

# MSCA COFUND Doctoral Fellowships "Affordable but High-Sensitivity NMR Spectroscopy"

## Summary

This PhD topic is part of the INNOCHEMBIO Doctoral Programme, which is funded through the Marie Skłodowska-Curie Actions (MSCA) COFUND action. The main objective of INNOCHEMBIO is to train future experts of sustainable chemistry and biotechnology, helping Europe to take the next steps in the green transition. The project will firstly focus on understanding the hyperpolarization process and its workings, optimizing it for different applications, metabolite classes, and biological sample types. And secondly, combine this expertise with benchtop NMR spectrometers. This PhD position will be hosted at National Institute of Chemical Physics and Biophysics with main supervisor Dr. Indrek Reile and will contain a secondment to co-supervisor Dr. Sören Lehmkuhl at Karlsruhe Institute of Technology (DE).

Research field: Chemistry and biotechnology

Supervisor: Dr. Indrek Reile

Availability: This position is available.

Offered by: National Institute Of Chemical Physics And Biophysics

Application deadline: Applications are accepted between July 01, 2025 00:00 and August 31, 2025

23:59 (Europe/Zurich)

## Description

# 1. General description of programme and host

The PhD fellowship is part of the Marie Skłodowska-Curie Actions (MSCA) COFUND doctoral programme IN-NOCHEMBIO (https://taltech.ee/en/innochembio), which is co-funded by the European Union (Grant agreement 101217295). The main objective of INNOCHEMBIO is to train future experts to help Europe take the next steps in the green transition. The solutions and trained experts can reduce the environmental impact of the chemical and agricultural industries, offer eco-friendly analytical techniques, and assess the safety of new materials. INNOCHEMBIO funding will co-finance **15 PhD positions**, for which the application process in the first call will start on the **1st of July in 2025**.

For 12 PhD positions the hosting institution will be Department of Chemistry and Biotechnology (DCB) at Tallinn University of Technology (TalTech) which combines three divisions – Chemistry, Gene Technology and Biomedicine, and Food and Biotechnology. DCB is developing solutions to the great challenges of the 21st century – climate change, environmental protection, carbon neutrality, renewable energy, and biodiversity conservation. DCB hosts the second biggest PhD programme in TalTech with nearly a hundred enrolled students.

For 3 PhD positions the hosting institution will be the implementing partner – National Institute of Chemical Physics and Biophysics (NICPB). NICPB is a public research institution that conducts both fundamental and applied research, developing novel directions in fields ranging from material sciences to informatics. NICPB houses the Laboratory of Environmental Toxicology and several laboratories focused on fundamental research in NMR technologies with expertise dating back decades. The PhD training activities conducted by NICPB are funded through TalTech.

Importantly, each PhD project has one co-supervisor from another European country, which is detailed under the specific offer (see under supervisors' section). In total, INNOCHEMBIO has **19 associate partners from 11 European countries**.

## 2. Description of specific PhD project

NMR spectroscopy is one of the most versatile analytical methods in the chemical laboratory. Its ability to provide users with reliable and easy to interpret information on the composition of even the most complex samples has allowed NMR to become an analytical workhorse that cannot be replaced in various fields of chemistry, from organic chemistry to biomedical studies. Practitioners of these fields have become used to the main drawback of NMR – its relative lack of sensitivity. This not an issue for organic chemistry where several milligrams of an analyte can usually be used for NMR analysis. This would, however, be impossible, when studying low concentration metabolites in the body or in biofluids – these analytes appear at their natural concentration and there is not much we can do about it. The result is that low concentration metabolites of living organisms cannot be analysed by NMR.



This PhD project will address this sensitivity limitation of NMR. The main supervisor has developed parahydrogen hyperpolarization based methods that boost NMR sensitivity by 1000-fold in biological sample analysis. This approach is built on dissolving a specific iridium metal-based catalyst in the NMR sample and bubbling parahydrogen gas through the sample in between NMR scans. The interaction of the gas and the catalyst with biological analytes will manipulate them to release orders of magnitude more NMR signal. This can be used to reduce the detectable concentration barrier and to make NMR measurements faster, recording more signal in a single NMR scan than a conventional NMR experiment would yield in thousands of scans. These NMR signal enhancement techniques are known as SABRE (10.1002/anie.201710406) and nh-PHIP (10.1021/acs.accounts.1c00796) in scientific literature.

The co-supervisor (Dr Lehmkuhl) is a leader in adapting parahydrogen hyperpolarization to affordable benchtop NMR spectrometers. Such machines are severalfold less costly to buy and operate, but are even less sensitive than regular NMR spectrometers. Combining them with hyperpolarization would allow to develop super-sensitive NMR methods on spectrometers that cost less. This leads to the essence of the project – combining the expertise in biological sample hyperpolarization with that of benchtop NMR spectrometers.

The PhD candidate will work on both high-end superconducting NMR instruments (in Tallinn) and compact benchtop machines (in KIT). The project will firstly focus on understanding the hyperpolarization process and its workings, optimizing it for different applications, metabolite classes, and biological sample types. Once accomplished (in Tallinn), we will port technology to benchtop instrumentation (in KIT). Development in Tallinn will focus on nh-PHIP, chemical development and understanding of the hyperpolarization process. Benchtop NMR experiments in KIT will develop nh-PHIP at low fields and also test SABRE in biological mixtures. The result will be a set on methods to detect biological information of benchtop NMR from samples that at the present state of the art cannot be analysed on affordable spectrometers or sometimes cannot be analysed by NMR at all. This project gives the PhD candidate an opportunity to participate in advancing the applications of NMR and expanding it towards new horizons in analytical chemistry and biomedical applications.

