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Similarity Metric for Automated FDMNES Parameter Optimization for XANES Simulations

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Abstract

X-ray Absorption Near-Edge Spectroscopy (XANES) is a key technique for studying the local structure of an atomic specie in matter. The technique provides information about the oxidation state, coordination number, and electronic configuration. Traditionally, XANES spectra are compared with those coming from model compounds, a process known as fingerprint analysis. However, for a deeper understanding of the electronic structure and when the experimental reference spectra are not available, *ab initio* simulations are mandatory. A well-known real-space density functional theory code for simulating XAS spectra is FDMNES1. To get the best simulation, the typical workflow requires manually running many simulations and comparing them with experimental spectra as a function of the input atomistic model and the code parameters, until a good match is found. To automatize such workflow, a comparison metric between the experimental and simulated spectra is required. Traditional numerical comparison methods, like normalized mean square error (NMSE), often do not capture important spectral differences needed for precise matching. To address this problem, we use a feature-based similarity approach inspired by machine learning. This method identifies key points in the spectrum such as local peaks, and inflection points. These features are combined into a single similarity score that is more sensitive to meaningful spectral details than traditional error metrics by comparing differences in energy and amplitude. By using such metric, an automated pipeline has been built in order to optimize the FDMNES input parameters. We will present this method applied to a series of gold-based compounds with diverse chemical characteristics, enabling us to unravel and interpret the structural details underlying the experimentally obtained spectra.

References

[1] Bunau, O. & Joly, Y. (2009). *Self-consistent aspects of x-ray absorption calculations*. *J. Phys.: Condens. Matter*, 21, 345501 (20).

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