Transforming the analysis of X-ray Absorption Spectra using Deep Neural Networks

Speaker: Tom Penfold (Newcastle University, UK))
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It is now possible for X-ray spectroscopy to deliver highly-detailed information about the local geometric, electronic and spin structure of matter in a broad range of different environments and under challenging operating conditions, e.g. in operando measurements of batteries and femtosecond time-resolved studies. However, to translate observation into scientific breakthroughs these experiments bring into focus a new challenge: How do we efficiently and accurately analyse these data to ensure that valuable quantitative information encoded in each spectrum can be extracted? In this presentation, I will discuss our recent work on supervised machine learning for X-ray absorption spectra through the development of a novel deep neural network (DNN). I show that we are able to estimate Fe K-edge X-ray absorption near-edge structure spectra in less than a second with no input beyond geometric information about the local environment of the absorption site. The performance of the DNN is promising, as illustrated by its application to the structural refinement of tris(bipyridine)iron(II) and nitrosylmyoglobin.