Machine Learning for X-ray Spectroscopy: Hero or Zero?

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Scientific breakthroughs are most commonly associated with developments in technology that enable the measurement of matter to an increased level of detail. A modern revolution, allowing more detailed insight into the structure of matter, is currently underway in X-ray spectroscopy (XS), driven by the transformative effects of next-generation, high-brilliance light sources. It is now possible for XS 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?

This increasingly demands detailed theoretical treatment to provide a firm link between the spectroscopic observables and the underlying structure and dynamics under study, but remains a far from trivial task. In this talk I will discuss our recent progress in using supervised machine-learning/deep learning algorithms to predict X-ray absorption near-edge structure spectra. Requiring only geometric information about the local environment of the absorption site, we demonstrate that we can predict peak positions with sub-eV accuracy and peak intensities with errors over an order of magnitude smaller than the spectral variations that the model is engineered to capture. The architecture will be discussed in detail and illustrated to applications over multiple absorption edges.

1. C. D. Rankine and T. J. Penfold *Accurate, affordable, and generalizable machine learning simulations of transition metal x-ray absorption spectra using the XANESNET deep neural network* J. Chem. Phys. 2022, **156**, 164102.
2. C. D. Rankine and T. J. Penfold *Progress in the theory of x-ray spectroscopy: From quantum chemistry to machine learning and ultrafast dynamics* J. Phys. Chem. A 2020, **125**, 4276-4293.