Summary of June 26, 2007 XAFS SIG Meeting

Present: Steve Heald, Nadia Leyarovska, Matt Newville, Robert Gordon, Shelly Kelly, Bruce Ravel, Julie Cross, Qing Ma.

Agenda

Thai lunch
Review applications for 2007 APS XAFS Summer School

1. All 35 applicants will be invited to participate.

As of the application deadline, the XAFS School received 35 applications. After a lively discussion, it was decided that because of the high level of experience of several applicants, the beamlines could accommodate seven students each. Therefore, the meeting proceded under the assumption that there could be as many as 35 students.

2. Students were tentatively assigned to beamlines.

Based on the information given in the application, Bruce Ravel grouped students by photon energy and research field. These groups were then assigned to beamlines, subject to final approval by the responsible beamline scientists.

Please look over these tables today, and call Julie at 2-0592 no later than COB tomorrow (6/28/07) if you see any obvious problems. The student data spread sheets and complete application information are attached to this meeting summary.

5-BM-D "High Energy"

Application #	Last Name	Fist Name	APS Badge #	Element	Level	Advisor	Field
1	Li	Wei	67521	?	Grad Student	Lane	Catalysis
3	Washington	Joseph	68937	Ge, Sb, Te	Grad Student	Paesler	Materials
9	Fox	Elise	81146	Pd, Rh	Government	n/a	Catalysis
15	Simonetti	Dante	81427	Pt, Re	Grad Student	Dumesic	Catalysis
19	Fawcett	Skya	69726	Sb	Grad Student	Jamieson	Geo/Enviro
30	Sanchez	Sergio	80989	Pt, Ru, Rh	Grad Student	Nuzzo	Chemistry
31	Zanella	Luciana	69509	Cr	Grad Student	Gaillard	Geo/Enviro

9-BM "Low Energy"

Application #	Last Name	Fist Name	APS Badge #	Element	Level	Advisor	Field
6	Murphy	Michael	68042	Zn	Grad Student	Sham	Chemistry
7	Ko	Peter	68041	?	Grad Student	Sham	Materials
16	Morris	Eric	81447	S	Grad Student	Jia	Geo/Enviro
20	Cai	Jenny	81487	S	Grad Student	Jia	Geo/Enviro
24	Fedor	Jan	55119	Co, Nb, Se	Post Doc	Iavarone	Materials
25	Merchan	Gregory	81600	all	Academic	n/a	Physics

10-ID "Platinum Beamline"

Application #	Last Name	Fist Name	APS Badge #	Element	Level	Advisor	Field
10	Setthapun	Worajit	57644	Pt, Pd	Post Doc	Marshall	Catalysis
13	Kunkes	Eduard		Pt, Re	Grad Student	Dumesic	Chemistry
14	Greenlay	Nan	67494	?	Industry	n/a	Catalysis
23	Beswick	Colin	81574	Novice	Industry	n/a	Catalysis
26	Guo	Neng	57950	Pt, Pd	Post Doc	Marshall	Catalysis
29	Nelson	Ryan		Pt	Post Doc	Scott	Catalysis
35	Lockard	Jenny		Pt, Fe	Post Doc	Wasielewski	Chemistry

12-BM "As/Zn/Ge and W"

Application #	Last Name	Fist Name	APS Badge #	Element	Level	Advisor	Field
2	Hayes	Sarah	67939	Pb, Zn	Grad Student	Chorover	Geo/Enviro
11	Moriarty	Maeve	69554	As	Grad Student	Reimer	
17	Liu	Yu-Ting	81448	As	Grad Student	Hesterberg	Geo/Enviro
21	Rekhi	Sandeep	87295		Academic	Chance	Bio/Biophys
22	Smith	Paula	63537	As	Grad Student	Reimer	Bio/Biophys
28	Zuzaan	Damdinsuren		As, Pb	Grad Student	Kersten	Geo/Enviro
33	Henderson	Eric	81511	Ge, Si, F, S	Grad Student	Veinot	Chemistry
34	Hessel	Colin	81472	Si, O, F	Grad Student	Veinot	Chemistry

20-BM "Fe/Re and W"

Application #	Last Name	Fist Name	APS Badge #	Element	Level	Advisor	Field
4	Mekki	Soufiane	68937	Lanthanides	Post Doc	Nagy	Geo/Enviro
5	Behrends	Thilo	81583	Fe	Academic	n/a	Geo/Enviro
8	Diallo	Mamadou	68992	Fe, Cu, Ag	Academic	n/a	Geo/Enviro
12	Johnson	Jacqueline	48925	Gd, Lanthanides	Government	n/a	Materials
18	Zelasko	Amanda	81446	Fe	Grad Student	Hesterberg	Geo/Enviro
27	Anastacio	Alexandre	81613	Fe, Cr	Post Doc	Stucki	Geo/Enviro
32	Quinn	Kelly	69635	Fe, Y	Post Doc	Byrne	Geo/Enviro

