Neutron PDF Technique and Its Application to Battery Materials

This technique consists of determining the correlations between pairs of atoms in the system under study. Specifically, the goal is to obtain the pair distribution function (PDF), which is a measure of the probability of finding a pair of particles at a given distance. Unlike diffraction, which reflects the average atomic order, this technique provides information about local order. Therefore, its field of application is primarily the study of the structure of disordered systems, such as liquids and amorphous materials, but it also extends to systems with long-range disorder, such as nanoparticles. This technique, also known as total scattering, can use different probes, such as photons or neutrons. In the case of neutrons, light elements like Li, a fundamental component of batteries, can be distinguished even when immersed in a matrix of heavier elements. Particularly for Li, isotopic substitution can be used to study the order around this ion in more detail. Isotopic substitution is a technique related to X-ray EXAFS.
In this lecture, the neutron PDF technique, the instruments where experiments are conducted, and basic data manipulation to obtain structure factors and correlation functions in real space will be presented. Finally, examples of materials used in battery electrodes will be shown.

Biography

Gabriel Cuello graduated with a degree in Physics from the National University of Córdoba (Argentina) and obtained his PhD in Neutron Physics at the Balseiro Institute of the National University of Cuyo in Bariloche (Argentina). In the late 90s, he completed a postdoctoral fellowship at the CSIC's Institute of Materials Science in Madrid, and after a brief return to Argentina as a CONICET researcher, he has spent 25 years working as an instrument scientist at the ILL, in charge of the diffractometer dedicated to the PDF technique. In 2009, he spent a sabbatical year at the University of the Basque Country as an Ikerbasque researcher.