Construction of XASDB

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Introduction

- X-ray Absorption Spectroscopy (XAS) involves the fingerprint features of the interested atom, is used in the characterization of sample for the local geometric and electronic structure at atomic scale, including bond lengths, coordination numbers, valence state, etc.
- The XAS database serves as a repository of experimental spectra for standards whose geometric structures are known, provides the possibility for users to find the spectra with absorber interested, to compare spectra with same absorbers, to judge or determine the spectrum line as features during the data analysis.
- The XAS database also provides the possibility for XAS data analysis based on machine learning(ML), where the experimental data can be used in the assessment of the ML model performance. A repository for the simulated XAS data designed in the plan will promote the application of our database into the online data analysis at synchrotron radiation beamlines by constructing the generalized ML models in the simulation of XAS for the interested elements.
- The XAS database provides sufficient toolkits for common XAS data treatments, including data normalization, background removal, Fourier transformation, principal component analysis, linear combination fit. A XASMATCH package helps user to find the most similar spectra in the database to the input spectroscopy line, which are listed with the coincidence scores.

Methods

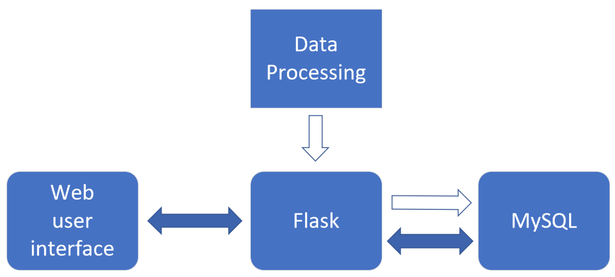

Figure 1: Database framework diagram.

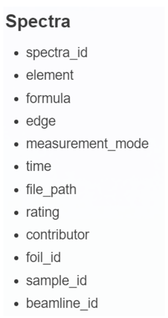

Figure 2: Table structure design diagram for MySQL database.

XASMatch is designed to identify the absorption spectrum within the database that exhibits the highest degree of similarity to the user-input spectrum line, providing detailed and specific information about the identified absorption spectrum.

- Integrate multiple matching algorithms
- Integrate three energy shift processing methods

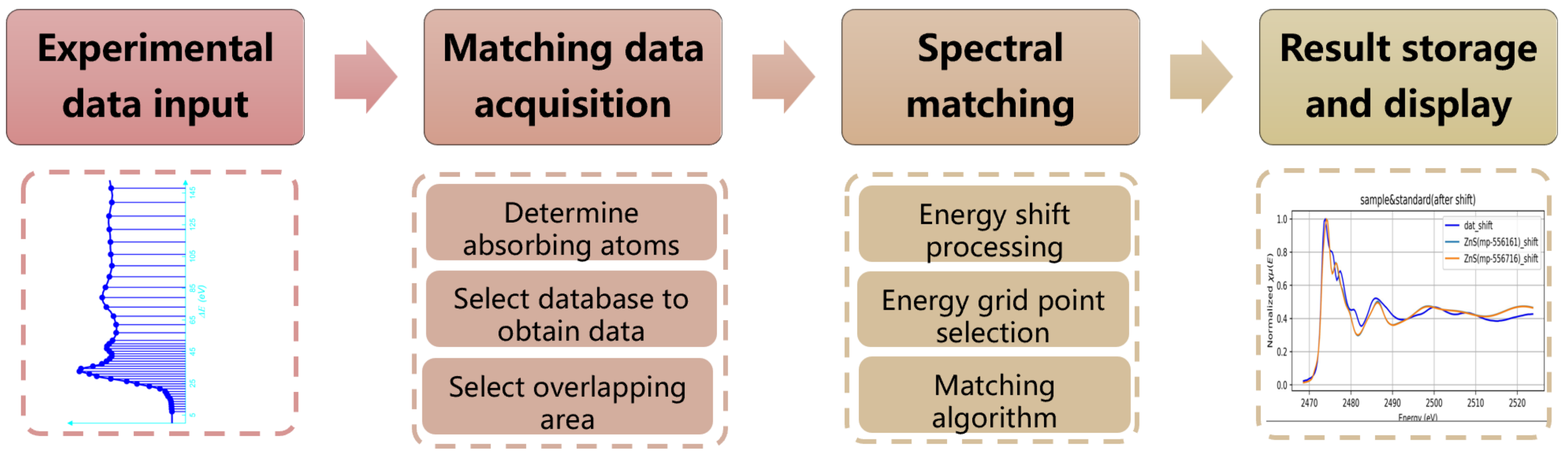

Figure 3: Technical roadmap for spectral matching function diagram.

