bringing a new approaches for calculation of electron-phonon hybridized spectra in oxides and *d*-electron metals [4]. We have discussed a lot with author of the manuscript J. Mentink about adapting his theories to static crystal field models and also *d*-electron systems.

Project strategy

Magnetoelastic effects are often overlooked and scientists still live in a world in which Born–Oppenheimer approximations are valid mainly because of the enormous demands placed on the experimental techniques used. There exist several direct or indirect ways of detecting the lattice vibration spectra of the material (phonons). There also exist a number of methods for detecting electronic levels in the material (CEF). But the only technique that can detect both together is **inelastic neutron scattering**. In addition, one needs to focus on specific positions in reciprocal space and study excitations on single crystal of the material. Such experiments are time-consuming, and it is only possible to realize them in **large neutron facilities**. The method also places demands on the size of the sample: mass of about 1 g is needed.

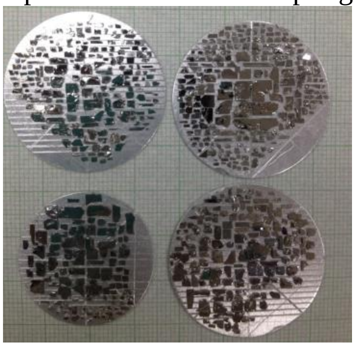


Fig. 2: Hundreds of tiny samples of $CeCoIn_5$ ready for neutron experimentation [44].

The requirement for the size of a single crystal is a tough proposition. More than a half of the single crystals we are going to investigate are **incongruently growing** (majority of correlated systems and all iron pnictides, see part B2 for details), so that the size of one crystal is in the order of milligrams. We need to co-align several hundred pieces to create a sample suitable for an inelastic neutron experiment (see Fig. 2, for example). Previously the preparation of one sample took several months of work and required a lot of manpower. MaMBA project is going **to change it**. We will fully automatize the co-alignment process by using a state-of-the-art X-ray Laue diffractometer, **robotized manipulators**, real-time camera recognition and AI for software analysis. The device ALSA (Automatic Laue Sample Aligner) will be truly revolutionary in the field of inelastic neutron scattering because it will drastically speed up the sample preparation process.

ALSA: A gamechanger in inelastic neutron scattering

The purpose of the ALSA device is to take several small single crystals with a known crystal structure but an unknown orientation, orient them and glue them together on an aluminium plate. Most of the single crystals grown using a flux growth technique are plate-shaped samples with a high symmetry crystallographic axis perpendicular to the surface of the sample. With this constraint, orientation and especially the gluing of the samples becomes a much easier task (since there is only one degree of freedom). The oriented crystals need to be glued very close to each other in order to keep the final sample as small as possible. The basis of the device will be a conventional Laue X-ray diffractometer. In addition, there will be a robotic arm with a tiny plastic straw. The arm will use suction to grab the sample, and a conventional industry camera will determine its detailed shape. Then the arm will take the sample to the X-ray beam, and specially developed software will automatically determine its crystallographic orientation from the Laue image. Software will match both microand macroscopic orientations together, and the arm will glue the sample in the correct place on the aluminium plate.

We are aware of **many challenges** connected with the development of ALSA. The crucial part of the device will be its software, which will be developed in cooperation with the Center for Machine Perception at the Czech Technical University in Prague. I am an expert on Laue image analysis as I co-developed the Esmeralda Laue Suite, which is state-of-the-art neutron Laue analysis software [38]. I also worked for almost one year for a private company where I developed automatic product recognition based on computer vision. The AI element will be taken care of by the team of Lukas Neumann, who is an award-winning [39] member of the Visual Recognition group at Czech Technical University and a lecturer at the University of Oxford.

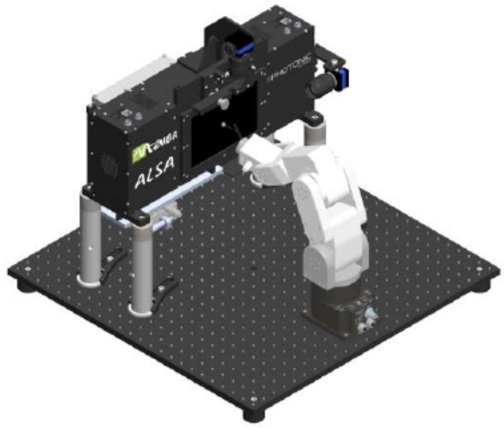


Fig. 3: Preliminary rendering of the ALSA device: The Automatic Laue Sample Aligner.

Theory and calculations

Successful neutron experimentation is not enough. We will develop a complex theory of phonon–CEF coupling. Up to now, there have only been theories describing how CEF spectra are influenced by phonons [2], but none of them have taken into account how phonon spectra are changed by their hybridization with electrons. We have started a collaboration with **K. Becker, M. Loewenhaupt and P. Thalmeier**, who are experts in crystal field excitations and coupling with phonons. K. Becker is already working on the extension of the famous Becker–Fulde–Keller theory [40] to describe changes in the phonon spectra: "Bound states of phonons and CEF excitations".

