

Ion Dynamics in Solid Electrolytes: Li^+ , Na^+ , O^{2-} , H^+

Sylvio Indris

Institut für Angewandte Materialien – Energiespeichersysteme (IAM-ESS), Karlsruher Institut für Technologie, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

E-Mail: sylvio.indris@kit.edu

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.

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. The local and long-range structures are investigated by multi-nuclear MAS NMR spectroscopy in combination with Mössbauer spectroscopy and diffraction techniques [1, 2].

Discontinuously generated forms of energy, *e.g.*, wind and solar energy, have to be stored in even larger energy storage systems. Na-ion batteries might offer less expensive solutions for these large systems due to the very high abundance of Na in the earth's surface and in the sea. Na-ion conductors with NASICON-type structure are investigated by ^{23}Na NMR relaxometry (Fig. 1) [3]. Furthermore, oxygen and proton conductors can be used as electrolytes in SOFC and PEM fuel cell systems. Ta-doped CeO_2 and PBA based electrolytes are investigated by ^{17}O and ^1H NMR spectroscopy/relaxometry, respectively [4].

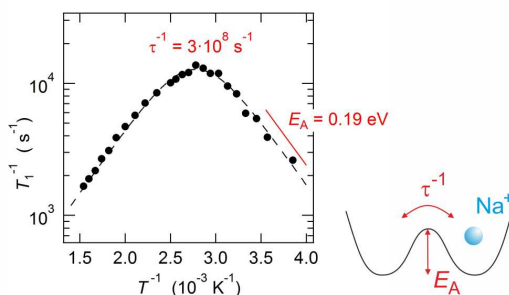


Figure 1: ^{23}Na NMR spin-lattice relaxation rates T_1^{-1} versus inverse temperature for $\text{Na}_{3.4}\text{Sc}_2(\text{SiO}_4)_{0.4}(\text{PO}_4)_{2.6}$ and the microscopic diffusion parameters deduced from this temperature dependence.

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- [2] Local Structural Investigations, Defect Formation, and Ionic Conductivity of the Lithium Ionic Conductor $\text{Li}_4\text{P}_2\text{S}_6$, C. Dietrich, M. Sadowski, S. Siculo, D. A. Weber, S. J. Sedlmaier, K. S. Weldert, S. Indris, K. Albe, J. Janek, W. G. Zeier, Chem. Mater. 28 (2016) 8764.
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- [4] Observing Local Oxygen Interstitial Diffusion in Donor-Doped Ceria by ^{17}O NMR Relaxometry, R. Heinzmann, I. Issac, J.-P. Eufinger, G. Ulbrich, M. Lerch, J. Janek, S. Indris, J. Phys. Chem. C 120 (2016) 8568.