Database Website - features

Website: http://xasdb.ihep.ac.cn/

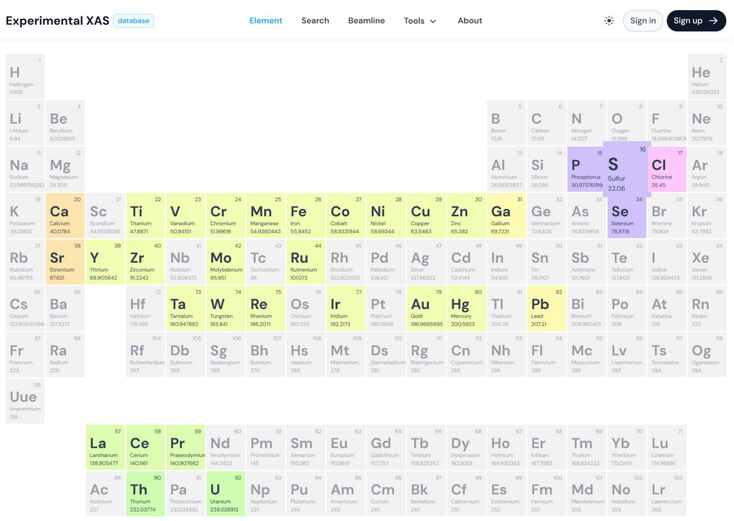

Figure 4: Database website homepage.

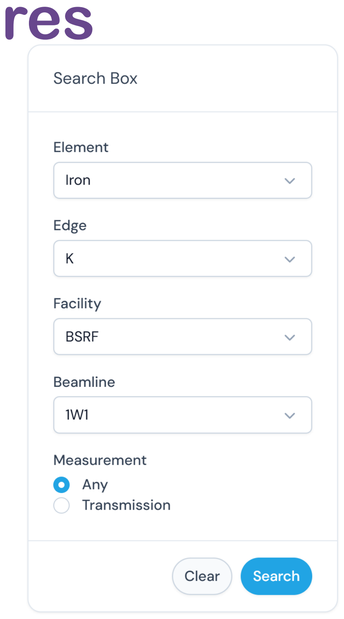

Figure 5: Compound search box.

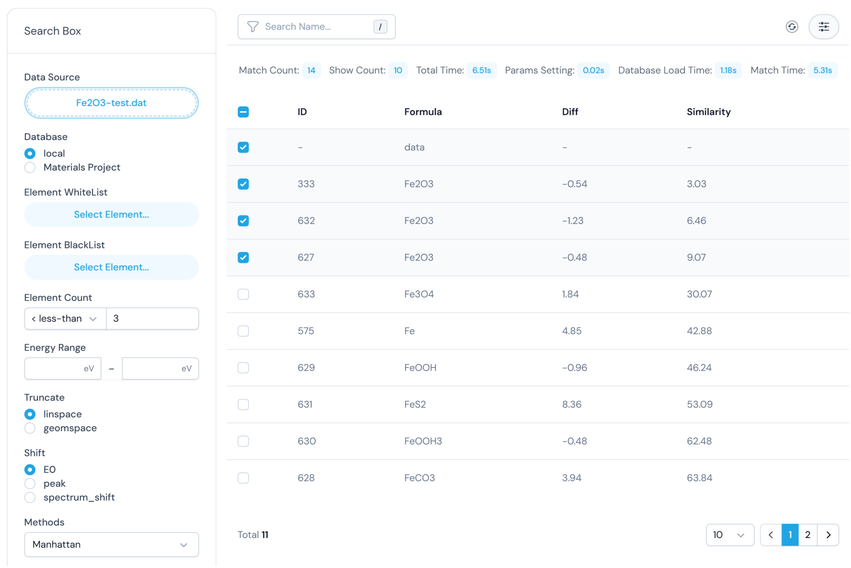

Figure 6: XASMatch function display.

Figure 7: Absorption spectra visualization function display diagram. Users can select multiple absorption spectra for comparison at the same time, and can choose Autoback or Mback method to normalize the absorption spectra. We provide the display of pre_edge and post_edge functions, as well as the offset function.

Conclusions

- Up to July, 2024, there are 154 spectra for 32 elements in the repository, including 131 with K-edge, 23 with L-edge.
- More spectra for other elements will be measured in Beijing Synchrotron Radiation Facility(BSRF) and High Energy Photon Source(HEPS) and included in our base, which will benefit for the construction of ML models for XAS data analysis.
- We hope our work will benefit the XAS community.

Acknowledgement

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