Priority Programme

“Material Synthesis near Room Temperature”

Project Description – Project Proposal

Solubility of molecular and ionic precursors in ionic liquids

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Summary of proposal

The success of ionothermal synthesis is crucially dependent on the creative choice of suitable precursors. The main goal of this project is the development of general thermodynamic procedure based on the predictive equation of state electrolyte PC-SAFT (ePC-SAFT). A model strategy will be developed and applied that allows predicting solubility of liquid or solid precursors in ionic liquids (ILs) used as suitable solvents for the ionothermal synthesis. As the solid precursors we consider inorganic salts, closely related to and motivated by the synthesis of metal nanoparticles in ILs. As the liquid precursors the homologous series of organic compounds (alkanes, alkenes, aromatics, alcohols, ethers, esters) will be studied.

Development and parametrization of ePC-SAFT will be performed by using reliable experimental data from literature and new data as well. In this context, the subsidiary goal of this project will be the extended experimental study of thermodynamic properties of pure ILs and precursors, as well as properties of their binary mixtures in order to provide reliable input data sets required for the model development and validation. This will allow model predictions in order to reliably screen ILs as synthesis medium for solid and liquid precursors. In order to propagate application of thermodynamic parameters obtained from binary

mixtures precursor-IL to multi-component systems, an additional validation of the model will be performed by the experimental and theoretical study of two reactive systems. These systems are composed of the reaction participants as well as the solvent (also ILs).
The establishment of thermodynamic results in the systems precursor/IL will allow developing of a general scale of solubility parameters, with the purpose of predicting the performance and to guide the selection of ILs for ionothermal synthesis and their use on reactive systems. This scale has huge potential to be extended and improved for application to a broad scope of molecular and ionic precursors.