Supplementary Information:

Soft X-Ray Spectroscopic Studies of the Electronic Structure of M-BiVO₄ (M = Mo, W) Single Crystals

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Supplementary Figure 1 – (a) Frequency Spectrum for a RIXS data of $BiVO_4$ recorded with a photon energy of 515.2 eV. (b) Example of an FIR LP filtered signal for the equivalent data set.

Alternative methods of Filtering and Data Analysis

It has also been demonstrated that filters based on different wavelets may be used to filter smooth chaotic signals from noise.¹ The following text describes this process for the same $BiVO_4 \ V \ L_3 \ RIXS$ spectrum ($hv = 515.2 \ eV$) used as an example for the FIR LP filter discussed in relation to Supplementary Fig. 1. In the filtering process, the first step involves converting the chaotic signal to wavelet domain and observation of its characteristics. Hard thresholding to zero is subsequently carried out on those parts of the signal which correspond to noise. Finally, the processed signal is converted back to its original form, demonstrating a possibility of filtering smooth chaotic signals.

Here we show that it is possible to use the wavelet filtering technique to successfully smooth the intensity signal by removing its noise components.¹ Firstly, the intensity signal is transformed to wavelet domain (Supplementary Fig. 2). Wavelet matrix rows 1-4, that is, bar graph columns of Supplementary Fig. 2, contained the fast varying noise component while rows 5-10 contained the slower varying signal component which we wish to extract and thus smooth the signal. We found that by hard thresholding rows 1-3 to zero and inverse transforming the wavelet matrix, the optimal smoothing of the intensity signal is obtained.¹ It was demonstrated that optimal noise filtering, or in our terminology signal smoothing, is achieved by using the Daubechies wavelet.¹ An advantage of using the described wavelet filter over an FIR filter is that the wavelet filter does not reduce the total number of samples of the original non filtered signal during the filtering process. Therefore, the technique may be useful in cases where only intensity signals of low number of samples are available.¹



Supplementary Figure 2 - Average power in each row of the wavelet matrix corresponding to the intensity signal.



Supplementary Figure 3 – Comparison of the FIR LP and Wavelet Filtering methods on a representative RIXS spectrum.



Supplementary Figure 4 – Representative V 2p core level XPS. The V 2p core level XPS for 0.3 at.% W:BiVO₄ is shown.

References

1. B. Jovic, *Synchronization techniques for chaotic communication systems*. Springer Science & Business Media: Auckland, New Zealand, 2011.