Master thesis in Computational Chemistry, UU

Rational Design of Liquid Metal Battery Electrolytes using Computer Simulations

Background
The increased use of intermittent renewable energy sources requires a more flexible and robust electrical grid and a large energy storage capacity in order to satisfy fluctuations in demand. Liquid metal batteries (LMBs) are a promising candidate for such large-scale grid energy storage. One way to tune the electrochemical performance of the LMB is to modify their salt mixture electrolyte, which will change the batteries properties. In particular the ternary and quaternary salt mixtures are largely unexplored, and there is in general a lack of data on physicochemical properties to guide development of LMBs.

Projects
Depending on your background and interests, we provide different projects:
(i) In this project, you will calculate melting points, conductivities and Gibbs energies of the melts with different compositions using the Molecular Dynamics simulation software GROMACS.
(ii) If you are interested in PYTHON programming, you can work on the development of a new force field for alkaline-earth cations that are relevant for LMBs.

If you are interested, please contact:

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