

Understanding Divergence In Modeling X-Ray Photoelectron Diffraction By Multiple Scattering Series Expansion

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X-Ray Photoelectron Diffraction (XPD) is a technique derived from X-ray photoemission, popularized in the 70s and 80s^[1]. Photoelectrons emitted by the sample act as a probe of their local environment and measuring them as a function of their escape direction can provide valuable information on the local structure with chemical resolution and with an extreme surface sensitivity.

Although a qualitative analysis of experimental data is possible, quantitative understanding of all the features of a diffraction pattern is only possible by comparing the observations with a model of the experiment^[2] based on multiple scattering theory (MST)^[3,4].

For photoelectrons in a typical 500-1500 eV energy range, the full multiple scattering calculation would require excessive computing resources but an approximation based on series expansion can make it feasible. We have however shown that the series expansion can diverge unexpectedly at certain kinetic energies. This is particularly true for complex oxide materials composed of heavy elements, which are currently being studied for their properties such as ferroelectricity, or for applications in photovoltaic devices (such as perovskites LaAlO₃, SrTiO₃...). This theoretical hurdle may precludes the use of MST to study these new materials, and thus limits the information we could obtain from electronic spectroscopy on a whole class of materials.

In this presentation, I will give a step-by-step overview of the origin of this divergence. Based on this analysis, I will show how a renormalized version of the series expansion can be optimized^[5] to finally make simulations converge.

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[4] <https://msspec.cnrs.fr>

[5] A. Takatsu, S. Tricot, P. Schieffer, K. Dunseath, M. Terao-Dunseath, K. Hatada & D. Sébilleau, *Phys. Chem. Chem. Phys.* **24**, 5658 (2022)