In order to test the theory, powerful simulation software is needed to confront the measured data. Existing software can simulate pure phonon spectra without a major external influence [6]. New software will be developed by Martin Rotter, developer of the well-known magnetism software McPhase [41]. The resulting code will be published under an open source licence and will be available for external use. In the second half of the project, we plan to involve angulon model [4] to our calculations. It will be needed especially for the calculation of the hybridized phonon spectra of iron pnictides and oxide materials. We will closely collaborate with Johan Mentink from Radboud University Nijmegen and needed software libraries will be again developed by Rotter.

Project organization

I will supervise five interrelated work packages (WP):

WP1 – Sample preparation and characterization (Crystal team)

High-quality single crystals will be grown at the MGML laboratory in Prague (https://mgml.eu). Its variety of equipment can meet our crystal growth needs. First, crystals will be prepared from the melt, and later from the flux (once ALSA is in operation). It will need **three PhD students**.

WP2 – ALSA team for AI development

ALSA team will kick-off the project and consist of **the engineer and the postdoc**. I will start to develop a computer vision algorithm for sorting the oriented crystals, while the engineer's and postdoc's main responsibility will be sample grabber and robotic arm movement.

WP3 – Neutron team

The crucial part of MaMBA. The team will perform neutron experiments to prove initial assumptions utilizing mainly European triple-axis and time-of-flight spectrometers. That approach requires experts in the field of inelastic neutron scattering: me and **two experienced postdocs**.

WP4 – Theory team

The theory and software for coupled magnetoelastic excitations will be developed through collaboration with external subjects. We will collaborate with experts in this field: K. Becker and M. Loewenhaupt and J. Mentink. First two are already working on the theoretical manuscript regarding magnetoelastic coupling; however, they need much more experimental input and measured data. Software will be developed by scientific programmer Martin Rotter.

WP5 – Administration team

The complexity of MaMBA requires solid administrative support. In the first year of the project, several public procurements for parts for the ALSA device need to be placed. A project manager will be also responsible for meeting all the ERC commitments and rules.

Timeframe

The project is designed for five years. The CRYSTAL and ALSA teams will start to work simultaneously. When the ALSA instrument is ready, the CRYSTAL team will switch to grow small flux samples for alignment in ALSA. The NEUTRON team will begin their measurements from the second year of the project when enough high-quality samples have been produced. See Gantt chart for details (Fig. 4).

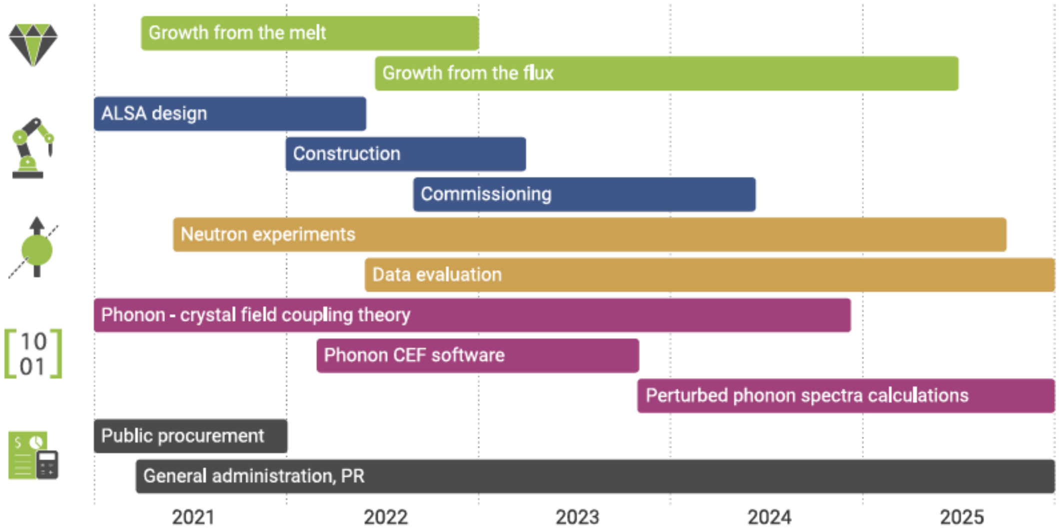


Fig. 4: Gantt chart of the project

Simplified risk analysis

1. The main risks are associated with the development of the ALSA device. Because of that, we have already started preparing the conceptual design (see Fig. 3), and we are having ongoing discussions with companies regarding the technical details. **We are certain of ALSA's feasibility** as it is a crucial part of the project, details are in part B2.
2. Access to the neutron beamtime is only possible via proposal process. The PI is experienced neutron users with more than 25 successfully accepted neutron proposals. In order to further mitigate the risk of losing beamtime due to potential problems with any neutron facility, the Neutron team will spread proposals over different facilities within Europe.
3. The last possible risk is failure to grow the samples. We are confident that we will succeed because all the studied samples are already well known, and the details of their preparation have been described in published papers.

Why me for ERC?

MaMBA is a **complex condensed matter proposal** with overlap to artificial intelligence and robotics. To be successful, such synergy project needs a PI with a very specific skills: neutron scattering, computer vision, Laue image treatment, software development, team leading.

