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Solid State Ion-dynamics in Materials for Future Energy Devices

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One of the most important scientific problems to solve for our modern society is how to convert and store clean energy. In order to accomplish a paradigm shift in this field we need to understand the fundamental dynamical processes that govern the transfer of energy on an atomic scale. For future energy devices like solid-state batteries (SSB) as well as solid-oxide fuel cells (SOFC) this means understanding and controlling the complex mechanisms of ion diffusion in solid matter. Only recently, developments of state-of-the-art large scale experimental facilities e.g. neutron/muon spallation sources as well as free electron lasers, have opened new possibilities for studying such intrinsic material properties in a straightforward manner.
Layered transition metal oxides (TMOs) have been extensively studied both for their correlated electronic properties (frustrated magnetism and superconductivity) as well as for energy applications e.g. Li-ion batteries or thermoelectrics. Recently these two fields have been unified under the framework of the layered NaxCoO2 family where Na-ion vacancy order as well as dynamics has been shown to tailor low-temperature magnetic and thermoelectric properties. In addition, room-temperature sodium batteries are currently receiving considerable attention since the available lithium reserves of our planet are very limited. In many ways the NaxCoO2 compound is the Na-analog of the most common Li-ion battery electrode LixCoO2. Hence, understanding Na-ion diffusion mechanisms of NaxCoO2 would seem a logical first step. Consequently, we have conducted systematic studies of this compound using neutron powder diffraction (NPD) [1], quasi-elastic neutron scattering (QENS) [2] and muon spin relaxation/rotation (μSR) [3-4] as a function of temperature as well as Na-content (x) and pressure [5].
In this talk I will show how our use of neutron scattering and μSR has established a novel and detailed insight into the ion diffusion mechanisms in this group of compounds. Further, such knowledge now allows us to contemplate and actively consider future possibilities for tuning fundamental physical properties as well as solid state engineering of energy related materials with improved functional properties.

REFERENCES
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