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Atom local environment student research project using Synchrotron X-Ray absorption with training based on open access databases for materials science

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***Abstract*—This Atom local environment using Synchrotron X-Ray absorption data provides important information for energy device design in materials engineering and the study of Carbon Cyle in life. A student research project can focus on EXAFS and XANES data analysis, upon completion of data collection by the professors in the National Synchrotron Radiation Facilities such as Brookhaven National Lab, Cornell Storage Ring, etc. A community college student's necessity of working part time to support food and rent could conflict with an approved synchrotron radiation beamline schedule. A toy model of a spectroscopy lab is deployed to simulate the missing data collection experience at the national synchrotron radiation facilities in student research. The recent release of open-access synchrotron radiation experiment databases for materials science enabled the repeated practice of analysis skill with many types of samples. In particular, the pre-edge data analysis practice using the open-access databases was found to be most beneficial in student research. The results of Fe and Zn local environment research projects of several types of samples are presented and discussed. A synchrotron radiation project has rich content for students to learn about the structure of a start-up research company. A project with students can be implemented via micro-internships in the learning of entrepreneurship. The company divisions could consist of sample preparation, spectroscopy instrumentation, data science, interpretation, billing, and reporting to clients. The sustainability aspect is discussed in terms of future synchrotron radiation projects in a start-up tech company and student career training in materials science and engineering, instrumentation, and AI-assisted data science.**

Keywords— Synchrotron X-Ray absorption data; open-access databases;, career training; AI-assisted tools

I. INTRODUCTION

Atom local environment using Synchrotron X-Ray absorption data provides important information for energy device design in materials engineering and the study of Carbon Cyle in life. Advances in material engineering using Synchrotron Radiation include cathode design application [1], and other applications described in two recent reviews [2, 3]. The key enzyme in the Wood-Ljungdahl pathway, the only known carbon fixation pathway that produces a net gain pf ATP, acetyl-CoA synthase (ACS) contains four iron and two nickel atoms. The full structure was solved using the Stanford Synchrotron Radiation Lightsource in 2021 [4]. The energy science and life science research projects are the two most popular topics for our engineering students in terms of career development.

II. IMPLEMENTATION

A student research project can focus on Synchrotron Radiation EXAFS and XANES data analysis, upon completion of data collection by the professors in the National Synchrotron Radiation Facilities such as Brookhaven National Lab, Cornell Storage Ring, etc. A community college student's necessity of working part time to support food and rent could conflict with an approved synchrotron radiation beamline schedule. A toy model of a spectroscopy lab is deployed to simulate the missing data collection experience at the national synchrotron radiation facilities in student research. Light sources such as dye lasers pumped by nitrogen lasers offer oscilloscope data collection experience. A spectrometer from 450 nm to 700 nm offers visible alignment experience.

III. SPECTROSCOPY DATA ANALYSIS

The recent release of open-access synchrotron radiation experiment databases for materials science enabled the repeated practice of analysis skill with many types of samples [5]. The Ritsumeikan SR Center Soft X-Ray XAFS Database of Japan offered the best resource in our experienced [6]. In particular, the pre-edge data analysis practice using the open-access database was found to be most beneficial in student research. The results of Fe local environment study of different regions of a carrot plant indicate that the amount of iron and immediate environment is different in different regions.

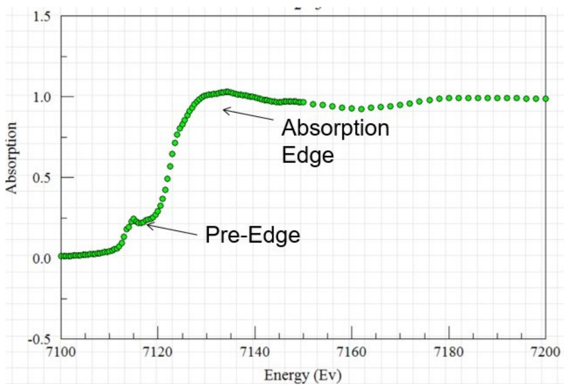
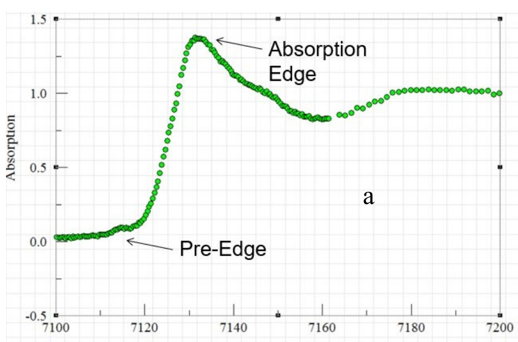


Fig1:X ray absorption near edge spectrum of iron oxide Fe_2O_3.

The small absorption peak, as shown in Fig 1, before the main absorption edge is known as pre-edge. This feature is due to 1s to 3d transition of electrons in iron atoms. This transition is known as forbidden under selection rules but becomes allowed when the iron atoms are bonded to oxygen atoms due to mixing of iron 3d and oxygen 2p orbitals. Therefore, pre-edge appears on Fe-O compounds. The main absorption edge intensity depends on the total amount of iron and pre-edge is only due to irons bonded to oxygen atoms. In the case of Fe_2O_3 all iron atoms are surrounded by oxygen atoms, and they are in octahedral co-ordination. Therefore, we can use this spectrum in iron oxide as a standard to compare unknown samples. X ray absorption near edge spectra of different regions of a carrot plant are shown in the Fig 2.



