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Fine-tuning ab-initio XANES spectra calculations using the Bayesian Optimization algorithm.

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First-principle calculations of near-edge absorption spectra are widely used for experimental data analysis. Finding simulation parameters for the best match with experimental data may often be a challenge due to insufficient computational resources, ambiguous interpretation of spectral similarity criteria, or lack of expertise. When considering the simulation codes, such as FEFF or FDMNES as a black-box software, in which the output is defined as a similarity measure between the theoretical spectrum and experimental one, a Bayesian optimization technique can be applied to optimize the input configuration yielding the output most resembling the target spectra. We test this method on several experimental K-edge transmission spectra of Ni, Fe, and Pd metals, trying to find the best fits between the calculated and experimental XANES spectra using different similarity metrics such as L2 Normalized distance, cosine similarity, and correlation coefficients. The fitting process successfully converges to qualitatively and quantitatively match the resulting spectrum, with the parameter sets being reproducible within a certain margin. The test results show that this algorithm consumes, on average, three times fewer resources than the random search algorithm.

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