2007 APS XAFS School
Applicant Data

Last Modified 6/27/07

Application No.	Last Name	First Name	APS Badge No.	Institution	Department	Tuition	APS User	Position	Advisor	Research Field	Notification	Confirmation	Payment	Housing	User Orientation	GERT	ESH100U	ESH223 (Cybersecurity)	ESH377 (Electrical Safety)	Sector Orientation
1	Li	Wei	67521	University of Alabama, Tuscaloosa	Chemical and Biological Engineering	375	YES	Graduate Student	Dr. Alan Lane	Catalysis					√	√	√		√	10
2	Hayes	Sarah	67939	University of Arizona	Soil, Water and Environmental Science	375	YES	Graduate Student	Dr. Jon Chorover	Geology / Environmental Science					√	√	√			13
3	Washington	Joseph	68937	North Carolina State University	Physics	375	YES	Graduate Student	Dr. Michael Paesler	Materials Science					√	√	√		√	10
4	Mekki	Soufiane	68937	University of Illinois, Chicago	Earth and environmental Sciences	375	YES	Post-Doctoral Fellow	Dr. Kathryn Nagy	Geology / Environmental Science					√	√	√	√	√	
5	Behrends	Thilo	81583	Utrecht University	Earth Sciences	375	NO	Scientist, Academia	n/a	Geology / Environmental Science	√	√								
6	Murphy	Michael	68042	University of Western Ontario	Chemistry	375	YES	Graduate Student	T. K. Sham	Chemistry					√	√	√		√	20
7	Ko	Jun Young Peter	68041	University of Western Ontario	Chemistry	375	YES	Graduate Student	T. K. Sham	Materials Science					√	√	√	√	√	20
8	Diallo	Mamadou	68992	California Institute of Technology	Chemistry and Chemical Engineering	375	NO	Scientist, Academia	n/a	Geology / Environmental Science										
9	Fox	Elise	81146	Savannah River National Laboratory	Materials Science and Technology	375	YES	Scientist, Government	n/a	Catalysis										
10	Setthapun	Worajit	57644	Argonne National Laboratory	Chemical Engineering Division (CMT)	98	YES	Post-Doctoral Fellow	Dr. Christopher Marshall	Catalysis					√	√	√	√	√	
11	Moriarty	Maeve	69554	Royal Military College of Canada	Chemistry	376	YES	Graduate Student	Dr. Ken Reimer	Choose One					√	√	√	√	√	20
12	Johnson	Jacqueline	48925	Argonne National Laboratory	Nuclear Engineering	98	YES	Scientist, Government	n/a	Materials Science						√	√	√	√	5
13	Kunkes	Eduard		University of Wisconsin, Madison	Chemical Engineering	375	NO	Graduate Student	Dr. James A. Dumesic	Chemistry										
14	Greenlay	Nan	67494	UOP, LLC Honeywell	Advanced Characterization	375	YES	Scientist, Industry	n/a	Catalysis					√	√	√	√	√	33
~~15~~	~~Simonetti~~	~~Dante~~	~~81427~~	~~University of Wisconsin, Madison~~	~~Chemical and Biological Engineering~~	~~375~~	~~NO~~	~~Graduate Student~~	~~Dr. James A. Dumesic~~	~~Catalysis~~										
16	Morris	Eric	81447	University of Toronto	Chemical Engineering & Applied Chemistry	375	YES	Graduate Student	Dr. Charles Q. Jia	Geology / Environmental Science										
17	Liu	Yu-Ting	81448	North Carolina State University	Soil Science	375	NO	Graduate Student	Dr. Dean Hesterberg	Geology / Environmental Science										
18	Zelasko	Amanda	81446	North Carolina State University	Soil Science	375	YES	Graduate Student	Dr. Dean Hesterberg	Geology / Environmental Science										
19	Fawcett	Skya	69726	Queen's University	Geological Sciences and Geological Engineering	375	YES	Graduate Student	Dr. Heather Jamieson	Geology / Environmental Science					√	√	√	√	√	20
20	Cai	Hui (Jenny)	81487	University of Toronto	Chemical Engineering & Applied Chemistry	375	YES	Graduate Student	Dr. Charles Q. Jia	Geology / Environmental Science										
21	Rekhi	Sandeep	87295	Case Western Reserve University	Center for Proteomics and Mass Spectrometry	375	YES	Scientist, Academia	Dr. Mark Chance	Biology/Biophysics					√		√			
22	Smith	Paula	63537	Royal Military College of Canada	Environmental Sciences Group	375	YES	Graduate Student	Dr. Ken Reimer	Biology/Biophysics						√	√		√	√
23	Beswick	Colin	81574	ExxonMobil	EMPR	375	NO	Scientist, Industry	n/a	Catalysis										
24	Fedor	Jan	55119	Argonne National Laboratory	Materials Science Division	98	YES	Post-Doctoral Fellow	Maria Iavarone	Materials Science								√	√	
25	Merchan	Gregory	81600	Louisiana State University	CAMD	375	NO	Scientist, Academia	n/a	Physics										
26	Guo	Neng	57950	Argonne National Laboratory	Chemical Engineering	98	NO	Post-Doctoral Fellow	Dr. Christopher Marshall	Catalysis										
27	Anastacio	Alexandre	81613	University of Illinois at Urbana-Champagne	Natural Resources and Environmental Sciences	375	NO	Post-Doctoral Fellow	Dr. Joseph W. Stucki	Geology / Environmental Science										
28	Zuzaan	Damdinsuren		Johannes-Gutenberg University of Mainz	Institute of Geosciences	375	NO	Graduate Student	Dr. Michael Kersten	Geology / Environmental Science										
29	Nelson	Ryan		University of California, Santa Barbara	Chemical Engineering	375	NO	Post-Doctoral Fellow	Dr. Susannah Scott	Catalysis										
30	Sanchez	Sergio	80989	University of Illinois at Urbana-Champagne	Chemistry	375	YES	Graduate Student	Dr. Ralph Nuzzo	Chemistry					√	√	√	√	√	33
31	Zanella	Luciana	69509	Northwestern University	Civil and Environmental Engineering	375	YES	Graduate Student	Dr. Jean-François Gaillard	Geology / Environmental Science					√	√	√	√	√	5
32	Quinn	Kelly	69635	University of South Florida	College of Marine Sciences	375	YES	Post-Doctoral Fellow	Dr. Robert Byrne	Geology / Environmental Science					√	√	√	√	√	13
33	Henderson	Eric	81511	University of Alberta	Chemistry	375	YES	Graduate Student	Dr. Jon Veinot	Chemistry										
34	Hessel	Colin	81472	University of Alberta	Chemistry	375	YES	Graduate Student	Dr. Jon Veinot	Chemistry										
35	Lockard	Jenny		Northwestern University	Chemistry	375	NO	Post-Doctoral Fellow	Dr. Michael Wasielewski	Chemistry										
audit	Osborn	Ray	38323	Argonne National Laboratory	Materials Science Division	0	n/a	Scientist, Government	n/a	Materials Science					√	√	√	√	√	
audit	Iovarone	Maria		Argonne National Laboratory	Materials Science Division	0	n/a	Scientist, Government	n/a	Materials Science										

Date: May 7, 2007 9:12:22 AM CDT

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Institution: The University of Alabama, Tuscaloosa
Department: Department of Chemical and Biological Engineering
Position: Grad Student, years 1-2
Advisor: Dr Alan Lane
Research Field: Catalysis

XAFS/Synchrotron Experience: I have used XAFS to in-situ investigate the electrocatalysis for Direct methanol fuel cell in Prof. Eugene Smotkin group. I had planned to attend the 2005 summer school to learn how to analysis our data. However, I missed it because of the visa delay. Now I work with Dr Alan Lane on the durability of electrocatalysis for Proton Exchange Membrane Fuel Cell (PEMFC). We have strong cooperation with Dr Theodore Krause at ANL.

