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TRANSPORT AND ENERGY CONVERSION IN NON-ISOTHERMAL BATTERY SYSTEMS. THE CASE OF THE LITHIUM BATTERY

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Electrochemical cells like batteries are complex heterogeneous layered structures, and each layer is frequently porous. This brings out central questions like; how many and which interfaces play a role in energy conversion? And, how do we define and measure this role? In other words, how do we describe the interplay between the various fluxes of heat, mass and charge in each layer? Most often the cell is treated as being isothermal, while this is clearly not the case when electric current is drawn. A systematic thermodynamic procedure is not only useful to model energy conversion and transport. It is needed, as current models and procedures frequently are insufficient. We have chosen to describe the energy conversion using non-equilibrium thermodynamic theory [1]. This classical theory offers a consistent way to obtain flux-force relations, whether they are based on ionic fluxes and their driving forces, or on the neutral component fluxes and their conjugate driving forces. The full set of transport coefficients can be derived directly from the entropy production [1], as well as from corresponding fluctuation dissipation theorems [2].

Using the lithium battery as an example, we first demonstrate how the various transport coefficients are interrelated [3]. We next present numerical values for a typical battery electrolyte as obtained from molecular dynamics simulations. Electrolyte models, assuming independent movement of ions, fail to capture the Onsager conductivities by a large amount. Using the solvent ethylene carbonate as a frame of reference, the co-solvent diethyl carbonate is moving across the electrolyte, contrary to current views, and create chemical potential gradients that need be overcome during operation. In addition, it is also likely that thermal gradients have an impact on battery voltage [4].

Participation

In-Person

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