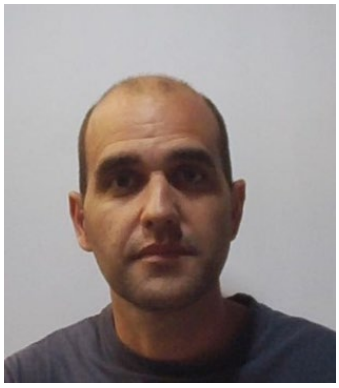
FullProfApp: an application for automating powder diffraction analysis with FullProf



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Abstract

In this talk we will present the FullProfApp, a software tool for conducting Rietveld refinements of powder diffraction data with minimal user intervention. FullProfApp is an easy way to introduce beginners to the use of FullProf, one of the world's most widely used software for diffraction data analysis. This talk will present the main features of the application: full-profile phase searches, sequential and high-throughput Rietveld refinements, background modelling, peak detection and user- interaction with crystallographic databases. We will illustrate the capabilities of the FullProfApp with a series of examples that will cover some potential use cases: i) a full-profile phase search to identify constituent phases from a pool of hundreds of candidates ii) several sequential refinements of powder diffraction data from electrochemical operando experiments with Li-ion and Na-ion solid state batteries.

Bio

Nebil A. Katcho has spent most of his scientific career in the field of molecular simulation applied to wide diversity of condensed matter physics problems. In the first part of his career (2004-2011), his work focused on structural modelling of disordered systems, ranging from liquids to amorphous solids to epitaxially strained nanostructures. These systems were modelled using both classical potentials and ab-initio approximations, depending on the nature of the problem, and studied experimentally using various diffractometric and spectroscopic techniques (EELS, GI-DAFS, X-ray and neutron diffraction). Subsequently, between 2011 and 2014 he worked at CEA-Grenoble on the theoretical quantification of the effect of point defects on the thermal conductivity of nanostructured materials with potential interest as thermoelectrics. Between 2014 and 2018 he worked at CIC-Energigune on the modelling of cathodes materials for Li and Na-ion batteries, focusing on the study phase transitions, the quantification of diffusion energy barriers and the determination of ion diffusion paths. Since 2018 he has been working at Institut Laue Langevin, developing software for single-crystal diffraction data

reduction, and developing the CrysFML08 crystallographic library which is intended to be the core of a completely new version of the FullProf suite.