I worked 5 years as an instrument responsible of inelastic spectrometer at neutron source in Garching, DE. I know the technique and **I know the people** in the field. **I am able to treat** the data in detail and because of my programming skills also to develop a software for data refinement. **I lead** the team developing automated product recognition device using computer vision in a big company. And finally – **I have an idea** how to co-align hundreds of tiny crystals in order to measure them with neutrons, which was never possible before.

ERC Starting Grant will allow me to develop **my own group** and establish magnetoelastic effects as an important property of solid-state physics.

Conclusion

In conclusion, allow me to summarize the idea of the project. We have shown in our recent study on $CeAuAl_3$ that it is hard to detect magnetoelastic effects, but even weak effects can have a significant impact on the properties of the compound. **The mission of MaMBA** is to show that magnetoelastic coupling and the existence of hybridized modes is a general property of solid-state physics, it just went unnoticed because it requires a very special technique to reveal it. We will prepare a set of single crystals suitable for inelastic neutron experimentation using ALSA, a state-of-the-art bespoke device. The measured neutron data will bring new insights to the topic and help with the confirmation of emerging theories.

MaMBA will offer **new perspectives on old theories**.

ALSA will be a **gamechanger in neutron experiment sample preparation**.

References

[1] M. Born and R. Oppenheimer, “Zur Quantentheorie der Molekeln,” *Annalen der Physik,* vol. 389, pp. 457-484, 1927.

[2] P. Thalmeier and P. Fulde, “Bound State between a Crystal-Field Excitation and a Phonon in $CeAl_2$,” *Physical Review Letters,* vol. 49, no. 21, pp. 1588-1591, 1982.

[3] M. Loewenhaupt and U. Witte, “Coupling between electronic and lattice degrees of freedom in 4*f*-electron systems investigated by inelastic neutron scattering,” *Journal of Physics: Condensed Matter,* vol. 15, no. 5, 2003.

[4] J. H. Mentink, M. Katsnelson and M. Lemeshko, “Quantum many-body dynamics of the Einstein-de Haas effect,” *Physical Review B,* vol. 99, no. 6, pp. 1-13, 2019.

[5] G. R. Stewart, “Unconventional superconductivity,” *Advances in Physics,* vol. 66, no. 2, pp. 75-196, 2017.

[6] A. Togo and I. Tanaka, “First principles phonon calculations in materials science,” *Scripta Materialia,* vol. 108, pp. 1-5, 2015.

[7] J. C. Tully, “Perspective on „Zur Quantentheorie der Molekeln“,” *Theoretical Chemistry Accounts,* vol. 103, pp. 173-176, 2000.

[8] I. Rahinov, R. Cooper, D. Matsiev, C. Bartels, D. J. Auerbach and A. M. Wodtke, “Quantifying the breakdown of the Born-Oppenheimer approximation in surface chemistry.,” *Physical Chemistry Chemical Physics,* vol. 13, no. 28, pp. 12680-12692, 2011.

[9] E. S. Kryachko, “Nonadiabatic Coupling: General Features and Relation to Molecular Properties,” *Advances in Quantum Chemistry,* vol. 44, pp. 119-133, 2003.

[10] A. Scherrer, D. Sebastiani, E. K. U. Gross, R. Vuilleumier and F. Agostini, “On the mass of atoms in molecules: Beyond the Born-Oppenheimer approximation,” *Physical Review X,* vol. 7, no. 3, 2017.

[11] M. Yang and S. R. White, “Density-matrix-renormalization-group study of a one-dimensional diatomic molecule beyond the Born-Oppenheimer approximation,” *Physical Review A,* vol. 99, no. 2, 2019.

[12] A. Abedi, E. Khosravi and I. V. Tokatly, “Shedding light on correlated electron–photon states using the exact factorization,” *European Physical Journal B,* vol. 91, no. 8, p. 194, 2018.

[13] P. Čermák, A. Schneidewind, B. Liu, M. M. Koza, C. Franz, R. Schönmann, O. Sobolev and C. Pfleiderer, “Magnetoelastic hybrid excitations in $CeAuAl_3$,” *Proceedings of the National Academy of Sciences of the United States of America,* vol. 116, no. 14, p. 201819664, 2019.

[14] S. Paschen, E. Felder and H. Ott, “Transport and thermodynamic properties of $CeAuAl_3$,” *European Physical Journal B,* vol. 2, no. 2, pp. 169-176, 1998.

[15] D. T. Adroja, C. d. l. Fuente, A. Fraile, E. Burzurí, F. Luis, J. I. Arnaudas and A. d. Moral, “Muon spin rotation and neutron scattering study of the noncentrosymmetric tetragonal compound $CeAuAl_3$,” *Physical Review B,* vol. 91, no. 13, 2015.

[16] A. Schneidewind and P. Čermák, “PANDA: Cold three axes spectrometer,” *Journal of large-scale research facilities JLSRF,* vol. 1, p. 12, 2015.