Durability is one of the most challenge barriers for PEMFC commercialization. There are hundreds of papers on the sintering degradation of the electrocatalyst durability in PEMFC. Most of them proved it with electrochemical methods and/or electron microscopy. Then they postulated the degradation mechanisms based on the results. However, there are no detail electrocatalyst structure change informations in the durability testing of PEMFC. XAFS can show what's going on about the electrocatalyst metals' atoms and chemical status during the degradation of PEMFC catalyst if we can set up an appropriate in situ experiment.

So I am really interested in this XAFS summer school. It is very important for my research and I think I can learn how to acquire and analysis the XAFS data. I also believe this experience will help me to design and improve our in situ PEMFC durability testing with XAFS. I am expecting it!

Date: May 7, 2007 12:23:56 PM CDT

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Institution: University of Arizona
Department: Soil, Water and Environmental Science
Position: Grad Student, years 1-2
Advisor: Jon Chorover
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: My research interest is on the effect of the rhizosphere on mineral transformations and metal bioavailability. Currently, I am studying the effects of phytostabilization on lead and zinc speciation in mine tailings. In this summer school, I anticipate building my theoretical understanding of EXAFS and obtaining assistance with the data that I have already accumulated from 4 trips to APS. I have also attended two O'Day group beamtimes at SSRL to gain experience.

Date: May 7, 2007 12:33:21 PM CDT

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Institution: North Carolina State University
Department: Physics
Position: Grad Student, years 1-2
Advisor: Michael Paesler
Research Field: Materials Science

XAFS/Synchrotron Experience: I am a current APS user. We predominantly use the MR-CAT ID10 to do EXAFS on Ge2Sb2Te5, as well as other variations of this material. It is a phase change memory material of considerable technological importance in DVD and phase change memory. In previous runs, I have used both transmission and floresence modes (depending on the sample) to analyze both crystalline and amorphous varitations of this sample from the Ge, Sb, and Te K edges.
I hope to gain a better understanding of the EXAFS technique from the summer school, so that I may gain enough confidence and familarity to run future experiments with limited supervision. I would also like to learn more about data interpretation, as well as the factors that can affect EXAFS spectra leading to better/worse results.

Date: May 8, 2007 10:06:08 AM CDT

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Department: Earth and environmental Sciences
Position: Post-Doctoral Fellow
Advisor: Kathryn Nagy
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: I experienced some collaboration in analyzing samples at the Synchrotron source of ESRF in France, Grenoble. I have a good background in understanding the technique with my master and PhD in radiochemistry (theoretical courses of EXAFS and XANES for actinide and lanthanide study). I would like to learn how to run a sample in an APS beam line. And then how to apply mathematical treatment of the raw data, and use EXAFS softwares, FEFF, etc... if possible.

Date: May 8, 2007 10:12:52 AM CDT

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Institution: Utrecht University
Department: Earth Sciences
Position: Scientist, Academia
Advisor:
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: My main research interests focus on redox transformations of metals in natural environments. In particular, I am interested in the role of microorganisms in redox reactions of metals and the interaction between biotic and abiotic reaction pathways. Projects along this research line include microbial induced iron mineral transformations, kinetics of bacterial reduction and oxidation of iron, and the effects of microbial activity on the mobility of uranium in subsurface systems.

In my research, improving the knowledge about speciation and redox states of metals became increasingly important for the interpretation of macroscopic observations. XAS is a very promising technique for this purpose and until now I performed two XAS experiments at the ESRF in Grenoble, France (ME1299 and EC120) in 2005 and 2006. The goal of the experiments was to investigate the fate of U(VI) in incubations with bacteria and hematite. The results of these experiments encouraged me to intensify my efforts to implement XAS in my research activities.

For the interpretation of the data I used several programs from the SixPACK package (E0 correction in SamView, Least Square fitting, and PC analysis). WinXAS was used for background correction, normalization, and data transformation for EXAFS analysis. However, regarding EXAFS analysis I still have to rely on my collaborators. My main expectation from the XAFS summer school is to become more independent in XAFS analysis. I hope to improve my understanding of the underlying principles of X-ray absorption, data treatment, and fitting procedures. Furthermore I am planning to spend my sabbatical next year in Chicago and to establish a cooperation with scientists from the Molecular Environmental Sciences group at the Argonne National Laboratory regarding the characterization of products of microbial U(VI) reduction. Within this cooperation I am also intending to submit a general user proposal at the APS. The XAFS summer school would give me an excellent opportunity to prepare myself for the planned activities.

Date: May 8, 2007 11:15:27 AM CDT

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Institution: University of Western Ontario
Department: Chemistry
Position: Grad Student, years 1-2
Advisor: T.K. Sham
Research Field: Chemistry

XAFS/Synchrotron Experience: Previously, I have used XANES and XEOL experiments to examine the opto-electronic properties of (doped) semiconducting nanostructures. These nanostructures include ZnS-ZnO, Si-Ge, ZnS, ZnS:Mn, ZnS:Cl, and ZnO. I also plan to due angle resolve XANES/XEOL experiments on aligned nanowire arrays. I am interested in using EXAFS to gather information on (Surface) bond lengths in these nanostructures. This workshop will allow me to learn valuable tools and analysis techniques to perform these experiments and increase my overall understanding of XAFS.

