

Scholarship for Student Position (Ref. M2ML-S-2025-3)

The Faculty of Mechanical Engineering at Silesian University of Technology (SUT) hereby announces competition for the student position (Ref. M2ML-S-2025-3). The successful applicant will participate in the research project titled: "Learning the Physics of Dendrite Growth in Lithium-Ion Batteries: An Attention Mechanism Approach for Prevention and Mitigation (DENDRITEPHASE)". The DENDRITEPHASE research project is jointly funded by the Narodowe Centrum Nauki (NCN), Poland and Fonds voor Wetenschappelijk Onderzoek Vlaanderen (FWO), Belgium. Within this project, researchers from SUT (Gliwice, Poland) and KU Leuven (Leuven, Belgium) will collaborate to investigate the mechanisms of dendrite growth in Lithium-Ion Batteries. The costs associated with the research stay of the successful applicant at SUT for the position Ref. **M2ML-S-2025-3** will be covered using funds from the grant (UMO-2023/51/I/ST11/02716) provided by the NCN.

Requirements:

1. Bachelor's degree awarded in any field of science or engineering including but not limited to chemistry, physics, technology, materials engineering, mechanical engineering, electrical engineering, biology, life sciences, agriculture engineering etc.
2. Proven background in at least four of the following scientific areas (refer Requirement 6.): (1) Density Functional Theory, (2) Molecular Dynamics, (3) Functional Materials, (4) Energy conversion technology or Energy Storage Materials, (5) Phase Field Method, (6) Machine learning;
3. Programming skills in one of the following languages (e.g. Python, C++). Experience in software app development in the applied engineering or applied science disciplines (the link to the data or code or the GUI or webapp of the software must be provided in the CV). Experienced in using Ubuntu OS;
4. Good command of spoken and written English language ;
5. Ability to work independently as well as work together in team.
6. Publication track record to justify the expertise required in 2.: The candidate has authored scientific research article(s) in SCI(E) journals.

Job description:

Lithium ion batteries (LIBs) are characterized with a large specific energy density ranging from 100 to 265 Wh/g. Rechargeable batteries, including LIBs, are considered as the most convenient and viable mobile energy storage devices of the present time. Dendrite growth is one of the serious reliability issues known to occur in the anode of LIBs. In spite of the several decades of continuous research on interfacial dynamics at electrode/electrolyte interface, the fundamental mechanism for the nucleation and growth process of Li dendrites is not yet fully understood. It is necessary to investigate these interfacial metallic structures at multi-scales through scale-bridging computations. Density functional theory (DFT) and molecular dynamics (MD) simulations can provide information about the property and structure of the electrode/electrolyte interface at atomic length scale. The insights from atomistic simulations could be imported into the phase field models for generating explainable data of dendrite evolution at continuum scale. To develop effective phase field model for energy storage materials, it is necessary to compare the thermodynamic formulations of free energies for LiB materials with those of ferroelectric materials or supercapacitor materials

In this research project, multiscale materials modeling as well as generative AI techniques will be utilized to study the dendrite formation and growth in LiBs. With the insights provided by these techniques, the research team will try to discover the mechanisms and ideas that help in the suppression of dendrite at the solid-electrolyte interface.

The main tasks for the scholar:

1. Perform DFT, MD and phase field computations for the **material candidates of energy storage devices (batteries, supercapacitors, and ferroelectric devices)**. (task 1 is 50 % of total task).

2. Integrate knowledge graphs and large language models to formulate the fact-finder generative AI model from the available **Electrochemical impedance spectroscopy (EIS) dataset** (task 2 is 50 % of total task).
3. Relay the data and results of task 1 and task 2 to other research team members.
4. Contribute to the publications of peer-reviewed articles in reputed scientific journals;

NCN call for proposals type: OPUS LAP – ST (NCN as lead agency*)

FWO call for proposals type: WEAVE (FWO as partner agency**)

Further information about the OPUS LAP/WEAVE:

* <https://www.ncn.gov.pl/en/ogloszenia/konkursy/opus26>

<https://ncn.gov.pl/en/wspolpraca-zagraniczna/wspolpraca-wielostronna/weave>

** <https://www.fwo.be/en/support-programmes/all-calls/senior-researchersresearch-teams/weave-fwo-partner/>

Form of tender submission: email (Ref. **M2ML-S-2025-3**)

Deadline for submission of tenders: 26.01.2025

Terms of Employment:

Announcement of competition results: As soon as possible

Number of position(s): 1

Place of work: Faculty of Mechanical Engineering, Silesian University of Technology, Gliwice, Poland

Duration of scholarship: 12 months

Working hours: Full time (40 h/week).

Date of commencement of employment: As soon as possible.

Additional Information:

The application should contain the following documents/information:

1. CV including the following information (list of scientific achievements, a list of publications, conference presentations, awards and distinctions for scientific activity, software and data processing skills) ;
2. Copy of the Bachelor's degree diploma or equivalent document or a document confirming the last year of Bachelor's studies;
3. Copy of the Bachelor's thesis abstract;
4. Application letter or letter of motivation (maximum 1 page)
5. Acronym for reference of this position (Reference: **M2ML-S-2025-3**).

In addition to the above documents, please prepare a document consisting of the following statement:

"I consent to the processing of my personal data for the purpose of recruitment in accordance with Art. 6 sec. 1 letter a of the Regulation of the European Parliament and of the Council (EU) 2016/679 of 27 April 2016 on the protection of individuals with regard to the processing of personal data and on the free movement of such data, and repealing Directive 95/46 /EC (general regulation on data protection)."

Application document (all of the documents combined together as a single pdf file) in English should be sent electronically to one of the Co-Principal Investigators (Co-PIs) of the project - Dr. Anil Kunwar (e-mail address: anil.kunwar@polsl.pl). This document must be also sent simultaneously as a CC email to another co-PI of the project - Professor Nele Moelans (e-mail address: nele.moelans@kuleuven.be). It is recommended to include the job reference (Reference: **M2ML-S-2025-3**) in the subject of the email message.