[17] C. Franz, A. Senyshyn, A. Regnat, C. Duvinage, R. Schönmann, A. Bauer, Y. Prots, L. Akselrud, V. Hlukhyy, V. Baran and C. Pfleiderer, “Single Crystal Growth of $CeTAl_3$ (T=Cu, Ag, Au, Pd and Pt),” *Journal of Alloys and Compounds,* vol. 688, no. 48, pp. 978-986, 2016.

[18] D. T. Adroja, A. d. Moral, C. d. l. Fuente, A. Fraile, E. A. Goremychkin, J. W. Taylor, A. D. Hillier and F. Fernandez-Alonso, “Vibron quasibound state in the noncentrosymmetric tetragonal heavy-fermion compound $CeCuAl_3$.,” *Physical Review Letters,* vol. 108, no. 21, p. 216402, 2012.

[19] L. Chapon, E. Goremychkin, R. Osborn, B. Rainford and S. Short, “Magnetic and structural instabilities in $CePd_2Al_2$ and $LaPd_2Al_2$,” *Physica B-condensed Matter,* vol. 378, pp. 819-820, 2006.

[20] T. Fennell, M. Kenzelmann, B. Roessli, H. Mutka, J. Ollivier, M. Ruminy, U. Stuhr, O. Zaharko, L. Bovo, A. Cervellino, M. K. Haas and R. J. Cava, “Magnetoelastic excitations in the pyrochlore spin liquid $Tb_2Ti_2O_7$.,” *Physical Review Letters,* vol. 112, no. 1, p. 17203, 2014.

[21] M. Ruminy, E. Pomjakushina, K. Iida, K. Kamazawa, D. T. Adroja, U. Stuhr and T. Fennell, “Crystal-field parameters of the rare-earth pyrochlores $R_2Ti_2O_7$ (R = Tb , Dy, and Ho),” *Physical Review B,* vol. 94, no. 2, p. 24430, 2016.

[22] J. Gaudet, A. Hallas, C. Buhariwalla, G. Sala, M. Stone, M. Tachibana, K. Baroudi, R. Cava and B. Gaulin, “Magneto-elastic induced vibronic bound state in the spin ice pyrochlore $Ho_2Ti_2O_7$,” *Physical Review B,* 2018.

[23] M. Naji, N. Magnani, J.-Y. Colle, O. Beneš, S. Stohr, R. Caciuffo, R. J. M. Konings and D. Manara, “Raman Scattering from Decoupled Phonon and Electron States in NpO_2,” *Journal of Physical Chemistry C,* vol. 120, no. 9, pp. 4799-4805, 2016.

[24] M. N. Popova, A. B. Sushkov, S. A. Klimin, E. P. Chukalina, B. Z. Malkin, M. Isobe and Y. Ueda, “Lattice vibrations of α-NaV_2O_5 in the low-temperature phase: An alternative interpretation to magnetic bound states,” *Physical Review B,* vol. 65, no. 14, 2002.

[25] K. N. Boldyrev, T. N. Stanislavchuk, A. A. Sirenko, D. Kamenskyi, L. N. Bezmaternykh and M. N. Popova, “Bifurcations of Coupled Electron-Phonon Modes in an Antiferromagnet Subjected to a Magnetic Field,” *Physical Review Letters,* vol. 118, no. 16, pp. 1-5, 2017.

[26] V. Aksenov, E. Goremychkin, E. Mühle, T. Frauenheim and W. Bührer, “Coupled quadrupole-phonon excitations: Inelastic Neutron scattering on van vleck paramagnet $PrNi_5$,” *Physica B-condensed Matter,* vol. 120, pp. 310-313, 1983.

[27] B.-Q. Liu, . P.Čermák, C. Franz, C. Pfleiderer and A. Schneidewind, “Lattice dynamics and coupled quadrupole-phonon excitations in $CeAuAl_3$,” *Physical Review B,* vol. 98, no. 17, p. 174306, 2018.

[28] F. Steglich, J. Aarts, C. D. Bredl, W. Lieke, D. Meschede, W. Franz and H. Schäfer, “Superconductivity in the Presence of Strong Pauli Paramagnetism: $CeCu_2Si_2$,” *Physical Review Letters,* vol. 43, no. 25, pp. 1892-1896, 1979.

[29] F. Steglich and S. Wirth, “Foundations of heavy-fermion superconductivity: lattice Kondo effect and Mott physics.,” *Reports on Progress in Physics,* vol. 79, no. 8, pp. 84502-84502, 2016.

[30] C. Pfleiderer, “Superconducting phases of f-electron compounds,” *Reviews of Modern Physics,* vol. 81, no. 4, pp. 1551-1624, 2009.

[31] N. K. Sato, N. Aso, K. Miyake, R. Shiina, P. Thalmeier, G. Varelogiannis, C. Geibel, F. Steglich, P. Fulde and T. Komatsubara, “Strong coupling between local moments and superconducting 'heavy' electrons in UPd2Al3.,” *Nature,* vol. 410, no. 6826, pp. 340-343, 2001.

[32] J. A. Mydosh and P. M. Oppeneer, “Hidden order behaviour in URu_2Si_2 A critical review of the status of hidden order in 2014),” *Philosophical Magazine,* vol. 94, pp. 3642-3662, 2014.

