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Understanding conductivity in liquids: From ion pairing to proton (and chirality) transfer

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Ion pairing is often used to explain a reduced electrical or ionic conductivity measured by impedance spectroscopy compared to ion diffusivities measured by pulsed field gradient. In this presentation we focus on the following questions: How are ion pairs defined? Ion pair versus ion association: Are there other effects like charge transfer, polarizability, or charge screening that should be considered? Is this related to charge scaling in force fields? How do we calculate electrical conductivity? How do we control uncertainties in this and other properties? Strutural diffusion in ionic liquids can enable fast transport. Mixtures of N-methylimidazole as well as similar cations and acetic acid show an unexpected high ionic conductivity. Is water addition necessary to enable a Grotthuss-like diffusion? Furthermore, we discuss the behavior of chiral solutes in different ionic liquids where the induction of optical acitivity is observed in achiral ionic liquids. We try to understand how chirality extend to solvents. Given time, we also present ionic liquids in confinement and discuss uncertainties in modellling of ionic liquid properties.