Postdoctoral Research Positions (Ref. DM-P-2025-3)

The Faculty of Mechanical Engineering at Silesian University of Technology (SUT) hereby announces competition for the postdoctoral research positions (**Ref. DM-P-2025-3)**. 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), 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 applicants at SUT for the position **Ref. DM-P-2025-3** will be covered using funds from the grant (UMO-2023/51/I/ST11/02716) provided by the NCN.

Requirements of the candidate(s):

1. PhD degree in mechanical engineering, materials engineering, chemistry, physics or a related discipline
2. Strong background in at least one of the following scientific areas: (1) Density Functional Theory or Molecular Dynamics, (2) Energy storage materials, (3) Statistics and optimization techniques, (4) Bayesian machine learning, (5) Natural Language Processing (MD or DFT related text datasets);
3. Programming skills in one of the following languages (e.g. Python, Fortran 90). Experienced in using VASP software for DFT calculations or Experienced in using LAMMPS software for MD calculations;
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: 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 the 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.

In this research project, the DFT method will be utilized to perform ab-initio study of the candidate LIB materials. The first-principles calculations will be combined together with MD simulations and/or machine learning to obtain the quantities such as migration energy barrier, free energy for electrochemical reactions, theoretical capacity prediction, Li adsorption energy, ion transport kinetics, structural stability parameter, electrodeposition probabilities at solid electrolyte interface etc. Two post-doctoral researchers will be involved in these tasks – one will perform the DFT computation and another will perform the MD computation. The main tasks for the postdoctoral researchers are as following:

A. Postdoctoral Researcher 1: DFT Specialist

1. Perform DFT computations to generate structure-property data for existing and candidate Li-ion battery materials.
2. Postprocess the generated data to make inferences regarding structural stability parameter and electrodeposition probability.
3. Relay the DFT- computed datasets to the team members performing mesoscale computations and/or machine learning methods
4. Contribute to the publications of peer-reviewed articles in scientific journals;

B. Postdoctoral Researcher 2: MD Specialist

1. Assess the feasibility of developing new interatomic potentials for use in molecular dynamics (MD) simulations and conduct benchmark MD simulations to validate these potentials.
2. Analyze the MD simulation outputs to derive insights into structural stability parameters and electrodeposition probabilities at the electrode/electrolyte interface, leveraging atomistic insights to inform dendrite growth mechanisms for integration into phase field models.
3. Share the MD-computed datasets with team members conducting mesoscale computations and/or machine learning methods.
4. Contribute to the publications of peer-reviewed articles in 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. DM-P-2025-3)

Deadline for submission of tenders: 30.07.2025

Terms of Employment:

Announcement of competition results: As soon as possible

Number of position(s): 2

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

Duration of employment: 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 PhD diploma or equivalent document or a document confirming the last year of master's studies;

3. Copy of the PhD thesis abstract;

4. Application letter or letter of motivation (maximum 1 page). In the first paragraph of the appliction letter, the preference for either the "**DFT Specialist**" or "**MD Specialist**" position has to be clearly stated.

5. Acronym for reference of this position (Reference: DM-P-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 in a single pdf file) in English should be sent electronically to one of the 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: DM-P-2025-3) in the subject of the email message.