Project: Transport and Reactions in Complex Heterogeneous Multiphase Systems

Summary: The goal of this project is to develop a reliable, theoretical, and computational framework for transport and reactions in Complex Heterogeneous Multiphase Systems (CHMSs) based on mathematical, physical, and thermodynamic principles.

The project consists of two main Themes with cross-linking throughout: 1. Modelling and analysis of novel effective transport formulations for CHMSs such as batteries, fuel cells, and solar cells. 2. Novel computational multiscale framework for transport and reactions in CHMSs.

We will apply rigorous, mathematical and physical modelling with state-of-the-art methodologies such as variational, physical, and thermodynamic analysis based on calculus of variations, gradient flows, statistical mechanics and thermodynamics as well as novel computational approaches allowing for the reliable and efficient discretisation of CHMSs.

The ultimate aim is the systematic and predictive theoretical and computational analysis as well as optimization of CHMSs with the goal of reducing material costs and of increasing longevity by a novel and general computational multiscale framework. As a consequence, the results from the proposed work shall guide experiments for gaining fundamental understanding of the underlying chemical, physical, and thermodynamic processes but shall ultimately recommend new design rules, materials, geometries, processes and operation strategies, as well as novel measurement techniques. Finally, this project builds the fundamental basis for the subsequent theoretical and computational investigation of random CHMSs which naturally occur in many applications.

Collaborations: The project is expected to foster national and international collaborations with Imperial College – London, ETH – Zürich, Simon Fraser University – Vancouver, University of Alberta, and École Polytechnique – Paris.

Educational background: We are looking for a Research Associate with a PhD in Mathematics (Analysis, Probability, Numerics & Computations), Computational Science, or any other equivalent field. Interested candidates should be enthusiastic to learn and understand new concepts and preferably have a fundamental understanding in one or more of the following fields: analysis, electrochemistry/thermodynamics & physics, finite element methods (preferably with experience with Python), and probability theory.

Project duration, funding source, and research group: This project is fully funded for 15 months by EPSRC and Heriot-Watt University. Opportunities for extending the contract beyond the 15 months are anticipated in another EPSRC or collaborative grants/projects. A Ph.D. project is closely linked to this research. There are two more Ph.D. students in the group which are part of the Maxwell Institute Graduate School in Analysis and its Applications.

If you are interested, please contact me (Dr. Markus Schmuck) by email (M.Schmuck@hw.ac.uk), and **send your application** as a pdf file (CV, motivation letter, BSc, MSc, and PhD theses, three recommendation letters, and brief research statement outlining your future interests) **until April 24, 2017**. For additional information about the group, see http://www.macs.hw.ac.uk/~ms713/index.html. The successful candidate will be based at the Maxwell Institute and the School of Mathematical and Computer Sciences at Heriot-Watt University. There are plenty of opportunities to collaborate with teams at national and international Universities. The successful candidate is also expected to present results at premier conferences in Applied Mathematics, Electrochemistry, and Computational Science as well as events of the American Physical Society, British Applied Mathematical Colloquium and publish in premier journals such as SIAM Journal of Applied Mathematics, Journal of Computational Physics, Journal of the Electrochemical Society, etc.