Date: May 8, 2007 11:15:38 AM CDT

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Institution: University of Western Ontario
Department: Chemistry
Position: Grad Student, years 1-2
Advisor: T.K. Sham
Research Field: Materials Science

XAFS/Synchrotron Experience: In my research, I have used XANES to characterize and examine opto-electronic properties of calcium-containing compounds. I am also interested in investigating optical properties of light-emitting materials using synchrotron radiation; XEOL has been used for such studies. From this we can measure specific relaxation channel (optical) after a sample has been excited by X-ray. Further, I plan to use EXAFS to determine bond lengths of samples of interest. From this workshop, I would like to gain valuable tools involving XANES and EXAFS analysis, ranging from data collection to analysis, and how I can improve my experimental and analysis technique.

Date: May 8, 2007 1:50:05 PM CDT

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Institution: California Institute of Technology
Department: Chemistry and Chemical Engineering
Position: Scientist, Academia
Advisor:
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: I am an Environmental Scientist and Engineer with background and experience in Molecular Physical Chemistry and Computational Chemistry. I hold a joint appointment between the California Institute of Technology and Howard University. I am currently the Principal Investigator of the NSF CTS Grant # 0506951 "Metal Ion Complexation by Dendritic Nanoscale Ligands in Aqueous Solutions: Fundamental Investigations and Applications to Water Purification." The characterization of the local structures of aqueous complexes of metal ions [(e.g., Cu(II), Fe(III) and Ag(I)] with poly(amidoamine) (PAMAM) dendrimers is a key objective of this project. Glenn Waychunas and I have been awarded beamtime by SSRL to carry out XAFS characterization of metal ion binding to PAMAM dendrimers in collaboration with Samuel Webb (SSRL). The first set of XAFS experiments, which focused on Cu(II) binding to PAMAM dendrimers terminal NH2 groups, was carried out on the SSRL beamline 2-3 in February 2-6, 2006. During these experiments, I got hands-on-experience on the set-up and implementation of an XAFS experiment. I was also introduced to the to use of Sam Webb's SixPACK XAS package. I also enrolled in the 2006 APS XAFS School. During this workshop, I also gained valuable knowledge on XAFS data analysis. Although my level comfort with all the XAFS technique has improved, I still feel that my overall knowledge of the technique is inadequate. Note that I have not previously enrolled in any XAFS introductory course that covered all the aspects of the techniques (e.g., sample preparation, experimental set-up, data acquisition, etc). Thus, I expect the completion of the 2007 APS XAFS School to provide me with the basic training on XAFS data so that I can work more efficiently with Glenn Waychunas, Sam Webb and graduate students at Caltech.

Date: May 8, 2007 2:06:20 PM CDT

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Institution: Savannah River National Laboratory
Department: Materials Science and Technology
Position: Scientist, Government
Advisor:
Research Field: Catalysis

XAFS/Synchrotron Experience: A journal article is in progress based on work done with Jeff Miller, from BP, on catalytic materials. The article will include XAFS data completed by Dr. Miller at APS. Otherwise, I do not have any direct experience with XAFS. My current research area is in understanding the hydrogen production reactions that take place in nuclear waste materials. Formic acid is added to high-level nuclear waste sludge during melter feed preparation for waste stabilization and storage. A portion of the formic acid has been found to react to produce molecular hydrogen during waste processing. This reaction presents a safety concern if hydrogen concentrations approach the lower flammability limit of four percent hydrogen in air in the process vessels. The presence of uranium fission product noble metals, such as Pd, Ru and Rh, have been shown to catalyze hydrogen generation. Yet, little information is known about the active state of the noble metals that c! atalyze the reactions. XAFS would be used to help determine the active state and coordination of noble metals in simulated nuclear waste materials before, during and after hydrogen generation. This information will be used to determine if other slurry components enhance the hydrogen production reactions. Hands-on experience is the best method to learn complicated techniques, such as XAFS. During the course, I expect to learn about fundamentals, which include theory, sample preparation, collection and analysis. Allotted beam time will be used to gain synchrotron experience, which supplements theoretical exercises. This information will help to determine the feasibility of future experiments and aid in sample acquisition and analysis. This knowledge will be used, not only for current projects, but future projects in materials science and catalysis.

Date: May 8, 2007 6:10:08 PM CDT

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Institution: Argonne National Laboratory
Department: CMT
Position: Post-Doctoral Fellow
Advisor: Christopher Marshall
Research Field: Catalysis

XAFS/Synchrotron Experience: Previous experience: I have help Dr. Marshall with the XAFS experiment for in-situ temperature program reduction of several catalyst samples. My responsibility was to prepare catalyst samples and help with the experimental set up.

My goal of this course is to learn how to perform the XAFS experiment and data interpretation. XAFS will be very useful for my research to determine the oxidation state and particle size of the metal on the catalyst support. Understanding the nature of these active species will serve as a guideline to synthesize a better performing catalyst.

Date: May 10, 2007 9:58:16 AM CDT

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Email: Maeve.Moriarty@rmc.ca
Institution: Royal Military College of Canada
Department: Chemistry
Position: Grad Student, years 1-2
Advisor: Dr. Ken Reimer
Research Field: Choose One

XAFS/Synchrotron Experience: I have visited the APS twice, and ran some fox hair and algae samples on the ID line at sector 20 on my last visit. I would like to use XAS mostly for XANES to compare speciation within tissues to speciation from extracted tissues, and why terrestrial birds have low extraction efficiencies using traditional techniques (~20%). From this course I hope to learn how to analyze data properly, and how to optimize sample set-up and data collection.

Date: May 10, 2007 12:49:03 PM CDT

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Institution: Argonne National Laboratory
Department: Nuclear Engineering
Position: Scientist, Government
Advisor:
Research Field: Materials Science

XAFS/Synchrotron Experience: I have run several experiemnets at the APS on XAFS, which have been analyzed my my postdoctoral associate. However, he is now moving on to a faculty position and I see this as the perfect opportunity to learn the analysis myself. I have lots of experience in diffraction and other synchrotron techniques and understand the basics of what is required. However, I wish to get a thorough grounding in the technique and make sure that my analysis is correct. This can only be done by total immersion in a course such as the one offered at Argonne.

