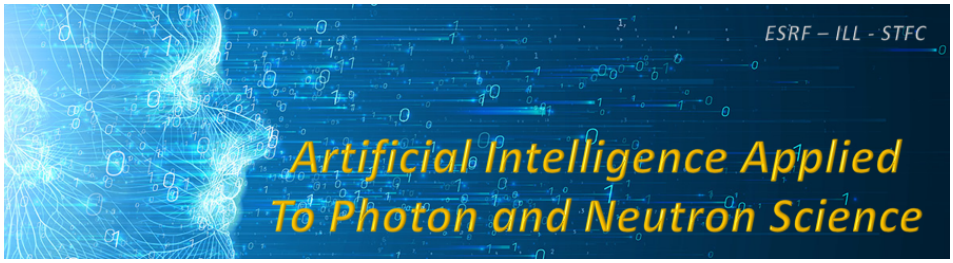


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# Machine Learning for Spectroscopy: From Spectra to Atomic Structures

*Thursday, 14 November 2019 11:25 (25 minutes)*

The vast majority of the scientific fields are currently experiencing the machine learning tsunami, as researchers try to exploit their unparallel ability to learn from data to give new insights and make fast predictions of target properties.

Spectroscopy using synchrotron radiation has also seen in recent years an increasing number of applications where machine learning techniques have been used to extract structural descriptors of materials from the experimental data.1,2 Most of these studies relied on supervised machine learning to train standard neural networks architectures. As the required amount of training data cannot be easily fulfilled using experimental measurements, the training sets are usually constructed using ab initio simulations. Using theoretical simulations allows to generate a large number of spectra corresponding to different structures, but this approach is not without its caveats. Also, the studies examine the application of machine learning to a limited subset of spectroscopic techniques.

In this contribution, I start by giving an overview of the different experiments performed at the ESRF's spectroscopy beamlines. Afterward, I will focus on the recent applications of machine learning in spectroscopy and discuss in more detail the use of theoretical simulations to train the artificial neural networks.

1 J. Timoshenko, D. Lu, Y. Lin, and A.I. Frenkel, J. Phys. Chem. Lett. 8, 5091 (2017).
2 A.A. Guda, S.A. Guda, K.A. Lomachenko, M.A. Soldatov, I.A. Pankin, A.V. Soldatov, L. Braglia, A.L. Bugaev, A. Martini, M. Signorile, E. Groppo, A. Piovano, E. Borfecchia, and C. Lamberti, Catal. Today 336, 3 (2019).

**Presenter:** Dr RETEGAN, Marius (ESRF)

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