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Electrodes and solid electrolytes for Li-ion batteries: Local structures, Li-ion mobility, and lithiation mechanisms

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Li-ion batteries are used extensively in mobile electronic devices and in electric vehicles due to their high energy and power densities. The performance of these storage systems strongly depends on the materials used inside these batteries as electrodes and electrolytes. In order to improve these batteries, it is important to understand the fundamental diffusion mechanisms and also the fundamental electrochemical reaction mechanisms that occur during charging and discharging of the batteries, i.e., during lithiation and delithiation of the electrodes, and that are responsible for function and degradation of these systems. The changes that occur in the electrode materials during electrochemical cycling are investigated by *in situ* techniques including diffraction as well as spectroscopic methods. These measurements are performed on olivine materials LiMPO_4 ($M=\text{Fe}$, Mn and Co) and high-voltage spinel materials $\text{LiM}'\text{M}''\text{O}_4$ (M' , $M''=\text{Mn}$, Co , Ni , Fe) and they reveal the details of the lithiation/delithiation mechanisms and how these are related to the performance of these materials in the batteries. Solid electrolytes might offer an enhanced safety for these systems. Different oxidic, sulfidic, and polymer systems are investigated with respect to Li^+ ion mobility by ^7Li NMR relaxometry and field-gradient NMR spectroscopy. From this, microscopic diffusion parameters such as the average Li ion jump rate τ^{-1} and the activation barrier E_A for single Li ion jumps can be extracted, but also the macroscopic transport of the Li ions can be observed. The results of these measurements are compared to those obtained by impedance spectroscopy.

Biography

Sylvio Indris is investigating materials that can be used as electrodes and electrolytes in Li-ion batteries. These materials are prepared by solvothermal/hydrothermal methods, sol-gel techniques, and solid-state reactions. The changes in these materials during operation in these batteries are investigated by diffraction techniques as well as X-ray absorption spectroscopy, solid-state NMR, and Mössbauer spectroscopy. Finally, the results of these investigations are used to optimize the performance of the complete Li-ion battery systems.

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