Date: May 10, 2007 2:05:16 PM CDT

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Institution: Univeristy of Wisconsin Madison
Department: Chemical Engineering
Position: Grad Student, years 3+
Advisor: Dr. James A. Dumesic
Research Field: Chemistry

XAFS/Synchrotron Experience: My previous XAFS experience involves collecting transmittance data on the Pt LIII and Re LIII edges at NSLS beam line X-18B at Brookhaven National lab. I studied supported Pt, Re and bimetallic PtRe catalysts used in the reforming of biomass derived molecules into synthesis gas. In reaction studies, we found that the bimetallic catalyst is an order of magnitude more active than Pt alone. Pt and Re edge data was recorded on the catalysts before, during and after an in-situ reduction. I have a little experience with Athena and Artemis in data reduction and fitting. My current objective involves investigating the interaction between Pt and Re (evidence for alloying through coordination number, nearest neighbor distances, etc) , and how this interaction leads to improved activity. Our group has collaborative projects with a theory group (DFT) that predicts the properties of bimetallic catalysts from first principles and another group doing TEM. I believe that XAFS characterization of catalysts, whose synthesis was based on theoretical predictions, will bring us one step closer towards bridging the gap between theory and experiment. In that respect, XAFS will serve to improve the rational design of catalysts. Therefore, in the long term, I plan to use XAFS to investigate other bimetallic catalysts systems. The APS XAFS summer course is a wonderful opportunity to interact with and learn directly from experts in the field. From this course, I would like to obtain the knowledge to better process the data I have already collected (background removal, fitting, etc) and learn more about fitting techniques. Of particular relevance to me, is to find a way of distinguishing Pt and Re backscatterers (since their backscattering characteristics are similar). I would also like to learn about fluorescence mode and in-situ XAFS on reacting systems.

Date: May 10, 2007 2:45:17 PM CDT

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Department: Advanced Characterization
Position: Scientist, Industry
Advisor:
Research Field: Catalysis

XAFS/Synchrotron Experience: I have been helping Simon Bare collect Xray absorption data at the APS for over a year. We generally collect data under simulated process conditions. This enables us to correlate oxidation state and coordination number with catalytic performance.

I hope to learn how to model and interpret the EXAFS data.

Date: May 10, 2007 2:48:19 PM CDT

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Institution: University of Wisconsin
Department: Chemical and Biological Engineering
Position: Grad Student, years 3+
Advisor: James A. Dumesic
Research Field: Catalysis

XAFS/Synchrotron Experience: Previously, I have studied carbon supported Pt, Re, and Pt-Re bimetallic catalysts both before and after reaction using XAFS at Brookhaven National Lab. This data has allowed us to identify the reactive phase of our catalyst as well as the oxidation state after reaction and any changes to metal particle composition during reaction. In the future, I plan to use XAFS to further investigate bimetallic catalysts and possibly perform in-situ XAFS experiments to determine what causes the catalyst to change during a reaction. I expect to learn more about XAFS spectra analysis and understand further the programs available for spectra analysis.

Date: May 15, 2007 6:17:53 PM CDT

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Department: Chemical Engineering & Applied Chemistry
Position: Grad Student, years 1-2
Advisor: Prof. Charles Jia
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: By the time that the 2007 XAFS School begins, I will have completed approximately five days worth of experiments at the Canadian Synchrotron Radiation Facility, which is part of the Synchrotron Radiation Center run by the University of Wisconsin at Madison. The purpose of my experiments is to use XANES to analyze the different forms of sulfur present in samples of petroleum coke that have been reacted with sulfur dioxide. The software needed to analyze the data, however, is quite complicated and, as yet, includes no 'help' file. In the XAFS course, I expect to gain more fundamental knowledge about the technique itself, as well as learn how to effectively utilize the Ifeffit software package to its full potential (or at least to the point where I know what I am doing). I anticipate that this experience will greatly enhance my research and prevent me from looking stupid during oral presentations.

Date: May 15, 2007 5:49:36 PM CDT

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Department: Soil Science
Position: Grad Student, years 1-2
Advisor: Dr. Dean Hesterberg
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: The XAFS is very a powerful and valid technique for atomic scale research. When I was a master student, I had participated in the project of Application of nano-materials in the remediation of polluted soils: sorption of arsenate on lithium-intercalated gibbsite: spectroscopic and macroscopic studies in beam lines of 17C1 / W20 – EXAFS and BL 15B DCM Tender X-ray in National Synchrotron Radiation Research Center (NSRRC) in Taiwan. It was about arsenate sorption on lithium/ aluminum layered double hydroxide intercalated by chloride (Li/Al LDH-Cl), and EXAFS technique was employed to analyze local coordination environments between arsenate and Li/Al LDH-Cl. Also, in 2004, I had joined the summer workshop: Training Course of X-ray Absorption Spectroscopy, held by NSRRC in Taiwan. In fall, 2006, I enrolled to Department of Soil Science, North Carolina State University, working with Dr. Dean Hesterberg. Our group have studied phosphate sorption behavior, and used XANES to distinguish phosphate sorption mechanisms. I am familiar with analyzing EXAFS data by feffit program; however, I am very interested in programs of ifeffit and Athena & Artemis. Therefore, I expect to learn how to use these programs to fit data, and also, I want to strengthen my knowledge about the theory of XAFS.

Date: May 16, 2007 9:02:00 AM CDT

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Department: Soil Science
Position: Grad Student, years 1-2
Advisor: Dean Hesterberg
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: For my MS degree in soil chemistry I am studying how oxidation-reduction cycles affect the chemical speciation of soil iron which is important for understanding how quickly restored wetlands begin to function like natural wetlands in terms of ecosystems and protection of water quality. Redox-induced changes in Fe-oxides and organic matter also regulate the mobility and environmental impacts of many soil contaminants. My master's research employed XAFS spectroscopy to determine the speciation of Fe in soil samples. XAFS analysis was more important than x-ray diffraction on these samples because concentrations of soil Fe were typically <1%, and a significant portion was likely bound with organic matter in non-crystalline species.
My laboratory studies determined how quickly microbial reduction of different soil samples occurred after water saturation. The aim of the XANES and EXAFS analysis was to determine changes in oxidation state and forms of soil iron after several redox cycles. The reduction, translocation, and re-oxidation of Fe are important processes for wetland soil development, which might affect the reactivity of soil Fe. The XAFS data have been collected but not fully analyzed, in part because of my lack of experience with EXAFS data analysis.
This fall I plan to begin work on my Ph.D. degree in soil chemistry. My research interests are in understanding bonding mechanisms of phosphate to Fe and Al metal centers in soil organic matter. The mechanisms of phosphorous bonding and dissolution under reducing soil conditions affect the potential of natural and restored wetlands to retard the migration of P to surface waters. Phosphorus XAFS will be an important tool for this research.
I have just begun my research using XAFS. Primarily, I need to learn more about the data analysis aspect of XAFS; however, I would also enjoy learning more about the theory and uses of XAFS

