INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Seminar

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Study of Heat Capacity and Phase Equilibrium Properties by Calorimetry and Monte Carlo Simulations

Calorimetry is a group of methods for measurement of heat absorbed or evolved in a process. In spite of the fact that basics of many calorimetric methods, for example, adiabatic calorimetry (AC), were developed many decades ago, nowadays it remains a powerful tool answering to the challenges of modern science. In this talk, the performance of calorimetry for studying of heat capacity and phase transitions of room-temperature ionic liquids (ILs) will be discussed.

The current status of heat capacity measurements for ILs and the problems related to the quality of these results will be considered. A self-consistent procedure will be presented which allows one to evaluate uncertainties of the reported experimental heat capacity data. The effect of the impurities on the temperature and enthalpy of fusion as well as the heat capacity of ILs will be considered as well.
Monte Carlo (MC) simulations are used in various fields of physical chemistry. Recent advances in computer hardware and algorithmic implementations of MC sampling techniques bring these methods closer to becoming a mainstream tool for prediction and extrapolation of thermophysical data. However, application of MC simulations to the calculation of thermophysical properties normally requires significant computational resources as well as substantial human expertise. In this talk a possibility of decreasing of the expert participation in the calculations by introducing a formal algorithm for determination of the force field parameters will be considered. A systematic procedure for determination of force field parameters is based on response surface mapping methodology that allows simultaneous parameter optimization against multiple property targets while constraining the number of required computationally-expensive numerical experiments. The approach was implemented for prediction of vapor-liquid equilibrium properties of alkanes, alkenes, and their fluorinated derivatives via Monte Carlo molecular simulations. To further reduce computational costs, a bootstrap procedure that involves a sequence of parameter optimization for groups of compounds was used.