

DC3 – JOB VACANCY

Position description

Reference:	DC3		
Title:	Multiscale modelling of ion transport and interfacial phenomena in Li-metal polymer batteries		
Hiring beneficiary:	UU		
Location:	Uppsala University, Uppsala, Sweden		
Start date:	01 October 2024	Duration:	48 months
Expected date of communication of results:	Less than 2 months after the application submission		

Job description

Objective:	DC3 will develop and apply multiscale modelling methodology to help understand the processes involved in the challenges and electrochemical bottlenecks of Li-metal polymer batteries. Overcoming these hurdles is vital for the commercial success and industrialization of these devices. The main problems is general electrochemical stability, surface decomposition of electrolyte component on Li-metal and formation of interphase layers at both electrodes, bulk and interface ionic transfer and transport, and finally how these parameters affect cell behaviour and ageing. Since these problems occur on several length- and time-scales in the battery cell, a multi-scale approach where these are interconnected becomes necessary.
Expected results:	DC3 will construct a multi-scale model comprising surface and bulk chemical processes for Li-metal batteries based on DFT, semi-empirical methods, MD simulations and FEM cell modelling. The model will iteratively interconnect the different techniques and conceptual designs developed by the <i>RIDERS</i> consortium, which separately address the critical processes in these devices at different length (Ångström for specific reduction/oxidation processes to hundreds of µm for the battery cell) and time-scales (ps for charge transfer to days/months for battery cycling). Suggestions of novel solid polymer electrolyte will be made based on the performance of the material and correlations to the chemical processes, which will target improved chemical stability and ionic transport. Ion-coordinating motifs in the polymer which undergo side-reactions at the anode and cathode, respectively, will be identified, thereby rendering suggestions for development of specific bilayer electrolyte systems and protective coatings for the electrodes.
Supervisors:	Dr. A. Mace (UU) Prof. D. Brandell (UU)
Secondments (short term academic and industrial internships):	2 months to GINP (Grenoble, France)– Correlation between MD simulations and experimental measurements of ionic charge transport in LMP batteries. 2 months to KIT (Ulm, Germany)– Correlation between DFT and AIMD surface chemistry phenomena and experimental data in Li/S batteries. 2 months to Volvo Personvagnar AB (VCC) (Göteborg, Sweden)– Exploration of FEM model and benchmarking of LMP model towards cell data.

Vacancy requirements	
Qualifications:	Not having resided in Sweden for more than 12 months in the 3 years immediately before the recruitment date, and not having carried out their main activity (work, studies, etc.) in Sweden during this period. Must be a doctoral candidate (not already in possession of a doctoral degree at the date of the recruitment)
Languages:	Good level in oral and written English is mandatory.
Skills/Experience	Chemist, physicist or materials science candidate with solid background on the computational chemistry and/or materials modelling methodology. Additional experience in electrochemistry or in electrochemical storage technologies are not mandatory however valuable as is a vast experience of different modelling techniques and programming.

Job details	
Salary:	Salary and benefits will comply with the rules of the DN-MSCA 2023, as foreseen in the Marie Skłodowska-Curie Actions Work Programme. Salary including living and mobility allowance before income tax will follow the local collective agreement in salaries for doctoral students at Uppsala University according the PhD salary ladder .
Other benefits:	<u>Gross family allowance (before income tax): 377 € per month - if applicable paid during the first 36 months</u> Family allowance: 'Family' means persons linked to the researcher by marriage (or a relationship with equivalent status to a marriage recognised by the legislation of the country where this relationship was formalised) or dependent children who are actually being maintained by the researcher.
Duration:	48 months
Starting date:	Ideally the 01/10/2024 – not after the 05/01/2025
Type of contract:	Full time position
Hours per week	40 hours
Place of work:	Ångström Laboratory, Polacksbacken, Lägerhyddsvägen 1, Uppsala
Local language:	Swedish

Application to be submitted through the recruitment page of Uppsala University website <https://www.jobb.uu.se> .