[33] J. A. Mydosh and P. M. Oppeneer, “Colloquium : Hidden order, superconductivity, and magnetism: The unsolved case of URu_2Si_2,” *Reviews of Modern Physics,* vol. 83, no. 4, pp. 1301-1322, 2011.

[34] M. M. Altarawneh, N. Harrison, G. Li, L. Balicas, P. H. Tobash, F. Ronning and E. D. Bauer, “Superconducting pairs with extreme uniaxial anisotropy in URu_2Si_2.,” *Physical Review Letters,* vol. 108, no. 6, p. 66407, 2012.

[35] G. Bastien, D. Aoki, G. Lapertot, J.-P. Brison, J. Flouquet and G. Knebel, “Fermi-surface selective determination of the g-factor anisotropy in URu_2Si_2,” *Physical Review B,* vol. 99, no. 16, 2019.

[36] L. A. Wray, J. Denlinger, S.-W. Huang, H. He, N. P. Butch, M. B. Maple, Z. Hussain and Y.-D. Chuang, “Spectroscopic Determination of the Atomic f-Electron Symmetry Underlying Hidden Order in URu_2Si_2.,” *Physical Review Letters,* vol. 114, no. 23, p. 236401, 2015.

[37] M. Wartenbe, R. E. Baumbach, A. Shekhter, G. S. Boebinger, E. D. Bauer, C. C. Moya, N. Harrison, R. D. McDonald, M. B. Salamon and M. Jaime, “Magnetoelastic coupling in URu_2Si_2: Probing multipolar correlations in the hidden order state,” *Phys. Rev. B,* no. 99, p. 235101, 2019.

[38] L. Fuentes-Montero, P. Cermak, J. Rodríguez-Carvajal and A. Filhol, “The Esmeralda suite for Laue diffraction data treatment,” p. 10.13140/RG.2.1.4954.1202, 2015.

[39] L. Neumann and J. Matas, “Efficient Scene text localization and recognition with local character refinement,” in *2015 13th International Conference on Document Analysis and Recognition (ICDAR),* 2015.

[40] K. W. Becker, P. Fulde and J. Keller, “Line width of crystal-field excitations in metallic rare-earth systems,” *European Physical Journal B,* vol. 28, no. 1, pp. 9-18, 1977.

[41] M. Rotter, “Using McPhase to calculate magnetic phase diagrams of rare earth compounds,” *Journal of Magnetism and Magnetic Materials,* vol. 272, 2004.

[42] T. Fennell, P. P. Deen, A. R. Wildes, K. Schmalzl, D. Prabhakaran, A. T. Boothroyd, R. J. Aldus, D. F. McMorrow and S. T. Bramwell, “Magnetic Coulomb Phase in the Spin Ice $Ho_2Ti_2O_7$,” *Science,* vol. 326, no. 5951, pp. 415-417, 2009.

[43] M. Wartenbe, R. E. Baumbach, A. Shekhter, G. S. Boebinger, E. D. Bauer, C. C. Moya, N. Harrison, R. D. McDonald, M. B. Salamon and M. Jaime, “Magnetoelastic coupling in URu_2Si_2: Probing multipolar correlations in the hidden order state,” *arXiv preprint arXiv:1812.02798,* 2018.

[44] Y. Song, J. V. Dyke, I. K. Lum, B. D. White, S. Jang, D. Yazici, L. Shu, A. Schneidewind, P. Čermák, Y. Qiu, M. B. Maple, D. K. Morr and P. Dai, “Robust upward dispersion of the neutron spin resonance in the heavy fermion superconductor $Ce_{1-x}Yb_xCoIn5$.,” *Nature Communications,* vol. 7, no. 1, pp. 12774-12774, 2016.

[45] P. M. Sarte, M. Songvilay, E. Pachoud, R. A. Ewings, C. D. Frost, D. Prabhakaran, K. H. Hong, A. J. Browne, Z. Yamani, J. P. Attfield, E. E. Rodriguez, S. D. Wilson and C. Stock, “Spin-orbit excitons in CoO,” *Physical Review B,* vol. 100, no. 7, 2019.

[46] D. M. Juraschek and N. A. Spaldin, “Orbital magnetic moments of phonons,” *Physical Review Materials,* vol. 3, no. 6, p. 64405, 2019.

[47] P. Fulde and M. Loewenhaupt, “Magnetic excitations in crystal-field split 4*f* systems,” *Advances in Physics,* vol. 34, no. 5, pp. 589-661, 1985.

[48] C. Dornes, Y. Acremann, M. Savoini, M. Kubli, M. J. Neugebauer, E. Abreu, L. Huber, G. Lantz, C. A. F. Vaz, H. Lemke, E. M. Bothschafter, M. Porer, V. Esposito, L. Rettig, M. Buzzi, A. Alberca, Y. W. Windsor, P. Beaud, U. Staub, D. Zhu, S. Song, J. M. Glownia and S. L. Johnson, “The ultrafast Einstein–de Haas effect,” *Nature,* vol. 565, no. 7738, pp. 209-212, 2019.

