

















Lightshow: a Python package for generating computational x-ray absorption spectroscopy input files

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Summary

First-principles computational spectroscopy is a critical tool for interpreting experiment, performing structure refinement, and developing new physical understanding. Systematically setting up input files for different simulation codes and a diverse class of materials is a challenging task with a very high barrier-to-entry, given the complexities and nuances of each individual simulation package. This task is non-trivial even for experts in the electronic structure field and nearly formidable for non-expert researchers. Lightshow solves this problem by providing a uniform abstraction for writing computational x-ray spectroscopy input files for multiple popular codes, including FEFF, VASP, OCEAN, exciting and XSpectra. Its extendable framework will also allow the community to easily add new functions and to incorporate new simulation codes.

Statement of need

First-principles simulations explore materials and molecular properties of a system by solving fundamental quantum mechanical equations numerically. Thanks to their predictive nature, first-principles simulations provide fundamental understanding into the physical origins of various phenomena at the microscopic level, making them a powerful tool at the forefront of a wide range of scientific research fields, including physics, chemistry, materials science and biology. They are also critical to accelerating new materials design. In comparison to experiments, which can be expensive and time-consuming, *in silico* materials design frameworks can quickly screen the most promising candidates for target applications by running high-throughput calculations, allowing for a systematic down-sampling of the intractably large chemical space. The emergence of high-performance computing hardware architecture combined with the development of efficient structure search algorithms continues to fuel the advance of first-principles simulations in materials design.

Spectroscopy is an important experimental characterization technique that probes a sample based on the physics of light-matter interaction. Different types of spectroscopy can be classified by the energy range they probe, such as X-ray, ultraviolet-visible, and infrared spectroscopy. Lightshow currently focuses on writing the input files for one type: X-ray

absorption spectroscopy (XAS), in which a deeply bound core level electron is excited to empty states in the conduction bands. XAS is particularly useful because it is element-specific and very sensitive to the local chemical environment of the absorbing sites, such as coordination number, charge state, and local symmetry (De Groot & Kotani, 2008). It has been widely used in condensed matter physics, geophysics, chemistry, materials science and biology for materials characterization. Recent instrument development at synchrotron light sources further improves the spatial, temporal and energy resolution of XAS, which opens new avenues in XAS research.

Despite the growing demands for first-principles XAS spectroscopy, carrying out practical calculations correctly is far from trivial and requires a great deal of expertise in electronic structure theory, creating a formidable barrier for non-expert researchers. Most of the practical challenges boil down to the proper choice of input parameters, which depends on the level of theory, details of the implementation of the simulation software, and the atomic structure of the system. A general purpose software package for generating XAS simulation input files for multiple codes does not exist. Lightshow has been developed to fill this gap. It provides not only sets of default input parameters based on a careful multi-code XAS benchmark project (Meng et al., 2023), but also exposes the entire suite of possible parameter choices to expert users to tune. Our goal is to provide an easy-to-use tool to the XAS community (for both newcomers and experts) for XAS simulation and analysis. This tool will also help to improve the data consistency and data reproducibility in the computational x-ray spectroscopy field, which are essential to data-driven applications.

Brief software description

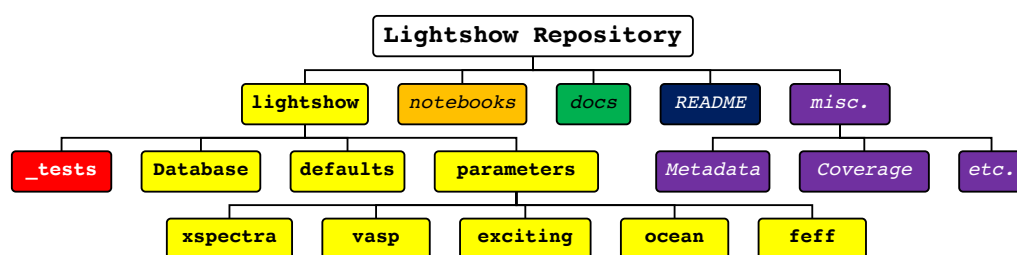


Figure 1: Graphical representation of the organization of the Lightshow repository.

We summarize the structure of Lightshow's application programming interface (API) in Figure 1. Lightshow's core design philosophy is built around two principal objects: the Database class and the _BaseParameters class. At a high level, the Database class interfaces primarily with Pymatgen and the Materials Project (Jain et al., 2011, 2013), allowing the user to easily utilize Pymatgen and pull a large number of materials structures quickly. Functionality is also available for instantiating a Database via loading, e.g., POSCAR-style structure files from local storage. Once a database has been created, code-specific simulation parameters inheriting the _BaseParameters base class interface with various methods in Pymatgen as well as in-house built software for systematically writing input files for multiple XAS simulation programs, including FEFF (Kas et al., 2021; Rehr et al., 2010), XSpectra (Bunău & Calandra, 2013; Gougoussis et al., 2009; Taillefumier et al., 2002), OCEAN (Vinson et al., 2011; Vinson, 2022), exciting (Vorwerk et al., 2019) and VASP (Karsai et al., 2018). We highlight the _tests directory, in which we maintain a suite of unit tests for individual functions and methods, as well as integration tests for the entire workflow. Lightshow is fully documented, and contains a simple example notebook for users to get started. Finally, we also note that Lightshow is designed to be part of larger workflows (including perhaps systematic comparison to experiment) in which users wish to abstract away the complicated and tedious task of generating input

files. Future work on the code will include designing modules for pre- and post-processing, allowing for more seamless integration into said workflows.

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Certain software is identified in this paper for clarity. Such identification is not intended to imply recommendation or endorsement by NIST, nor is it intended to imply that the materials or equipment identified are necessarily the best available for the purpose.

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