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MODELLING AND SIMULATION OF POROUS BATTERY ELECTRODES WITH MULTI-SCALE HOMOGENISATION TECHNIQUES

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In this talk I will give an overview on the modelling procedure of porous insertion electrodes with homogenisation techniques. Foundation for this approach is a sophisticated modelling framework for electrochemical systems on the basis of non- equilibrium thermodynamics [1-4].

Some key aspects of this model framework are (i) thermodynamically consistent boundary conditions taking into account charge transfer reactions and capacitive effects at the electrode-electrolyte interface [5-7], (ii) the dependence of the conductivity and the transference number on the (local) ion concentration, (iii) predictivity and validation of the thermodynamic factor, (iv) accounting for incomplete electrolyte dissociation [8], and (v) self-consistent incorporation of the open circuit potential for various electrode materials.

The homogenisation of this model framework for a porous medium allows then the determination of the porosity, tortuosity, and interfacial area based on representative and real micro-structure models, as well as the derivation of homogenised equations for this porous electrochemical system.

Numerical simulations of charge/discharge cycles show the validity of this approach, and potential extensions regarding ageing effects are finally discussed.

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