Modeling and Validation of Material and Transport Models for Electrolytes

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In this talk, I will show some general aspects of modeling ionic species in liquid electrolytes which are subject to solvation effects. Based on non-equilibrium thermodynamics, the derivation for a material model of an incompressible solvation mixture is thus sketched. I will show how such a material model can be validated in thermodynamic equilibrium on various electrochemical measurement techniques and deduce some results regarding the modeling perception. Building on this, I will discuss several models for ionic flux relations, including Nernst–Planck-type fluxes and Onsager-type cross-diffusion models. I will show some shortcomings of the classical Nernst–Planck-flux in terms of measurable quantities and provide an interpretation of the Kohlrausch law for electrolytes on the basis of cross-diffusion effects.