Link to the project: https://taltech.ee/en/innochembio/reile

## 3. Supervisory team

- National Institute of Chemical Physics and Biophysics (main supervisor): Dr. Indrek Reile
- Karlsruhe Institute of Technology (Germany): Dr. Sören Lehmkuhl (The length of the long-term mobility will be 16 months of the whole 48 months PhD period. The PhD candidate will be based in Tallinn in the National Institute of Chemical Physics and Biophysics, but will be travelling to the Karlsruhe Institute of Technology on several occasions (for combined 16 months), as required by results and progress).
- National Institute of Chemical Physics and Biophysics: Dr. Kerti Ausmees

### 4. Requirements

- · Excellent command of written and spoken English.
- · MSc degree or equivalent in chemistry or biotechnology, or equivalent.
- Compliance with the rules of INNOCHEMBIO (e.g. eligibility, adhering to MSCA mobility rules, etc.).
- The primary workplace will be in Estonia. Therefore, candidates from outside the EU must be eligible to obtain a visa. The position is expected to start in the first half of 2026.
- The candidate should enjoy practical labwork at the interface of metalorganic and analytical chemistry. Work will include the study of organometallic catalysts and kinetics that influence hyperpolarization. Prior experience in metalorganic chemistry (possible work in inert gas atmosphere) is desirable, but focus will be on analytical chemistry methods that utilize metalorganic catalysts.
- The candidate can interpret NMR spectra and has completed a course in principles of NMR.
- He/she should be able to communicate freely in English and be prepared to work in an interdisciplinary and multinational environment.
- · Project will involve biological fluids and training for their safe handling.

### 5. Duties and Responsibilities

- Undertake postgraduate research for specific doctoral research project at TalTech or NICPB, respectively.
- Present and publish research in both academic and non-academic audiences. Attend and participate in academic and non-academic conferences, events and seminars.
- Attend and participate in all training events and supervisory meetings.
- Be seconded to the associated partner as necessary to fulfil the grant obligations.



- Prepare progress reports and similar documents on research for funding bodies, as required.
- · Actively contribute to the public engagement and outreach activities of the project.
- The above job descriptions are not exhaustive, the PhD candidate may be required to undertake other tasks, which are broadly in line with the above duties and responsibilities.
- Full-time employment (40 hours per week), temporary contract for 4 years.

## 6. Eligibility requirements

- The applicant must be a doctoral candidate (i.e. not already in possession of a doctoral degree at the date of the recruitment).
- At the time of recruitment, the researcher must not have resided or carried out their main activity (work, studies, etc.) in Estonia for more than 12 months in the three years immediately prior to the recruitment date. Compulsory national service and/or short stays such as holidays are not taken into account.

#### 7. Benefits

- Competitive funding scheme, with a minimum gross monthly salary of EUR 2500. Topped by additional mobility allowances as well as optional family allowances (if applicable).
- Covered tuition costs, research costs and funding for short term mobility (i.e. conference attendance).
- Interdisciplinary and international research projects.
- Early-stage researcher position, with corresponding social and medical benefits in Estonia.
- · Becoming a Marie Skłodowska-Curie PhD fellow.

### 8. How to Apply

All applications must be sent through TalTech's official application platform Glowbase and only applications submitted here will be considered for the programme. We ask the candidates not to contact the supervisors directly, in case of questions please write at innochembio@taltech.ee. Each application must include the following material: CV, 1-page motivation letter, copies of BSc and MSc study records and diplomas, scanned copy of valid photo ID, 2 reference letters, eligibility statement.

NB! The INNOCHEMBIO programme has additional requirements compared to the standard TalTech application process. Details on the exact nature of these documents and how to insert them in Glowbase can be found at our official INNOCHEMBIO website: <a href="https://taltech.ee/en/innochembio/application-process">https://taltech.ee/en/innochembio/application-process</a>. If any of the required documents are missing, the candidate will not be eligible to proceed to the selection stage.

#### 9. Selection Process

The selection and recruitment process will be in accordance with the European Charter and Code of Conduct for the Recruitment of Researchers. The recruitment process will be open, transparent, impartial, equitable, and merit-based. There will be no overt/covert discrimination based on race, gender, sexual orientation, religion or belief, disability or age. To this end, the following selection criteria will be considered.

The application deadline is 31 August 2025. The application process will be carried out in 3 steps. In short, first an eligibility check is performed. All eligible candidates will proceed to stage 1, where they will be evaluated by independent evaluators based on the application documents. Lastly, shortlisted candidates from stage 1 will proceed to stage 2, where they will be interviewed via teleconference, which will be used to determine a candidate to whom an offer will be made. All candidates will be informed about the progress in due course after each step of the process. The selection process is described on the guide for applicants available here: https://taltech.ee/en/innochembio/application-process.

### 10. Disclaimer

By applying for this position, the applicants

- 1. give their consent to circulate their application and personal data within the INNOCHEMBIO consortium and with the evaluators:
- 2. confirm that the data provided is valid and accurate:
- 3. confirm compliance with the eligibility requirements;



4. commit to undertaking the planned secondment at the co-supervisor's institution.



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