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Na+ diffusion in Na-ion battery materials investigated by neutron diffraction

Batteries are playing prominent role in energy storage technology, both for portable devices and large-scale stationary storage. Presently, most battery technologies are based on diffusion of light Li-ions between the host materials at the anode and the cathode. Given the scarcity and the increasing price of lithium, cheaper and more abundant sodium, that has close chemistry but bigger in size, is emerging as alternative at least for use in large-scale high-energy batteries that are needed to achieve sustainable energy development.
The main goal of this work is to investigate the Na+ diffusion in layered oxide NaxCoO2. This material is the Na-analogue of LixCoO2, one of the most popular cathode materials in mobile and laptop batteries. The results of the work are supposed to shed light upon ionic diffusion in Na cobaltites, help to understand the relationship between Na-vacancy order and Na dynamics in NaxCoO2. Furthermore, fundamental principles of ion-diffusion could further open the way to design tailored energy materials with improved functional performance.
Keywords: Sodium-Ion Batteries, Cathode materials, Na+ diffusion, Neutron diffraction
The project is being realized at PSI under the supervision of Dr. Marisa Medarde (Group Physical Properties of Materials) and Dr. Claire Villevieille (Battery Materials Group). The detailed work plan is listed below:
- Synthesis of the layered oxide NaxCoO2 with x = 0.72 and 0.66;
- Investigation of the Na+ diffusion using neutron diffraction. The experiments are performed at the neutron diffractometer HRPT (SINQ);
- Data analysis: to determine the changes in the structure and the diffusion paths of Na+ ions for each composition as a function of temperature the set of programs FullProf Suite is used;
- Electrochemical assessment of cobaltites'performance and it comparison with NaFeO2 and NaFe1/2Co1/2O2 is going to be carried out with the collaboration of University of Montpellier.

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