[49] P. P. Deen, T. Fennell, H. Schober, A. Orecchini, S. Rols, K. H. Andersen and J. R. Stewart, “PANTHER-Polarisation Analysis with Thermal neutron.,” *ILL2020 Vision: Future directions in neutron science, France* , 2011.

Section b: Curriculum vitae (max. 2 pages)

PERSONAL INFORMATION

Family name, First name:	**Čermák, Petr**
Researcher unique identifier:	https://publons.com/researcher/S-6152-2016/ https://orcid.org/0000-0002-4176-6905
Date of birth:	[redacted]
Nationality:	Czech
URL for web site:	https://cermak.science/

- **EDUCATION**

2014	PhD in Physics of Condensed Matter and Materials Research Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic Prof. Pavel Javorský
2010	Master in Physics Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic

- **CURRENT POSITION(S)**

2018 – now	PostDoc / Scientific researcher in the group of Magnetic studies Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Czech Republic *I am employed at MGML national research facility, mainly responsible for* 20T *magnet and dilution refrigerator. I help our users and students to perform their bulk measurements. Important part of my job is development and maintenance of our user office system Prius.*

- **PREVIOUS POSITIONS**

2018	Head developer of the automated camera recognition software (**computer vision**) for production line. Label Design, Czech Republic (producer of high-quality self-adhesive labels) *After leaving FZ Jülich I had 2-month gap before starting my job at Charles University. Initialy 2-month contract at private company was prolonged for almost 1 year in order to finish the project. I learned how to lead the team and develop commercially feasible device. I plan to valorize gained computer vision knowledge in MaMBA project.*
2013 – 2018	Instrument Responsible at Three Axis Spectrometer PANDA Forschungszentrum Jülich GmbH outstation at MLZ, Garching, Germany *My task was to operate, maintain and develop state of the art neutron spectrometer. Only three such machines exist in Europe (PANDA, ThALES and IN12)*
2012 – 2013	PhD fellowship Institute Laue Langevin, Grenoble, France *I was developing spectrometer ThALES and measuring data for my thesis.*

- **TEACHING ACTIVITIES**

I enjoy teaching although it is not my primary activity. Helping students allows me to relax from research.

2018 – now	Mechanics: Exercise Seminar, Charles University, CZ (50 – 90 students per year)
2013 – 2017	Tutor of JCNS Laboratory Course - Neutron Scattering, FZ Jülich, Garching, DE

- **ORGANISATION OF SCIENTIFIC MEETINGS**

I feel important to exchange knowledge between different group of scientists and I am experienced with neutron scattering. Therefore, I am organizing events to strengthen Czech neutron community. I also organized workshops about neutron resolution calculation where I co-develop software suite.

2017	Triple Axis Resolution Workshop, MLZ, Garching, DE (30 participants) https://doi.org/10.1080/10448632.2017.1342483
2018	The triple axis resolution workshop, Charles University, Prague, CZ (20 participants) https://www.illcz.cz/
2019	EHPRG satellite workshop "Modern trends in Neutrons under Extreme Pressures", European High Pressure Research Group Meeting 2019, Prague, CZ (50 participants) https://neutron.press/

- **INSTITUTIONAL RESPONSIBILITIES (if applicable)**

2018 – now	**Local Contact** at Materials Growth & Measurement Laboratory (MGML.eu), Prague, Czech Republic
2018 – now	Implementation of the **open source instrument control software** NICOS at MGML (see software section below), Prague, Czech Republic
2019 – now	Organizer of **regular Czech Neutron Community meetings** (see https://neutron.beer/), Department of Condensed Matter Physics, Charles University, CZ

- **REVIEWING ACTIVITIES**

2017 – 2020	Member of FAP 4 (Facility access panel), ISIS Neutron and Muon Source, UK https://www.isis.stfc.ac.uk/Pages/FAP-Members.pdf
2018	Outstanding reviewer status, Elsevier (Intermetallics, J. Magn. Magn. Mater, Physica B)

- **MAJOR COLLABORATIONS**

See track record for details common papers and details about collaboration.

Prof. Pfleiderer, **Multi-Component Electronic Correlations**, TU Munich, Germany
Prof. Loewenhaupt, **Crystalline electric field broadening**, TU Dresden, Germany
Prof. Jinsheng Wen, **Inelastic neutron experiments**, Nanjing University, China
Prof. Dr. Huiqian Luo, **Neutron experiments on heavy fermions**, Chinese Academy of Sciences, Beijing

- **FUNDING (not ongoing)**

2011 – 2013	Charles University Grant Agency #348511 (as PI) "Study of magnetic structure of $R_2T\mathrm{In}_8$ materials" 32 k€
2005 – 2019	**Neutron facility experiments**: over 25 funded neutron experiments (neutron sources: ILL, MLZ, ISIS, PSI, HZB) roughly 130 beamdays, cost equivalent equiv. 1.3 M€.
2013 – 2018	I was employed in Forschungszentrum Jülich, member of Helmholtz association. Employees of Helmholtz association are **not allowed to ask for external funding**. See more in track record.

