CO2-derived carbon electrodes for lithium and sodium-ion batteries

Summary

The National Institute of Chemical Physics and Biophysics (NICPB) invites applications for a PhD position in the Energy Technologies Laboratory to develop high-performance anode materials from CO2-derived carbon for lithium-/sodium-ion batteries. The project focuses on molten salt electrolytic synthesis (CO2MSE) of nanostructured carbon and its optimization for energy storage, aiming to replace fossil-based graphitic carbons with sustainable, high-capacity alternatives. Particular attention will be given to tuning porosity, heteroatom doping, and surface chemistry to improve capacity, rate performance, and cycling stability in Li-ion and Na-ion systems. The successful candidate will address the following research questions: 1. How do molten salt electrolysis conditions and post-treatment strategies affect the microstructure, porosity, and sodium/lithium storage capability of CO#-derived carbon? 2. Can heteroatom doping or co-deposition strategies enhance charge carrier intercalation mechanisms in hard carbon-like materials? 3. What are the structure–function relationships governing electrochemical performance in Li-ion and Na-ion cells with molten-salt synthesized carbon electrodes?

Research field:	Chemical, materials and energy technology
Supervisors:	Kätlin Kaare Sander Ratso
Availability:	This position is available.
Offered by:	School of Engineering National Institute Of Chemical Physics And Biophysics
Application deadline:	Applications are accepted between June 01, 2025 00:00 and June 30, 2025 23:59 (Europe/Zurich)

Description

The research

As battery technologies expand beyond lithium-ion systems to sodium-ion and multivalent alternatives, there is an urgent need for low-cost, sustainable anode materials that combine high capacity, structural stability, and abundant availability. Hard carbon (HC) has emerged as the most promising anode for sodium-ion batteries (SIBs), offering high reversible capacities and excellent stability. However, commercial HC materials are typically derived from fossil precursors through energy-intensive pyrolysis. Similarly, mined and synthetic graphite dominate the market for Li-ion battery (LIB) anodes, but each come with enormous CO_2 footprints.

This PhD project proposes an alternative route: the direct electrochemical conversion of CO# into functional carbon via molten salt electrolysis. This method, developed in our lab under the CO2MSE framework, yields turbostratic, porous carbon structures with tunable morphology, heteroatom contents, and crystallite size—all key parameters influencing sodium and lithium storage mechanisms.

The candidate will first optimize electrolysis conditions in carbonate melts to tailor key material features: specific surface area, d-spacing, and degree of graphitization. Subsequent post-treatments (e.g., KOH activation, air/CO# oxidation) will be applied to fine-tune pore architecture and surface chemistry. Heteroatom doping (e.g., N, S) via in situ precursors or co-electrolysis will be explored to further improve electronic conductivity and pseudocapacitive contributions.

The synthesized materials will be characterized by XRD, Raman spectroscopy, BET, and XPS to determine key structural properties including L_c, L_a, I_D/I_G ratios, pore size distributions, and functional group compositions. Full electrochemical evaluation in half-cell and full-cell configurations will follow using LiPF# and NaPF#-based electrolytes, examining rate capability, cycling stability, and coulombic efficiency. The student will explore the dual-storage mechanisms in Na-ion systems (intercalation and pore filling), benchmarking performance against commercial hard carbon and other state-of-the-art materials.

Ultimately, this research aims to develop carbon electrodes that not only match but exceed the performance of conventional fossil-based carbons while offering a carbon-negative lifecycle. A study on the environmental impacts of CO_2-derived battery carbons will be a part of the project, looking at eelectricity sources and energy intensity of the process, CO# capture routes (e.g., direct air vs. point-source), purification processes, end-of-life recycling assumptions.

Responsibilities and (foreseen) tasks

- Synthesis of CO#-derived carbon materials via molten salt electrolysis.
- Apply thermal, chemical, and electrochemical post-treatments to control porosity and surface functionality.
- Characterization of materials using structural, spectroscopic, and microscopy techniques.
- Fabricate and test Li-ion and Na-ion half-cells and full-cells.
- Present research results in international journals and conferences.

Applicants should fulfil the following requirements:

- MSc in natural sciences.
- Strong interest in electrochemistry, carbon materials, and sustainable energy technologies.
- Excellent level of English and a collaborative spirit
- Ability to work independently and as part of an interdisciplinary research team.

(The following experience is beneficial:)

- Previous experience with electrochemical methods, fuel cell or battery systems is highly desirable.
- Proven track record of independently designing experiments and/or instrumentation.
- Experience in the physical characterization of carbon materials.
- Experience in working with molten salts or high-temperature chemical equipment.

We offer:

- A 4-year PhD position in a lab with cutting-edge infrastructure.
- Active participation in multiple international collaborations.
- Work with unique molten salt electrolysis systems and energy devices.
- Opportunities for conference visits, research visits to partnering institutions.
- A dynamic, innovative research environment focused on real-world CO# mitigation technologies.

About the department

The **National Institute of Chemical Physics and Biophysics (NICPB)** in Tallinn, Estonia is an independent research institute, which carries out basic and applied research in materials science, genetic engineering and biotechnology, environmental technology, in the field of particle physics and informatics, employing researchers from all over the world. The **Energy Technologies Laboratory (ETL)** at NICPB focuses on furthering fundamental understanding of electrochemical processes both at low and high temperatures, recycling of Li-ion batteries and developing novel functional materials with a minimal CO_2 equivalent. Key aspects of the research at ETL include the synthesis of carbon nanomaterials from CO_2 and biomass, battery recycling and advanced electrochemical testing, physical characterization and production scale-up. Our core aim is to replace the high CO_2 equivalent carbon materials in fuel cells, batteries and supercapacitors with sustainable alternatives.

(Additional information)

For further information, please contact Sander Ratso sander.ratso@kbfi.ee

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