Monday, 19th November 2018
12.00h CIC energiGUNE
Seminar room

Host:
Dr. Marine Reynaud

Seminar: "Examples of Complex Structural Modelling of Crystallographically Challenged Materials"

Speaker:
Dr. María Díaz López

From:
ISIS Neutron and Muon Source & Diamond Light Source, Didcot, United Kingdom

For a long time, the field of structural analysis has been partitioned into crystalline and amorphous materials, whose structures are well described by crystallography and local probes, respectively. However, new materials are being increasingly discovered that lie between these two extremes. This is the case of highly defective materials where the local structure does not follow the periodicity of the lattice, and nanostructured materials where the atomic ordering is only limited to a few nanometres. Traditional crystallography fails to describe these types of materials. Due to the complexity of these materials there are not generic analytical methods for their structural characterization. Instead, we have to design a structural solution strategy in a case by case basis.

During this presentation I will introduce two examples of complex structural modelling of Crystallographically challenged materials for energy applications. The first example will deal with the structural characterization of a novel oxide ionic conductor via a multi-technique approach were a model was proposed by Density Functional Theory that was then validated by high-resolution neutron powder diffraction and Nuclear Magnetic Resonance.

In the second example the structure of a novel nanostructured and highly disordered electrode material was elucidated by Neutron and X-ray total scattering data that were inputted in a global optimizer where constraints from other experiments (near-edge absorption spectroscopy) and theory were also taken into consideration.

Short biography

Present – PDRA in total scattering at POLARIS (ISIS) and I15-1 (Diamond)

Activities:

- New refinement strategies for complex structural modelling.

- RMCProfile software development
- Development of new set ups for the study of Li/Na ion batteries in operando XPDF.

2016-2018 Post-doc at Institut Neel Studying battery materials

2012-2016 PhD student at Matt Rosseinsky and John Claridge group at the University of Liverpool

BSc Chemistry at UPV-EHU Leioa