- **SCIENTIFIC SOFTWARE DEVELOPEMENT**

2012 – 2013	Esmeralda Laue Suite (https://lauesuite.com)
2015 – 2019	CrysFiPy – Crystal Field Python package (https://crysfipy.rtfd.io)
2014 – now	NICOS contributor (https://nicos-controls.org)
2018 – now	Python Research Infrastructure User System (https://github.com/me2d09/prius and released version at https://user.mgml.eu)

Section c: Early achievements track-record

The course of my scientific career was clear early on from the time when I performed my **first neutron experiment** alone at the large-scale facility Helmholtz Zentrum Berlin as a master's student. During my doctoral studies at Charles University in Prague, my interest in neutron scattering grew. I was selected for a one-year PhD fellowship at the world's largest neutron source, ILL, in France (https://www.ill.eu), as a representative of the Central European Neutron Initiative (CENI). There, I become an **expert on neutron scattering**, and already during my PhD, I moved to Heinz Meier-Leibnitz Zentrum (MLZ) in Garching as a second instrument responsible for the PANDA spectrometer. My task was to operate, maintain and develop the state-of-the-art neutron spectrometer.

I worked for five years on PANDA, employed by Forschungszentrum Julich, which is a member of the German Helmholtz Association. Employees of the Helmholtz Association are not normally allowed to ask for external funding, so I have none of my own grant applications from this period. Our work was evaluated as part of the program-oriented funding and was always rated as excellent. My duty was to support MLZ users from various fields of condensed matter physics and develop the instrument. I was part of the German Federal Ministry of Education and Research (BMBF)-supported €1.4M project **BAMBUS**, where we developed a state-of-the-art multianalyser for the PANDA spectrometer. I gained a tremendous amount of experience and started collaborating with several **world-leading neutron scattering groups** (the Inosov group at TU Dresden, the Janoschek group at the Paul Scherrer Institute, the Pfleiderer group at TU Munich and the Jinsheng Wen group at Nanjing University).

- I have substantial knowledge of advanced crystal field treatment, phonon–crystal field coupling, data visualization, magnetic structures refinement, Laue neutron diffraction and data evaluation — **see my list of publications**.
- I am an expert in neutron triple-axis spectroscopy, resolution calculations and advanced data reduction and fitting and organized several workshops on it — **see my CV**.
- I actively participated in development of the ThALES spectrometer at ILL and the PANDA spectrometer at MLZ — **see my instrument development publications below**.
- I am a programmer, and I contribute to several open source Python and Fortran projects — **see my CV**.
- I know solutions. **I lead the development** of computer vision solutions for a private company in past. Now I have decided to fully engage in science and ended private sector activities.

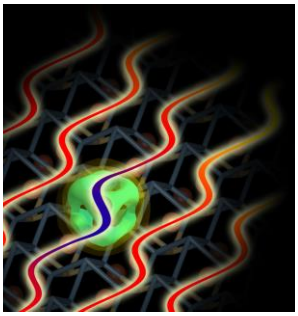
Total publications in peer-reviewed journals: 25

10x first author, 2x **Nature Comm.**, 1x **PNAS**, 2x **PRL**, 6x **PRB**, **h-index** = 7 (ISI)/9 (Google Scholar).

Full list:

https://publons.com/researcher/S-6152-2016/ or https://scholar.google.cz/citations?user=TJRuzI4AAAAJ

Five most important publications:



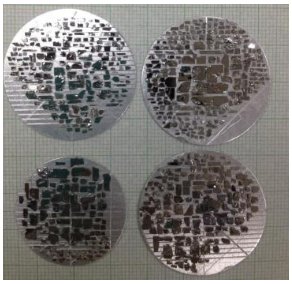
The coupling of phonons to the crystal electric field are much more generic than hitherto thought.

1) **P. Čermák**, A. Schneidewind, B. Liu, M. M. Koza, C. Franz, R. Schönmann, O. Sobolev, C. Pfleiderer, Magnetoelastic hybrid excitations in $CeAuAl_3$, **Proceedings of the National Academy of Sciences** **116** (14) (2019) 6695-6700.
2) B. Liu, **P. Čermák**, C. Franz, C. Pfleiderer, and A. Schneidewind, Lattice dynamics and coupled quadrupole-phonon excitations in $CeAuAl_3$, **Phys. Rev. B** **98** (2018) 174306.

These two publications deal with magnetoelastic coupling, and the published results motivated MaMBA. We have revealed new excitations and started to deal with them in more detail. It took three years of measurement and discussions with theoreticians to explain the measured data. I formed a team with my colleagues B. Liu and A. Schneidewind (first instrument responsible for PANDA). B. Liu developed the theory (paper 2), and I did all the measurements and supervised the project. A. Schneidewind supported the whole team with her instrumentation knowledge. We heavily conferred with "the owner" of the sample, Prof. Pfleiderer, and our efforts finally resulted in the PNAS publication (paper 1). Our work was mentioned in the press: [1], [2], [3 German], [4 German]

