Postdoctoral Research Position (Ref. DM-P-2026-10)

The Faculty of Mechanical Engineering at Silesian University of Technology (SUT) hereby announces competition for the postdoctoral research positions (**Ref. DM-P-2026-10)**. 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 applicant at SUT for the position **Ref. DM-P-2026-10** 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 obtained not earlier than 7 years before employment start date.
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) Retrieval Augmented Generation Method, (5) Natural Language Processing (MD or DFT related text datasets), (6) 2D Materials;
3. Programming skills in one of the following languages (e.g. Python, Fortran 90). Experienced in using VASP software or Quantum Espresso or any relevant software for DFT calculations or Experienced in using LAMMPS software or any relevant 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 by a high specific energy density, typically ranging from 100 to 265 Wh/kg (Note: energy density is usually measured in Wh/kg or Wh/L, rather than Wh/g). Rechargeable batteries, including LIBs, are currently considered the most convenient and viable mobile energy storage devices. Dendrite growth remains a serious reliability issue known to occur at the LIB anode. Despite several decades of continuous research on interfacial dynamics at the electrode/electrolyte interface, the fundamental mechanisms driving the nucleation and growth of lithium (Li) dendrites are not yet fully understood. To address this, it is necessary to investigate these interfacial metallic structures across multiple scales using scale-bridging computations. Density functional theory (DFT) and molecular dynamics (MD) simulations will provide insights into the properties and structures of the electrode/electrolyte interface at the atomic length scale. These atomistic insights will be integrated into phase-field models to generate explainable data regarding dendrite evolution.

In this research project, DFT methods will be utilized to perform ab-initio studies of candidate LIB materials. These first-principles calculations will be combined with MD simulations and/or machine learning (ML) to determine key quantities, such as: migration energy barriers, free energy for electrochemical reactions, theoretical capacity predictions, Li adsorption energy, ion transport kinetics, structural stability parameters, electrodeposition probabilities at solid electrolyte interface etc. A postdoctoral researcher will be involved in these tasks, performing both the DFT and MD computations. The main tasks for the postdoctoral researcher are as follows:

A. Role as a DFT Specialist

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

B. Role as a 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 them.
2. Analyze MD simulation outputs to gain insights into structural stability parameters and electrodeposition probabilities at the electrode/electrolyte interface. Utilize the knowledge from these 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.
4. Contribute to the publications of peer-reviewed articles in scientific journals;

It is expected that a candidate proficient in Category A (DFT) will be able to perform the tasks of Category B (MD) after minimal on-the-job training, and vice versa. Demonstrable expertise in one of the fields is sufficient to fulfill both roles effectively within the scope of the DENDRITEPHASE project.

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-2026-10)

Closing timeline for submission of tenders: 29.06.2026

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 employment: 24 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 PhD studies;

3. Copy of the PhD thesis abstract;

4. Application letter or letter of motivation (maximum 1 page). In the first paragraph of your application letter (maximum 1 page), please clearly state which of the two fields,- DFT Specialist or MD Specialist, best matches your primary expertise.

5. Acronym for reference of this position (Reference: **DM-P-2026-10**).

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-2026-10**) in the subject of the email message.