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Institution: Queen's University
Department: Geological Sciences and Geological Engineering
Position: Grad Student, years 3+
Advisor: Heather Jamieson
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: My research involves the determination of the solid-state speciation of antimony (Sb) in environmental and mill samples from the Giant Mine, Yellowknife, NWT (Canada). On the basis of our previous work, we anticipated multiple, fine-grained Sb hosts in the sediments and mill samples and recognized that the most powerful tools for identification of those Sb hosts are microXANES and microXRD. Our initial work with Sb was carried out at 20-ID-XOR in November 2006 with more time allotted at this beamline in August 2007. XANES and XRD analysis was conducted on model compounds, and on multiple spots on sediment, and mill samples. Our initial work indicates that we can distinguish the Sb-bearing sulfides/sulphosalts, the Sb(III) oxide, the mixed Sb(III)/Sb(V) oxide, and the Sb(V) oxide edges unambiguously. We have also identified two forms of Sb-bearing solids in the sediments never reported previously in environmental samples. This research into!

Sb solid-state is proving to be very exciting. However, we are struggling with the data processing aspect of the project. For this reason I am most interested in the data processing and analysis part of the XAFS course. Our research group has been using WINXAS for data processing. We have recently been considering learning a new data analysis program. I am also interested in different methods of sample preparation to evaluate the most effective preparation methods for my experiments. Although I have yet to collect data in the EXAFS region, it may prove useful in the near future; any instruction on EXAFS data collection and analysis should prove useful.

Date: May 22, 2007 12:47:29 PM CDT

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Department: Chemical Engineering and Applied Chemistry
Position: Grad Student, years 3+
Advisor: Charles Q. Jia
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: My project is about using high sulphur petroleum coke to produce sulphur impregnated activated carbon (SIAC) for effective mercury adsorption. In this study, the mechanisms of chemical activation of high sulphur petroleum coke are investigated, with a focus on sulphur roles in coke activation. In order to gain detailed knowledge about sulphur compounds in SIAC, the technique, X-ray Absorption Near Edge Structure (XANES) is applied. As I know, XANES is the best available tool for characterizing sulphur species in solid samples. I was using XANES to analyze my sample in SRC for one week. However, at that time I only got a very short training on how to use the device without giving lectures to help understand the whole technique. Besides, when I used the software, Athena, to analyze my data, I was so confused with it. Since I was back to Toronto, I could not get sufficient help from SRC, and had to learn almost all by myself. Therefore, I think the!
summer school that you provide should be suitable for me to learn more about XAFS, not only the XANES. I hope through this course I can obtain systematic knowledge of XAFS, and more importantly, to understand how to analyze the data. I hope to learn how to use the whole package of Ifeffit, not only Athena.

May 30, 2007 8:48:12 AM CDT

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Position: Scientist, Academia
Advisor: Mark Chance
Research Field: Biology / Biophysics

XAFS/Synchrotron Experience: I am working on X3B beamline at NSLS. I have attended the summer school last year at APS on Artemis and that was a great learning experience. The last EXAFS school was bit advanced and one of the hand on example by Scott on Athena was of great help. During this course I expect to learn more on XAS analysis using Athena and EXAFS interpretation. I am also looking forward to do some data collection and analysis on real sample with the help of EXAFS team at the course.

Date: June 4, 2007 10:37:15 AM CDT

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Advisor: Dr. K. Reimer
Research Field: Biology / Biophysics

XAFS/Synchrotron Experience: For the past five years I have used XAS to determine the distribution of arsenic compounds in a variety of samples. This work has involved mainly XANES analysis and micro-imagining techniques, and has been applied to samples from terrestrial organisms, as well as bioreactors and soils. During these experiments which are part of the Environmental Sciences Group (ESG) research program, XAFS data were collected for a variety of samples.
One focus of my current research will be to address the analysis of these XAFS spectra. In some cases, it is possible that the nearest-neighbour information provided by XAFS may provide a means of distinguishing between arsenic compounds with similar K-edge energies. In addition, XAFS results now appear more frequently in biological and environmental literature, and I believe that a basic understanding of this type of analysis would be invaluable for interpreting such results.
From the XAFS summer school I am particularly interested in learning how to correctly analyze XAFS data such that I can apply these skills to the XAFS spectra already collected by ESG and be confident in my interpretation of the results. This will involve addressing not only how to use whatever software is provided but understanding the steps involved in the analysis. I have already made some attempts at XAFS analysis; however, this experience has left me with the impression that a large portion of XAFS analysis relies upon experience therefore it will be important to learn to recognize whether the final interpretation of XAFS data is acceptable or unacceptable, and what should be reported in a publication to indicate the quality of the data. While my focus is on data analysis, I anticipate that the XAFS course will also demonstrate methods for sample preparation and collection that provide the best possible XAFS data.

Date: June 6, 2007 3:28:51 PM CDT

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Research Field: Catalysis

XAFS/Synchrotron Experience: Novice User
Spend some time at the beamline at BNL
Proposal File: null
Received at 15:28:51 on 6-Jun-107

Date: June 11, 2007 2:47:14 PM CDT

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Position: Post-Doctoral Fellow
Advisor: Maria Iavarone
Research Field: Materials Science

XAFS/Synchrotron Experience: I have no experience for XAFS, but we are planning to do an XAFS experiment on CoxNbSe2 to evaluate if Co is clustering.

