Modelling of Lithium Ion Batteries with Silicon Anode and Ionic Liquid Electrolyte

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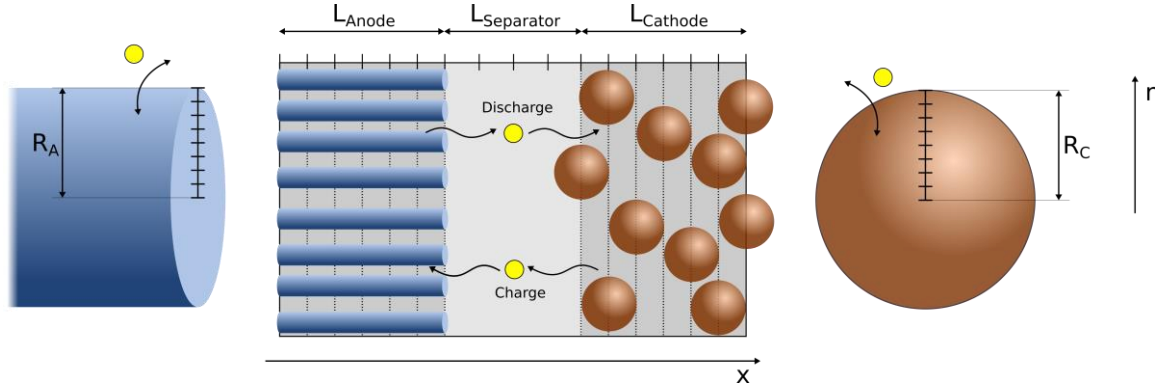
Silicon anodes are studied to boost lithium storage capacity. Standard organic electrolytes, however, are incompatible with silicon anodes due to the large volumetric changes of silicon. Thus, the solid electrolyte interface is unstable. As promising alternatives, novel electrolytes like ionic liquids offer desirable characteristics such as high chemical, thermal and electrochemical stability as well as high ionic conductivity.

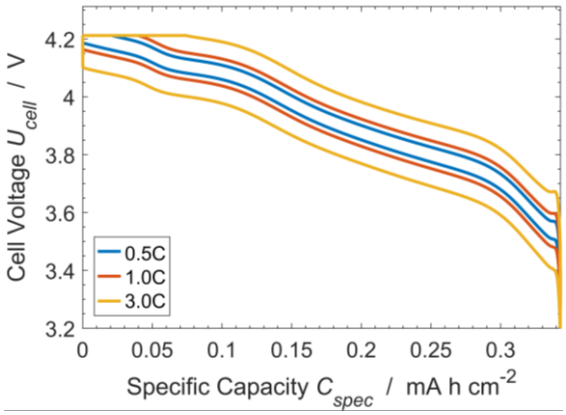
Our theoretical work aims at providing full cell simulations of lithium ion batteries with silicon anodes and ionic liquid electrolytes on the continuum level. The modelling framework is based on our recent development of a thermodynamically consistent transport theory for ionic liquids.[1] The theory was validated in the bulk phase and at interfaces where it captures effects like crowding and overscreening.[2] On the anode side, mechanical effects due to lithium insertion are coupled to the electrochemical model. Lithium ion transport through the cell is thus captured in a macro-homogenized 1d+1d model.

The modelled battery consists of a silicon nanowire anode, an ionic liquid electrolyte and a standard lithium cobalt oxide cathode. We model the nanowire structure of the silicon anode in a cylindrical geometry. Simulations are carried out with MATLAB.

This work is supported by the European Union's Horizon 2020 research and innovation programme via the "Si-DRIVE" project (grant agreement No 814464).



Top: 1d+1d model scheme; Right: Discharge-charge curves for different C-rates.



***Keywords**:* 1d+1d cell model, lithium ion battery, silicon anode, ionic liquid electrolyte, transport theory.

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[2] V. Hoffmann et al., *Phys. Chem. Chem. Phys.*, 2018, **20**, 4760.