Molecular Artificial Intelligence in the Design of Concentrated Electrolyte Fluids for Energy Storage

Summary

The combination of stochastic machine learning and experimental work in the design of ionic liquids (ILs) and deep eutectic solvents (DESs) for latent heat thermal energy storage (LHTES) represents an innovative approach to materials science. This interdisciplinary research not only advances our understanding of electrolyte fluids but also contributes to the development of more efficient and sustainable energy storage solutions. Therefore, the results of this research have the potential to impact several sectors, including renewable energy, industrial processes, and beyond. The aim of the PhD project is to use available datasets to develop and apply stochastic machine learning models to predict the properties of ILs and DESs, followed by the design and synthesis of the most promising new ILs and DESs based on the model predictions. The relevant physicochemical properties of the synthesised materials will be measured experimentally to validate the modelling results. The PhD project is co-supervised by Oliver Järvik (Department of Energy Technology, Tallinn University of Technology, Estonia) and Dinis Abranches (CICECO - Aveiro Institute of Materials, University of Aveiro, Portugal).

Research field:	Chemical, materials and energy technology
Supervisors:	Dr. Oliver Järvik Dr. Dinis Abranches
Availability:	This position is available.
Offered by:	School of Engineering Department of Energy Technology
Application deadline:	Applications are accepted between January 01, 2025 00:00 and January 24, 2025 23:59 (Europe/Zurich)

Description

The research

Thermal energy storage (TES) is a critical technology for improving the efficiency and reliability of renewable energy systems. By storing excess thermal energy generated during periods of low demand and releasing it when needed, TES systems help to balance energy supply and demand, reduce reliance on fossil fuels, and improve the overall stability of the power grid. In addition to energy applications, LHTES materials can be used in many other fields.

Ionic liquids (ILs) are a unique class of materials composed entirely of ions that can be used for TES as they have several advantageous properties over conventional LHTES materials, including low volatility and high thermal stability. Most importantly, since theoretically trillions of ILs can be created, the IL can be designed to have the physicochemical properties required for the specific application. The same is true of deep eutectic solvents (DESs), which are mixtures of solid precursors that yield liquid systems upon physical contact. Related to ILs, the design space of DESs, encompassing the chemical structure and relative composition of their precursors, is virtually infinite.

The design of new ILs and DESs for LHTES involves a complex interplay of factors, including molecular structure, thermal properties, and stability. Traditional experimental approaches to discovering and optimising ILs are time-consuming and resource-intensive. Machine learning models can analyse large datasets to identify patterns and correlations that may not be immediately apparent from experimental work alone. These models can then be used to predict the properties from the structure of ILs before they are synthesised, significantly reducing the trial-and-error aspect of experimental research.

Key responsibilities and (foreseen) tasks:

- Development of stochastic machine learning models to predict IL and DES properties following the design of candidate ILs and DESs.
- Synthesis of new ILs and DESs based on model predictions.
- Experimentally validate the properties of the synthesised ILs and DESs.
- Collaborate with a multidisciplinary research team.
- Publication of research results in high-impact journals and presentation at international conferences.
- Collaborate with other PhD students and colleagues in the department.

- Supervision of BSc and MSc students.

Applicants should fulfil the following requirements:

- A master's degree in chemistry, chemical engineering, material science, or other engineering subjects related to the PhD project topic.
- A clear interest in the topic of the position.
- Strong background in machine learning, preferably in related Python packages (e.g., TensorFlow or PyTorch).
- Hands-on experience in the synthesis and characterization of ILs and/or DESs.
- Excellent problem-solving skills and the ability to work independently.
- Strong written and verbal communication skills in English.

Applicants should submit:

1. A cover letter outlining the motivation and relevant experience.
2. A research plan for the topic, including the overall research and data collection strategy. The candidate can expand on the listed research questions and tasks.
3. Possible titles of at least three articles to be published on the project topic.
4. Previous work (e.g., thesis/dissertation, scientific articles, conference communications) that demonstrates proficiency in machine learning.

We offer:

- 4-year PhD position in the Department of Energy Technology at Tallinn University of Technology.
- Short-term stays abroad, namely at the University of Aveiro.
- A stimulating research environment with access to state-of-the-art facilities.
- Opportunities for professional development and networking.
- Full-time paid employment with a competitive salary and benefits.
- Support for conference travel and research dissemination.

About the department

The Department of Energy Technology is a research-focused department with robust connections to the Estonian chemical industry as well as the heat and power sectors. Our areas of expertise encompass chemical engineering, environmental engineering, thermal engineering, thermal power plants, heat economy, and thermal energy.

CICECO - Aveiro Institute of Materials at the University of Aveiro is a multidisciplinary research institution with a strong emphasis on materials design and artificial intelligence for engineering applications. CICECO is currently the largest Portuguese institute in the field of materials science and engineering, with a staff of almost 500 persons from the Departments of Chemistry, Physics, Materials and Ceramic Engineering, along with the School of Design, Management, and Production Technologies Northern Aveiro from the University of Aveiro.

Additional information

For further information, please contact Associate Professor Oliver Järvik at oliver.jarvik@taltech.ee or visit https://taltech.ee/en/department-energy-technology.

To get more information or to apply online, visit https://taltech.glowbase.com/positions/891 or scan the the code on the left with your smartphone.