Date: June 12, 2007 12:43:13 PM CDT

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Position: Scientist, Academia
Advisor:
Research Field: Physics

XAFS/Synchrotron Experience: I've been a research associate at LSU/CAMD for just over a year, primarily helping users collect XANES and EXAFS spectra in transmission, fluorescence, and (rarely) electron yield. I do not currently pursue my own research, but I must support many users of varied experience from many fields. I expect to learn proper analysis techniques and get a new perspective on the work I do.

Date: June 12, 2007 1:57:53 PM CDT

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Department: Chemical Engineering
Position: Post-Doctoral Fellow
Advisor: Christopher L. Marshall
Research Field: Catalysis

XAFS/Synchrotron Experience: I don't have any hands-on XAFS or synchrotron experience, however, one of my coworkers at Northwestern is doing XAFS work at Argonne APS facility. From his group meeting presentations, I learned that XAFS can be used to determine the oxidation state, coordination number, and chemical environment of essentially all the elements. Furthermore, the sample does not have to be crystalline. I am going to be a postdoctoral appointee at the Argonne National Lab, chemical engineering division, working with Dr. Chris Marshall. Our future project is to synthesize homogeneous organometallic complexes, support them on the metal oxides surface, and study their catalytic properties. XAFS would be an vital tool for us to understand how the active species look like on the surface and the oxidation state of the metal centers before and after catalysis.
From this summer course, I expect to learn the fundamental theory of EXAFS, how to prepare the samples, how to do the measurements at the beamline, and how to collect and analyze the data. Most importantly, I hope I can use EXAFS as a complimentary technique to investigate the mechanism of certain catalytic reactions.

Date: June 14, 2007 9:23:09 AM CDT

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Position: Post-Doctoral Fellow
Advisor: Joseph W. Stucki
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: I performed some experiments in powder X-ray diffraction at LNLS (Brazilian National Synchroton Light Source) but I do not have any experience in XAFS, except mainly in data processing. I have some background knowledge from having submitted a proposal to LNLS to investigate coordination of iron oxides. Now I would like to use XAFS to investigate mechanism of adsorption of Chromium and/or Uranium in clay minerals and iron oxides.
I would like to attend the workshop to learn more about the theoretical aspects of the technique, sample preparation methods, and how to handle data fitting and interpretation.

Date: June 14, 2007 3:27:54 AM CDT

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Position: Grad Student, years 1-2
Advisor: Michael Kersten
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: I am PhD student at the Institute of Geosciences, Johannes-Gutenberg University of Mainz, Germany. My PhD project is “Spatially resolved speciation of heavy metals in soil samples using X-ray absorption spectroscopy (µ-XAS)” under supervision of Professor Michael Kersten. The environmental impact of potentially toxic elements, which is determined by their toxicity, mobility, distribution, and bioavailability, is not simply dependent on their total concentration but, most critically, on the element species. This realization has spurred the development of many different methods of elemental speciation.
X-ray Absorption Fine Structure(XAFS) is a direct, non-destructive method of speciation analysis suitable to determine the valence state and coordination of elements directly in solid matrices on a molecular level. This information is essentially needed to parameterize the mobility of toxic metals like arsenic or lead as well as their pathways inside of soils. Also µ-XAFS provides information to improve the current understanding of metal-associated complexes at the mineral oxide/water interface. Also µ-XRF or µ-XRD will be used to further characterize the solid constituents of my soil samples. So I am very interested to participate this course and most important points for me from this course is sample preparation and interpretation of measured data using Athena and Artemis.
In conclusion I believe that this summer school will be good benefit to my future work.

Date: June 13, 2007 5:09:12 PM CDT

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Advisor: Susannah Scott
Research Field: Catalysis

XAFS/Synchrotron Experience: My research project is on surface-supported catalysts for alkene metathesis. I have been to the Stanford Synchrotron Research Labs (SSRL) on three occasions to collect XAFS data. Unfortunately, my understanding of both the physical principles governing XAFS and data collection is rudimentary. In addition, I would like to learn more about correct processing and interpretation of the data I have already collected, especially using Athena and Artemis.

Date: June 13, 2007 3:37:58 PM CDT

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Advisor: Ralph Nuzzo
Research Field: Chemistry

XAFS/Synchrotron Experience: On a recent visit Argonne I studied the structural changes of platinum nanoclusters after oxidation, reduction and exposure to different temperatures. My current project will also involve similar experimental controls to study the structure and behavior of bimetallic nanoclusters (i.e. Pt-Ru, Pt-Rh etc).
In this course I expect to get a more thorough, hands-on understanding of working with XAFS. Of most interest to me is developing better intuition for data analysis and learning how to navigate through the software (Artemis, Athena).

Date: June 18, 2007 11:16:13 AM CDT

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Department: Dept. of Civil and Environmental Engineering
Position: Grad Student, years 1-2
Advisor: Jean-Francois Gaillard
Research Field: Geology / Environmental Science

XAFS/Synchrotron Experience: I am a first year graduate student in the Department of Civil and Environmental Engineering at Northwestern University. My background is in Chemistry, and my current area of study is Environmental Sciences with focus on metal speciation. I have attended a Structural Inorganic Chemistry course at Northwestern, which covered topics from group theory to basic background on spectroscopic techniques such as EXAFS.

XAFS is one of the most important tools to be used during my graduate studies, but my only previous experience with the technique has been at the Advanced Photon Source. I have used the DND-CAT beamline for preliminary studies of chromium speciation in paint samples. I participated in these experiments twice and I see a need for training in both how to set up an experiment and how to analyze XAFS data. By participating in the 2007 APS XAFS Summer School, I expect to obtain this introductory training.

The hands-on practice offered by this summer course will be of great value for my (very) near future experiments. From my two previous experiments, I understand that many steps are involved in the operation of a beamline, and the only way to learn these steps is by literally doing them.

I have had initial contact with the program Athena and I know that it is one of the key tools in data treatment. Training with experienced users in the many operations that this and other programs can perform will provide me with a more solid knowledge on their basis and on the results that they may enable me to obtain. I look forward to participating in this Summer School, since it will reserve time for practical operation of a beamline and for data processing, with the instruction of well-known researchers in the area, certainly fulfilling my expectations.

