Abstract

Development of new, safe, highly efficient, and environmentally friendly energy storage and conversion devices is demanded in today's world. This includes the synthesis, characterization, and application of new advanced materials. Promising materials such as polymer electrolytes, conductive polymers, and perovskites have drawn the great attention of scientists worldwide and are under intensive investigation. These substances are believed to be capable of solving some issues and improving the existing energy storage and conversion technologies.

The presented thesis is dedicated to the investigation of above-mentioned materials for energy applications. The research was focused on the elucidation of structure-properties relation in the compounds of interest and optimization of their composition to get better properties in terms of potential application in the energy field. Among all experimental techniques used within the thesis, NMR spectroscopy was comprehensively employed and chosen as the main tool for the structural characterization of the investigated samples. Various liquid-state as well as solid-state NMR techniques were used, and some of them were optimized for specific purposes of the research.

During the investigation of polymer electrolyte systems, NMR spectroscopy was utilized to study the structure of the polymer matrixes and for investigation of ions mobility (PFG NMR, relaxation measurements) and exchange (^{7}Li-^{7}Li EXSY NMR) providing insights into conductivity mechanism. Further, a multinuclear NMR approach (including ^{17}O natural abundance experiments) was used to study coordination among cations, anions, and solvent (water) in electrolytes used in symmetrical PANI-based electrochemical cell. In the case of characterization conductive polymers, the effect of sample conductivity on NMR signals was observed. A relation between the structure of the sample, its conductivity, and the halfwidth of the respective NMR signals has been found. In the case of perovskites, NMR spectroscopy of "exotic" nuclei such as ^{133}Cs and ^{209}Bi was used to get insights into the structure of the investigated materials. Additionally, ^{35}Cl ultra-wideline spikelets NMR spectra were recorded using WURST-QCPMG NMR experiments with variable offset. Such spectra provided additional structural information and were found to be very benefical for this case. Finally, in order to optimize the processing of such spectra, a piece of software (USS software) was developed, tested, and published. This software allows fast and simple handling of any spikelets spectra with further accurate fitting in conventional NMR software and extraction of required NMR parameters.

Keywords: NMR spectroscopy, Li-ion batteries, gel polymer electrolytes (GPEs), composite polymer electrolytes (CPEs), conductive polymers, solar cells, perovskites.