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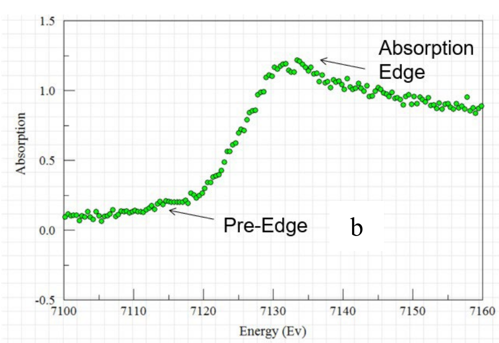

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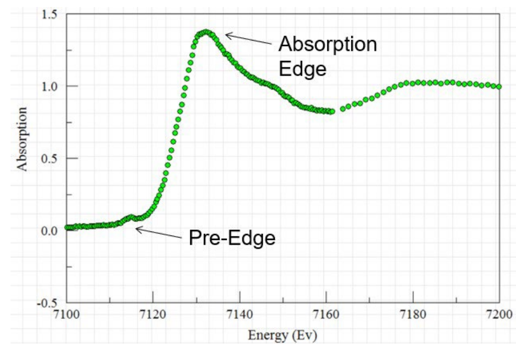

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Fig 2: X ray absorption near edge spectra of (a)-carrot leaf (b)- stem (c)- root

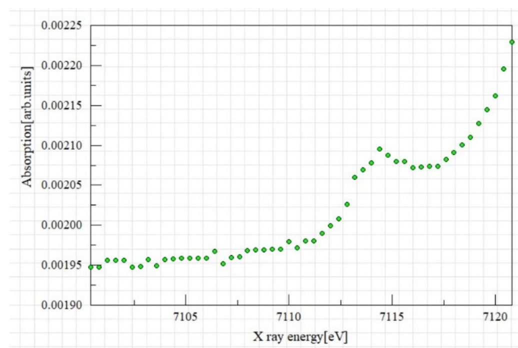

Fig. 3: X-ray absorption pre-edge isolated from X ray absorption spectrum.

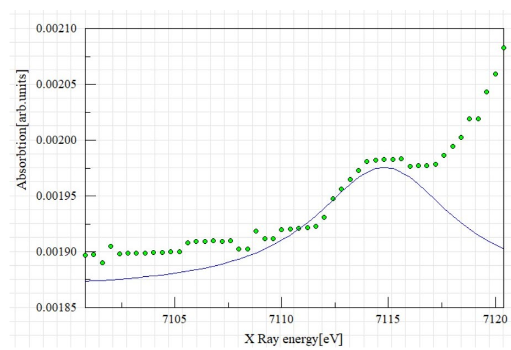

Fig. 4: X ray absorption pre-edge and Lorentzian fit to the pre edge.

From these spectra only the pre-edge regions were extracted, for an example Fig 3, and Lorentzian functions were fitted to pre-edge peak (Fig 4). Then the intensities of Lorentzian were normalized to the height of main absorption edge intensity. If all iron atoms of samples were surrounded by oxygen atoms, these normalized pre edge intensities should be the same. But as shown in the table 1, normalized pre edge intensities of different regions of the carrot plant are slightly different. It appears that the stem region has highest amount of iron atoms surrounded by oxygen atoms. Main edge intensity indicates that carrot leaf has the lowest amount of iron. Also normalized pr edge intensity indicates that the iron in carrot root has the smallest percentage (7.4%) of oxygen atoms as near neighbor atom.

Sample	Main edge Intensity	Pre-Edge intensity	Normalized pre edge Intensity	% of iron surrounded by oxygen
Iron oxide	92	24	0.2609	100
Carrot leaf	1.5	0.049	0.0327	12.5
Carrot stem	1.69	0.069	0.0408	15.6
Carrot root	1.79	0.0346	0.0193	7.4

Table 1: X ray absorption near edge and pre edge results of different parts of a carrot plant.

IV. Career Training

A synchrotron radiation project has rich content for students to learn about the structure of a start-up research company. A project with students can be implemented via micro-internships in the learning of entrepreneurship. The company divisions could consist of sample preparation, spectroscopy instrumentation, data science, interpretation of analysis results, cost and billing, and reporting to clients. A minimum of two professors would be needed. A professor serves as the CEO of the start-up company and another professor serves as the representative of a client company. AI-assisted writing is used to enhance reporting.

IV Sustainability

The sustainability issue is fulfilled by the need of using Synchrotron Radiation data in materials science and engineering, as described in the introduction section. With a campus location in New York City, the Brookhaven and Cornell Synchrotron Radiation Facilities are within driving distance for continuous data collection.
The advances in AI diffusion model in text to image technology have helped Microsoft to develop MatterGen to predict inorganic compounds with targeted properties [7]. The MatterGen prediction results necessitate the use of instrumentation tools such as synchrotron radiation spectroscopy to access the local atomic environment. For instance, the high magnetic energy density and low risk supply chain criteria were modeled by MatterGen, with the local impurity issue of Fe as an important fabrication issue that can be solved with Synchrotron Radiation data.

V DISCUSSION

The student research projects using Synchrotron Radiation data complement the computational experience in Microsoft MatterGen products and other AI-assisted products such as Google AlphaFold protein products. On the one hand, our campus can only run simple AI models as demonstrations. On the other hand, we can go to Brookhaven and Cornell to conduct first-rate Synchrotron Radiation data collection and analysis to upkeep the student research projects as first-rate with some computational experience in AI-assisted models in material designs. The training in the Synchrotron Radiation student research projects with world-class Synchrotron Radiation databases would provide R-1 university authentic experience in our pedagogy.

CONCLUSIONS

Synchrotron Radiation X-Ray absorption data collection and analysis is a world-class analytical tool and a marker of an activity of R-1 university. Coupled with an understanding of AI-assisted tools such as Microsoft MatterGen, students will be fully engaged in career training related to materials science and engineering

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