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Combinatorial Approach for solving complex structures from low resolution data

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Crystal structure solution from diffraction experiments is an essential step in materials science, chemistry, physics and geology. Unfortunately, numerous factors render this process in some cases quite complex. Experimental conditions, such as high pressure or poor crystallinity, often complicate characterization. Furthermore, many applied materials such as batteries and/or energy storage materials, contain light elements such as Li and H that only weakly scatter X-rays. In that case a combined X-ray /neutron analysis is required. Moreover, the quality of charge-discharge cycling of these materials is at the cost of the crystallinity which brings more complexity to have a good level of understanding of the cycling process. Similar issues could also be raised for the analysis of some minerals which possess numerous phases which could be eventually amorphous. Finally, structural refinements generally require significant human input and intuition, as they rely on good initial guesses for the target structure. To eliminate part of these guesses, we are supporting a more combinatorial approach which uses X-ray and Neutron scattering experiments but also theoretical tools such as DFT and/or Molecular dynamics calculations as well as data mining tools. This presentation will mainly focus on recent experiments performed on two different high intensity/medium resolution T-o-F neutron diffractometers at LANSCE: HIPPO (High Pressure Preferred Orientation) and HIPD (High Intensity Powder Diffractometer). Examples will be used to highlight the level of information which can be achieved using these combined strategies and how we can connect it to the physical properties.

Keywords: Neutron and X-Ray diffraction, Low resolution, Combinatorial approach