Date: June 22, 2007 8:51:47 AM CDT

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Advisor: Robert Byrne
Research Field: Geology / Environmental Science
XAFS/Synchrotron Experience: My research involves studying yttrium and rare earth element (YREE) sorption onto a variety of solids (e.g., Fe(OH)3, Al(OH)3, silica gel) over a range of solution conditions, such as pH, alkalinity, and temperature. Through my research a molecular model of YREE sorption by amorphous ferric hydroxide has been developed. The underlying assumption for the model is that YREEs, as free ions or simple solution complexes, interact with one or two surface hydroxyl groups. I want to verify this assumption by using EXAFS to observe the coordination of individually sorbed YREEs. Initially, samples would be prepared according to a set of stable solution parameters (i.e., at a single pH and alkalinity) but eventually, these parameters would be varied to determine their effect on YREE coordination.

I recently gained some XAFS experience at the APS on the GSECARS beamline 13-BMD. I was there with my advisor on June 13-15 to collect EXAFS spectra of individual REEs pre-sorbed onto amorphous ferric and aluminum hydroxides. Since this was our first visit to a Synchrotron facility, we learned about sample preparation and basic operation of the beamline. While our results require improved counting statistics, we determined which experimental conditions need to be adjusted for increased success in future work.

During this course, I expect to learn more about the theory behind XAFS measurements. I am particularly interested in obtaining guidance on all aspects of data analysis, including data processing and interpretation. My hope is to start analyzing the data we recently collected. If possible, I would also like to collect preliminary data on samples generated from our recent findings. This course is a wonderful opportunity to learn about innovative methods that will benefit my research, as well as other research being done at the APS.

Date: June 25, 2007 1:46:36 PM CDT

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Department: Chemistry
Position: Grad Student, years 1-2
Advisor: Dr. Jon Veinot
Research Field: Chemistry

XAFS/Synchrotron Experience: I am currently a registered user at the Canadian Light Source (CLS) synchrotron facility. Over 4 sessions in the past 8 months, I have been working alongside Dr. Ronald Cavell, member of the CLS Beamline Advisory Committee, to investigate the source and mechanism of the optical emission from oxide-embedded and freestanding silicon nanocrystals, nc-Si/SiO2 and FS-nc-Si, respectively. Our initial focus was to identify the silicon and silicon oxide species present in various nc-Si/SiO2 composites and FS-nc-Si through X-ray absorption spectroscopy. This was successfully accomplished by performing XANES experiments on the High Resolution Spherical Grating Monochromator (SGM) beamline. We subsequently investigated the optical response of these systems through X-ray excited optical spectroscopy (XEOL). By selectively exciting the various silicon and silicon oxide species and monitoring the optical response, we were able to identify that both sur!
face oxide states and quantum confinement effects play crucial roles in the optical properties of nc-Si.

My current focus is to investigate the optical properties of germanium nanocrystals, nc-Ge, through XANES, XEOL, and XAFS experiments. I believe that XAFS would provide unparalleled insight into the structural and chemical environments within the nc-Ge crystalline core and the nc-Ge/oxide interface. Specifically, it will allow the investigation into the presence of crystal defects and the composition and abruptness of the core/oxide interface, both of which are thought to be crucial in the optical properties of semiconductor nanocrytals.

I hope to learn a lot from the APS XAFS School, both in terms of background theory and experimental details. State-of-the-art X-ray spectroscopy techniques are powerful characterization tools, and it would be very beneficial to understand their mechanism in depth. Learning proper sample preparation techniques and the analysis and interpretation of XANES and XAFS data will give me the knowledge and expertise I need to perform these experiments.

Date: June 25, 2007 3:39:59 PM CDT

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Position: Grad Student, years 3+
Advisor: Dr. Jonathan Veinot
Research Field: Chemistry

XAFS/Synchrotron Experience: The Canadian Light Source (CLS) in Saskatoon, Canada has provided me with X-ray safety training and 96 hours of beamline experience. I am currently working with Dr. Ron Cavell on an active project entitled, "Electronic Structure, Chemical State and Emission Properties in Size Regulated Silicon Nanoparticles Probed With Soft X-ray Spectroscopy." All experimentation for this project was performed on the spherical grating monochrometer (SGM) beamline in order to access the appropriate core-electron binding energies for silicon, oxygen and fluorine. During this study we employed X-ray absorption near edge spectroscopy (XANES) to examine the chemical environment of oxide-embedded and freestanding silicon nanocrystals. As well, to study the optical response of these luminescent silicon nanocrystals we used X-ray excited optical luminescence (XEOL) in an attempt to characterize the source of photoluminescent emission. Using these two techniques we !
have determined that the emission from silicon nanocrystals arises from both the nanocrystals/oxide interface, and quantum confinement within nanocrystals.

I plan to use X-ray absorption-based spectrocopies to gain electronic and bonding information for silicon nanocrystals in specific chemical environments. Etching away the surface oxide and attaching various functional groups to the nanocrystals will change the surface chemistry and subsequently alter the emission properties of these materials. XANES spectroscopy will help determine how the bonding environment of chemically altered silicon interfaces changes when different functional groups are attached. XEOL measurements will quantify the effects that the surface functionalization has on the emission properties of silicon nanocrystals.

I hope to take away a significant amount of knowledge from the APS XAFS School, both in terms of background theory and hands on instruction. I plan to enhance my understanding of sample preparation, data analysis and interpretation of experimentally obtained data. I am also interesting in learning the basics behind modeling theoretical XANES and XAFS spectra, and comparing these plots to experimental data.

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Research Field: Chemistry

XAFS/Synchrotron Experience: I have no previous XAFS or Synchrotron experience but this fall I plan to begin working for Lin Chen in the Chemistry Department at Argonne who highly recommended me taking this course as an introduction to the types of experiments that I will be doing in her lab. My proposed research includes using Laser-Initiated Time-Resolved X-ray Absorption Spectroscopy (LITR-XAS)to study excited state structural changes of organometallic molecules. I hope that through this course i will build a foundational understanding of XAFS and other X-ray experiments using the Advanced Photon Source at Argonne.