Synthesis and characterization of novel functional materials obtained by esterification of cellulose

Summary

Cellulose, as the most abundant, naturally occurring biopolymer in the world, is an important resource for replacing fossil-based plastics, as it has good mechanical properties and chemical durability, it is nontoxic and is not competing food resources. However, only minor amount of global plastic production is covered by cellulose derivatives or regenerates up to now. This is pointing strong need to increase utilisation of this sustainable, carbon neutral raw material for plastics. Unlike most of the commodity plastics, cellulose is not intrinsically thermoplastic and must be chemically modified to achieve melting behaviour, expected by plastics processing industry. The cellulose modification methods known so far are resource- and energy-intensive. This stimulates development of more sustainable routes. The modern society, from other hand is suffering due to intensive use of fossil-based plastics causing littering and pollution in soils, sediment and water, contamination of food and living tissues with plastic particles and leeched additives. Cellulose based bioplastics are sustainable solution for this problem. Therefore, the study is devising and demonstrating novel, sustainable esterification routes for preparing thermoplastic cellulose esters and their potential application in several commodity and high-tech applications.

Research field:	Chemical, materials and energy technology
Supervisors:	Andres Krumme Omar Parve
Availability:	This position is available.
Offered by:	School of Engineering Department of Materials and Environmental Technology
Application deadline:	Applications are accepted between January 01, 2025 00:00 and January 24, 2025 23:59 (Europe/Zurich)

Description

These PhD studies are targeted on the synthesis of novel reagents for esterification of cellulose in order to produce novel functional cellulose based biopolymers. The protocols of the syntheses to be developed should be as green and technically simple as possible in order to allow technological upscaling. Regarding reactivity of the reagents, the best putative solution would be successful use of alkyl esters in base-catalyzed transesterification, however, in several cases use of different structurally modified more reactive esters is expected. The use of novel reagents requires identification of a suitable reaction medium together with a sufficiently potent basic catalyst. Alternatively, reagents could be tailored to a suitable reaction medium.

The third part of the thesis would be dedicated to thorough characterization of the novel functional derivatives of cellulose to identify their potential fields of application. This study has to start from proving the structure of the derivative by using NMR spectroscopic methods followed by studying solubility, thermal and mechanical properties, viscosity etc. The main research questions are:

- Which are the most sustainable synthesis protocols for preparing mostly biobased reagents for esterification of cellulose?
- Which is the most suitable reaction medium, catalysts etc?
- How the esterification reagents affect chemical and physical properties of the cellulose derivatives?
- What is the environmental effect of the synthesis protocols, how to reduce it?

Responsibilities and (foreseen) tasks

- Collecting state-of-the-art knowledge of the recent trends in the field of cellulose chemistry and reaction medium.
- Conducting intensive research program in the laboratory of cellulose chemistry.
- Characterizing the novel reagents and materials regarding their chemical composition and physical properties.
- Publishing the results in field specific journals and conferences.
- Participating in teaching activities and supervision of masters and bachelor students.

Applicants should fulfil the following requirements:

- a master's degree in chemistry (preferably in organic chemistry or biochemistry)
- practical skills of laboratory of organic chemistry
- a clear interest in the topic of the position
- excellent command of English
- strong and demonstrable writing and analytical skills
- capacity to work both as an independent researcher and as part of an international team
- capacity and willingness to provide assistance in organizational tasks relevant to the project
- capacity and willingness to participate in relevant teaching activities

The following experience is beneficial:

- experimental and/or theoretical understanding of cellulose chemistry
- NMR, FTIR experience
- knowledge of thermal and mechanical characterization methods of polymeric materials

The candidate should submit a research plan for the topic, including the overall research strategy. The candidate can expand on the listed research questions and tasks, and propose theoretical lenses to be used.

We offer:

- 4-year PhD position in a fast-growing competence center of wood valorization in Estonia with a broad network of R&D partners in Baltic and Nordic countries.
- The chance to do high-level research in one of the most perspective directions for replacing fossil plastics with biopolymers.
- Opportunities for conference visits, research stays and networking with globally leading universities and research centers in the field of cellulose chemistry.

About the hosting laboratory

The main focus of research of Laboratory of Biopolymer Technology of TalTech is valorizing bio-based environmental resources in everyday and high-tech applications. The aim is to find sustainable alternatives to fossil-based polymeric materials by using bio-based alternatives and recyclables.

The team is looking for novel ways to sustainably valorize cellulose by applying new, recyclable solvent systems, bio-based chemical modification reagents, and energy-saving technologies. New, bio-based or well-recycled solvent systems are used. Plant oils are being used for the esterification of cellulose, and reactive extrusion technology is being developed as a synthesis medium.

The laboratory has a unique pilot production capability in Estonia in essential areas of polymer technology such as hot mixing, extrusion, and injection moulding. Thermoplastic or thermosetting polymer composites with inorganic or bio-based additives are being developed to efficiently use secondary raw materials in the circular economy.

The laboratory is the only one in Estonia that can pilot electrospinning. This method develops triboelectric materials and filter materials based on cellulose derivatives.

Additional information

For further information, please contact Prof. Andres Krumme (andres.krumme@taltech.ee) or visit https://biopolymer.taltech.ee/en/

To get more information or to apply online, visit https://taltech.glowbase.com/positions/881 or scan the the code on the left with your smartphone.