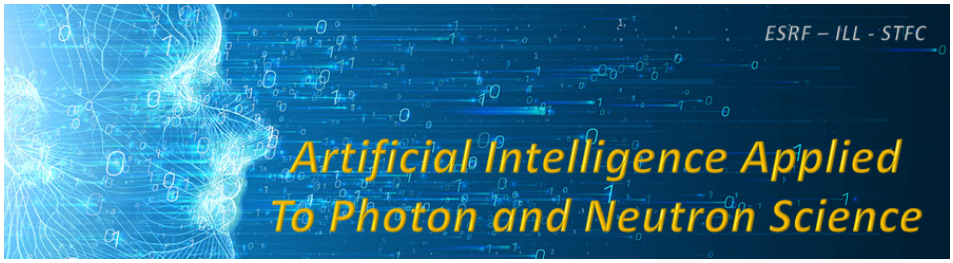

Contribution ID: **73** Type: **not specified**

PyFitit: the software for quantitative analysis of XANES spectra using machine-learning algorithms

Wednesday, 13 November 2019 12:15 (25 minutes)

X-ray absorption near-edge spectroscopy (XANES) is becoming an extremely popular tool for material science thanks to the development of new synchrotron radiation light sources. It provides information about charge state and local geometry around atoms of interest in operando and extreme conditions. However, in contrast to X-ray diffraction, a quantitative analysis of XANES spectra is rarely performed in the research papers. The reason must be found in the larger amount of time required for calculation of a single spectrum compared to a diffractogram. For such time-consuming calculations, in the space of several structural parameters, we developed an interpolation approach proposed originally by Smolentsev et al. The current version of this software, named PyFitIt, is a major upgrade version of FitIt and it is based on machine learning algorithms. We have chosen Jupyter Notebook framework to be friendly for users and at the same time being available for remastering. The analytical work is divided in two steps. First, the series of experimental spectra are analysed statistically and decomposed into principal components. Second, pure spectral profiles, recovered by principal components, are fitted by theoretical interpolated spectra. We implemented different schemes of choice of nodes for approximation and learning algorithms including Gradient Boosting of Random Trees, Radial Basis Functions and Neural Networks. The fitting procedure can be performed both for a XANES spectrum or for a difference spectrum, thus minimizing the systematic errors of theoretical simulations. The problem of several local minima is addressed in the framework of direct and indirect approaches.

Presenter: Dr GUDA, Alexander (The Smart Materials Research Institute, Southern Federal University)

Session Classification: Morning 2