

TITLE: Multivalent (Mg, Ca) electrolytes with improved ion-pair dissociation

Summary: Multivalent batteries are seen as next generation technology based on abundant resources. However, their practical application is lagging behind due to lack of suitable electrolytes. In this thesis, novel multivalent electrolytes based on magnesium and calcium salts with weakly coordinating anions (WCA) will be synthesized and characterized. Mg and Ca salts based on WCA have shown good electrochemical performance in terms of plating/stripping efficiency, cell overpotential and oxidative stability. However, further steps forward are needed to achieve practical battery cell benchmarks through improved ion-pair dissociation. In this thesis, new Mg and Ca salts from class of fluorinated alkoxy class based on aluminate and borate salts with different ligands will be synthesized. Their ion-pair dissociation will be studied in different solvents and solvent mixtures through a combination of IR and Raman spectroscopy. This will allow fine tuning of ion-pair dissociation, a key factor governing electrolyte stability, as well as improved performance in practical multivalent cells with organic cathodes.

Research techniques used: Organic synthesis and solvent distillation in specially equipped glove-box for chemical synthesis and their chemical analysis with NMR, IR and TGA. Cell testing in Swagelok or pouch cell setups with a range of different electrochemical techniques (cyclic voltammetry, electrochemical impedance spectroscopy, galvanostatic cycling). IR and Raman spectroscopy measurement in conventional setups as well as in situ and operando cell setups. Use of DFT computational modelling tools to assign and fit the obtained spectroscopy measurements.

The reason why the topic is innovative: The PhD topic will move beyond the existing knowledge on the multivalent battery electrolytes by joining state-of-the-art salt synthesis and connecting it with the advanced spectroscopy characterization of electrolyte. Advanced spectroscopy characterization will be enabled by application of advanced spectroscopy setups and expertise of the Theory Department providing key insights into electrolyte speciation. This PhD topic will through detailed analysis and identification of governing principles, create guidelines for future synthesis of multivalent as well as other battery electrolytes.

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