Scholarship for Students/PhD students (Ref. PFML-S-2024-1/Ref. BAP-2024-574)

The Faculty of Mechanical Engineering at Silesian University of Technology (Gliwice, Poland) and the Department of Materials Engineering, KU Leuven (Leuven, Belgium) hereby jointly announce scholarship competition for two students/PhD students. The successful applicants 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) and Fonds voor Wetenschappelijk Onderzoek Vlaanderen (FWO).

The scholarship competition in connection to the research stay at Gliwice is represented by the reference (**PFML-S-2024-1)**. Similarly, the announcement related to the research stay at Leuven is represented by the reference (**BAP-2024-574**).

Requirements of the candidate(s):

1. MSc degree in mechanical engineering, materials engineering, chemistry, physics or a related discipline
2. Strong background in at least four of the following scientific areas: (1) Feature engineering, (2) Uncertainty Analysis, (3) Energy storage materials, (4) Phase Field Method (5) Statistics and optimization techniques (6) Bayesian machine learning;
3. Programming skills in one of the following languages (e.g. Python, C++). Experienced in using TensorFlow and PyTorch libraries to develop machine learning models. Proficient in utilizing the MOOSE Framework for finite element analysis. ;
4. Good command of spoken and written English language (IELTS: average of 6.5 or more; TOEFL: average of 79 or more, or Equivalent);
5. Ability to work independently as well as work together in team.
6. Publication track record: The candidate(s) has/have authored scientific research article(s) in SCI(E) journals.

Job description:

Lithium ion batteries (LIBs) are considered as the materials of the future when it comes to efficient energy storage. One of the remaining problems limiting their lifespan is the formation of lithium dendrites. They are responsible for problems such as short circuits, failures and fires, electrolyte decomposition, and loss of active lithium in these batteries. Dendrite formation is an interfacial process spanning numerous length- and time scales. Despite decades of research, their composition, structure and formation still present a significant conundrum. Achieving completely dendrite-free battery interfaces can only be possible only the correct understanding of the fundamental mechanisms governing dendritic evolution.

In the PhD research, you combine multi-physics finite-element simulations with the use of (generative) AI models. Within the multi-physics finite-element model, the morphological evolution of the dendrites due to electrochemical reactions, diffusion, convection and other physical effects will be simulated for two contexts – **liquid (Type A)** and **solid (Type B)** electrolytes. The resulting computational datasets will be combined with experimental datasets to train attention mechanism (AM) based generative and/or discriminative machine learning (ML) models. The list of ML models will include but is not limited to MeshGraphNet, variational autoencoder, transformers etc. The objective is to generate in-silico novel battery architecture or structures that are resistant to dendrite growth, as well as narrowing down the list of features required for outlining the conditions favorable for suppressing the dendrite growth.

The main tasks for the PhD students:

1. Perform multi-physics simulations,including phase field models for electrochemical migration in LIBs with either Type A or Type B electrolyte, and tally them with available experimental data.
2. Quantify the dendrite evolution pattern in the computational model.
3. Blend the computational and experimental data associated with lithium ion battery to create a feature pool of influential attributes.
4. Train generative and/or discriminative AI models with the datasets obtained in 3. Use these models to generate structures/architecture or predict conditions that can ensure the prevention of dendrite growth in LIBs.
5. 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. PFML-S-2024-1), online application (Ref. BAP-2024-574)

Deadline for submission of tenders: 25.09.2024

Terms of Employment:

Announcement of competition results: As soon as possible

Number of position(s): 2

During research stay for first 24 months at KU Leuven :

Place of work: Department of Materials Engineering, KU Leuven, Leuven, Belgium

Duration of scholarship: 24 months

Working hours: Full time

Further Information: Information on salary and working conditions under a doctoral scholarship at KU Leuven: https://www.kuleuven.be/personeel/jobsite/en/phd/phd-information#working-conditions

During research stay for remaining 24 months at Silesian University of Technology:

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

Duration of scholarship: 24 months

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

Date of commencement of employment: As soon as possible.

Further Information: Detailed information about NCN scholarships is available at https://www.ncn.gov.pl/sites/default/files/pliki/uchwaly-rady/2022/uchwala124_2022-zal1_ang.pdf . We kindly request the applicant to read the NCN's announcement on exemption from income tax from the NCN research scholarship: https://www.ncn.gov.pl/en/aktualnosci/2021-12-30-stypendia-ncn-podatki

Additional Information:

As these are joint PhD positions at the two universities, the candidates must submit their applications to both universities:

i. Application procedure (Ref. PFML-S-2024-1):

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 MSc diploma or equivalent document or a document confirming the last year of master's studies;

3. Copy of the MSc/ BSc thesis abstract;

4. Application letter or letter of motivation (maximum 1 page)

5. Acronym for reference of this position (Reference: PFML-S-2024-1).

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 in a single pdf file) in English should be sent electronically to the Co-PIs of the project Dr. Anil Kunwar (e-mail address: anil.kunwar@polsl.pl) and Professor Nele Moelans (e-mail address: nele.moelans@kuleuven.be). It is recommended to include the job reference (Reference: PFML-S-2024-1) in the subject of the email message.

ii. Application Procedure (Ref. BAP-2024-574):

Prospective applicants are requested to visit the link https://www.kuleuven.be/personeel/jobsite/jobs/60373107?lang=en) for obtaining further information about Ref. **BAP-2024-574.**