

Postdoctoral position in multiscale modelling of battery materials (BIG-MAP)

Uppsala University, Department of Chemistry-Ångström Laboratory, Sweden

Context and research focus: The Battery Interface Genome – Materials Acceleration Platform (BIG-MAP) project (<http://www.big-map.eu>) is a large consortium of academic and industrial partner groups funded by the European Commission. The announced position is part of BIG-MAP and is placed at the Department of Chemistry at the Ångström Laboratory of Uppsala University (Sweden), where the host group (<http://www.teoroo.kemi.uu.se>) of the announced position is located. Within BIG-MAP we collaborate with the Karlsruher Institut für Technologie (KIT) and École polytechnique Fédérale de Lausanne (EPFL) on multiscale modelling workflows and interoperability as well as with University of Cambridge and the University of Vienna on the development of machine-learning potentials and property prediction of battery materials and molecules. The current research project concerns the exploration of data interoperability and interaction models at different levels of the multiscale ladder with a focus on electronic structure-based methods of different flavours and applications in the area of battery materials (electrodes, electrolytes, and interfaces) consistent with the goals of the BIG-MAP project.

Contacts: To perform this work we are looking for a talented postdoctoral candidate with suitable background and ambition who would be interested to work with us in this project. The recruitment will be carried out as a 2-stage process. If you are interested, please contact the PI (kersti.hermansson@kemi.uu.se) with a cover letter and a CV, preferentially by 20 July 2021.

The host group: The host group is strongly involved in research on –combinations of– electronic structure methods (DFT, ab initio and semi-empirical), atomistic advanced (reactive) force fields and kinetic modelling. A range of applications involving interface chemistry, redox properties, energy materials and intermolecular interactions are being explored. The starting data is as soon as possible.

Desired skills: (i) A solid background in quantum chemistry modelling of materials and molecules, (ii) at least moderate skills in the application of machine learning to scientific problems, (iii) good working skills in programming/ scripting, data handling and interoperability, and (iv) some experience with atomistic (force-field) models, MD simulations and multi-scale modelling. Finally, (v) the applicant is also expected to have a very good command of written and spoken English and (vi) possess good collaborative skills, drive and independence. Greater importance will be attached to the ability to conduct independent research of high quality than to the number of publications.