

A wavelet analysis for X-ray absorption spectra

T.J. Penfold,^{a,b,c} I. Tavernelli,^b U. Rothlisberger,^b R. Abela,^c M. Chergui^a

a) Laboratoire de spectroscopie ultrarapide, EPFL, CH-1015 Lausanne, CH.

b) Laboratoire de chimie et biochimie computationnelles, EPFL, CH-1015 Lausanne, CH.

c) SwissFEL, Paul Scherrer Inst, CH-5232 Villigen, CH.

X-ray absorption spectroscopy (XAS) is a powerful tool for the investigation of molecules in solution, but the complex origin of these spectra means that theoretical simulations are critical. Presently, calculations are most reliable when the photoelectron is not sensitive to the fine details of the atomic potential, i.e., in the EXAFS region which is the most attractive for local structural analysis. Here, the initial step in obtaining a qualitative description of the structure is achieved using a Fourier transform (FT) which yields a pseudo-radial distribution. However, for systems containing many scattering paths of different atomic species, and/or single and multiple scattering pathways which contribute to the same region of R -space, an unambiguous assignment of the peaks can be difficult.

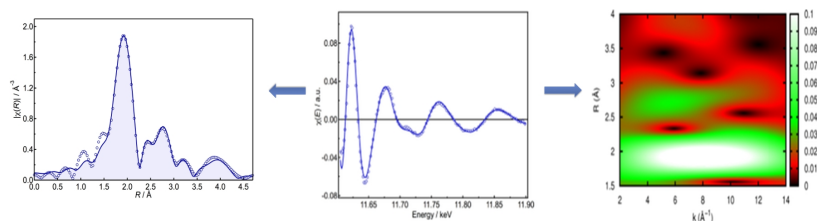


Figure 1: *Left*: A radial distribution function from the Fourier transform of an EXAFS signal (*center*) in contrast to the Wavelet transform approach (*right*).

Here I will present our recent development of a new analysis approach based upon Wavelet transform [1]. In contrast to the traditionally used FT approach, this analysis yields a 2D correlation plot in both R - and k -space (Fig. 1). As a consequence, it is possible to distinguish between different scattering pathways at the same distance from the absorbing atom and between the contributions of single and multiple scattering events, making an unambiguous assignment of the fine structure oscillations for complex systems possible. Following its introduction I will present some examples, for both static and time-resolved spectra before finally presenting a fitting scheme.

1. Penfold, T. *et al.*, *The Journal of Chemical Physics*, **138**, 014104 (2013)