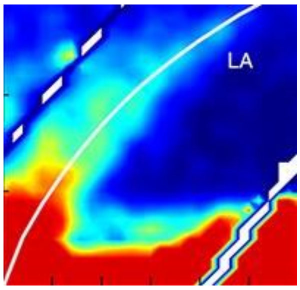
***IF* 2017: 9.504, *Altmetrics*: 30**

3) Y. Song, J. Van Dyke, I. K. Lum, B. D. White, S. Jang, D. Yazici, L. Shu, A. Schneidewind, **P. Čermák,** Y. Qiu, M. B. Maple, Dirk. K Morr, P. Dai, Robust upward dispersion of the neutron spin resonance in the heavy fermion superconductor $Ce_{1-x}Yb_xCoIn_5$, **Nat. Commun. 7** (2016) 12774.
As an instrument scientist, I am the co-author of several high-ranked papers, but this one is special because we invested a lot of effort and I was not only "the local contact". $CeCoIn_5$ is a prototypical unconventional superconductor that has been known for decades, but we have revealed details about it that had not been observed before. We faced several challenges during the measurements, the most difficult of which was to get enough of the sample. I learned how to manually co-align small crystals. The MaMBA will deal with this issue by developing ALSA. Press coverage here: phys.org, **IF 2017: 12.353, Altmetrics: 19**



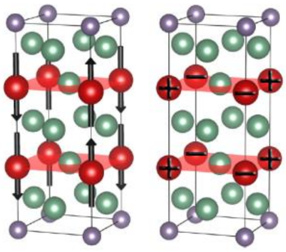
Hundreds of tiny samples co-aligned and glued onto aluminium plates.

4) J. Wang, K. Ran, S. Li, Z. Ma, S. Bao, Z. Cai, Y. Zhang, K. Nakajima, S. O. Kawamura, **P. Čermák**, A. Schneidewind, S. Savrasov, X. Wan, J. Wen, Evidence for singular-phonon-induced nematic superconductivity in a topological superconductor candidate $Sr_{0\,1}Bi_2Se_3$, **Nat. Commun. 10** (2019) 2802.
Cooperation with Prof. Wen's group deals with unconventional superconductors. By performing inelastic neutron measurements on a prime candidate for realizing topological superconductivity, we revealed highly anisotropic phonons with increasing linewidths at long wavelengths. Such observation indicates a large ME coupling, which we propose gives rise to the exotic p-wave nematic superconducting pairing. It creates an open question which should be answered by MaMBA. **IF 2017: 12.353**



Measured phonon dispersion along [001] direction.

5) **P. Čermák**, P. Javorský, M. Kratochvílová, K. Pajskr, M. Klicpera, B. Ouladdiaf, M.-H. Lemée-Cailleau, J. Rodriguez-Carvajal, M. Boehm, Magnetic structures of non-cerium analogues of heavy-fermion Ce_2RhIn_8: The case of Nd_2RhIn_8, Dy_2RhIn_8, and Er_2RhIn_8, **Phys. Rev. B 89** (2014) 184409.
The fifth highlighted paper is the last paper published together with my PhD supervisor and the last paper coming from my doctoral thesis. It summarizes the results that I obtained during my stay at the ILL neutron source. It helped me to start my career in the field of neutron scattering.



Determined magnetic structures.

Instrument development publications:

1) **P. Čermák**, M. Boehm, J. Kulda, S. Roux, A. Hiess, P. Steffens, J. Saroun, Optimizing monochromatic focusing on ThALES, **J. Phys. Soc. Jpn. 82** (2013) SA026.
I performed Monte Carlo simulations of the elliptical focusing guide with a novel "inner lamella" approach. The guide is in use for ThALES at ILL – the world most intense cold triple-axis spectrometer.
2) J. A. Lim, K. Siemensmeyer, **P. Čermák**, B. Lake, A. Schneidewind, D. S. Inosov, BAMBUS: A new inelastic multiplexed neutron spectrometer for PANDA, **J. Phys. Conf. Ser. 592** (2015) 012145.
I was part of the BAMBUS team to develop a unique neutron multi-analyser. I am the author of a concept of rotated detectors in order to save space. A prototype will be commissioned in 2020.

Invited lectures:

1. LNS seminar, Paul Scherrer Institute, Villigen, Switzerland, 2019, https://www.psi.ch/
2. SwedNess course in neutron spectroscopy, Chalmers, Göteborg, 2018, https://swedness.se/

Total presentations at international conferences: Seven oral and more than 30 posters.
Selected **invited speaking engagements and contributing talks** made to international conferences:

1. "Hybridized excitations in $CeAuAl_3$" (**invited**, https://indico.frm2.tum.de/event/171/)
@ Frontiers in Quantum Condensed Matter Research with Neutrons 2019, Garching
2. "Neutrons as a key method for accessing magnetoelastic effects"
@ ECNS 2019, St. Petersburg, http://ecns2019.com/
3. "Analysis of magneto-elastic hybridized effects due to the CEF"
@ ICM 2018, San Francisco, http://www.icm2018sf.org/
4. "Magnetoelastic hybrid excitations in non-centrosymmetric tetragonal $CeTAl_3$"
@ SCES 2017, Prague, http://sces2017.org/
5. "A novel hybridized crystal field–phonon excitations"
@ JEMS 2016, Glasgow, http://jems2016.iopconfs.org/