

Summary of the 3rd Penn State Bioinorganic Workshop

The 3rd Penn State Bioinorganic Workshop took place in early June 2014 and was combined with the 3rd Penn State Frontiers in Metallobiochemistry Symposium. The workshop was even larger than the 2nd Penn State Bioinorganic Workshop we offered in 2012. It had even more participants (162 rather than 123 in 2012). Like the 2012 workshop, the 2014 workshop had three parts. The first part consisted of 16 90-min lectures presented by faculty experts on the topic of their expertise (see below). Based on the suggestions from the 2012 workshop, we have recorded all 16 lectures professionally and make them available to the entire bioinorganic community via online streaming. In addition, hard copies of the recordings are available as backup.

1. Introduction to coordination chemistry (Neese)
2. Introduction to quantum chemistry (Neese)
3. X-ray spectroscopy (DeBeer)
4. Biological Electron transfer (Dutton)
5. Resonance Raman spectroscopy (Neese)
6. EPR spectroscopy (van der Est)
7. Pulse EPR spectroscopy: ENDOR/ESEEM/DEER (Stoll)
8. Mössbauer spectroscopy (Münck)
9. MCD spectroscopy (Lehnert)
10. Protein electrochemistry (Armstrong)
11. Isothermal titration calorimetry (Wilcox)
12. Transient state methods (Bollinger)
13. X-ray crystallography (Boal)
14. Small-angle X-ray scattering (Ando)
15. Mass spectrometry (Agar)
16. Bioinformatics methods (Babbitt)

The second part (the center piece of the workshop) provided hands-on training in 21 (up from 16 in 2012) different methods to small groups (6 or less “students” taught by 1-3 “teachers”). The various experimental topics were offered up to 12 times in 2-h blocks over the next 4 days. Regular participants thus had the opportunity to learn up to 12 new methods. The “teachers” included 74 participants (up from 55 in 2012). In other words, nearly half the participants served as teachers. The “teachers” included 16 faculty, 17 postdocs, 39 graduate students, and 2 undergraduate students. The following 16 sections were offered:

1. Basic EPR (John Golbeck and members of his group)
2. Pulse EPR (Stefan Stoll and Alexey Silakov)
3. Transient state EPR (Art van der Est and Sam Mula from his group)
4. FQ method (members of the Bollinger/Krebs group)
5. SF-abs spectroscopy (members of the Bollinger/Krebs group)

6. Anaerobic protein purification (members of the Booker group)
7. Resonance Raman spectroscopy (members of the Green group and Bo Zhang from the Bollinger/Krebs group)
8. Mössbauer spectroscopy (members of Bollinger/Krebs group and Alex Guo)
9. MCD spectroscopy (Nicolai Lehnert and members of his group)
10. X-ray spectroscopy (Serena DeBeer and members of her group)
11. Introduction to the DFT package ORCA (members of the Neese group)
12. Cryoreduction (Candace Davison from the Breazeale Nuclear Reactor and members of the Bollinger/Krebs group)
13. ENDOR/ESEEM spectroscopy (Alexey Silakov from the Green group and Stefan Stoll)
14. Protein electrochemistry (Sean Elliott and members of his group)
15. X-ray crystallography (Oliver Einsle, Amie Boal and members of her group)
16. High-resolution mass spectrometry (Tatiana Larenov from the Penn State Huck Institutes and Jeff Agar with Jared Auclair from his group)
16. QQQ mass spectrometry for analysis of small molecules (members of the Booker group)
17. Isothermal titration calorimetry (Dean Wilcox and members of his group and Booker group)
18. Small-angle X-ray scattering (Nozomi Ando)
19. Bioinformatics I (Patsy Babbitt and members of her group)
20. Bioinformatics II (Patsy Babbitt and members of her group)
21. Bioinformatics III (Patsy Babbitt and members of her group)

For most experimental sections, there were enough “teachers” available, so each individual teacher taught her/his method of specialty on average half of the time (6 times of the 12 times a method was offered). For the remaining 6 times, the teachers had the opportunity to become students and learn up to 6 other methods. The boundaries between the “teachers” and “students” were severely blurred, to the extent that even undergraduate students trained faculty, as described below.

Personalized schedule for hands-on training for

Compton, Ashley

teaching: Stopped-flow absorption spectroscopy

Personalized schedule for hands-on training for

Einsle, Oliver

teaching: X-ray crystallography

Sunday	Monday	Tuesday	Wednesday	Sunday	Monday	Tuesday	Wednesday
8:30 am - 10:30 am	Stopped-flow absorption spectroscopy	Stopped-flow absorption spectroscopy	EPR II - Pulsed EPR techniques	8:30 am - 10:30 am	X-ray crystallography	X-ray crystallography	X-ray crystallography
10:45 am - 12:45 pm	Stopped-flow absorption spectroscopy	Freeze-quench method	EPR III - Time-resolved EPR spectroscopy	10:45 am - 12:45 pm	Resonance Raman spectroscopy	X-ray crystallography	X-ray crystallography
2:00 pm - 4:00 pm	X-ray crystallography	MCD spectroscopy	EPR I - Fundamentals of EPR spectroscopy	2:00 pm - 4:00 pm	X-ray crystallography	DFT calculations with ORCA	Protein electrochemistry
4:15 pm - 6:15 pm	Stopped-flow absorption spectroscopy	Mössbauer spectroscopy	Stopped-flow absorption spectroscopy	4:15 pm - 6:15 pm	Stopped-flow absorption spectroscopy	DFT calculations with ORCA	X-ray spectroscopy

Ms. Ashley Compton was at that time an undergraduate student working under the tutelage of Prof. Kathryn Haas (participant of the 2012 and 2014 workshops). Ashley was an NSF-sponsored REU student in the summer of 2013 (based on Kathryn Haas' advice to do research at Penn State, which is likely fueled by Kathryn's participation in the 2012 workshop). During that time, Ashley became so proficient in stopped-flow absorption spectroscopy that we had offered her to be a teacher in that method. As can be seen from the Ashley Compton's schedule, she learned on Sunday, June 1 2014 from 2-4 pm X-ray crystallography. Her teacher was Prof. Oliver Einsle. Right after Oliver taught Ashley X-ray crystallography, they walked together to the stopped-flow instrument, where their roles reversed. The undergraduate student Ashley Compton taught Prof. Oliver Einsle stopped-flow absorption spectroscopy.

In the hands-on section of the workshop, a total of ~1,200 2-h person-training-units were administered to "students" by the 74 "teachers". The total number of 2-h person-training-units increased by more than 50% from 2012 (~750)! Originally, we had intended each participant to enroll in 9 different units, because (i) we did not want to overwhelm the participants, preferring to keep schedules flexible for the important informal networking that goes on in such settings and (ii) we sought flexibility with the daunting task of creating a master schedule that ensured that each participant could enroll in her/his 9 top choices without requiring the number of students in any given installment of any unit to exceed 6. We intended that participants could network amongst themselves during their "bye rounds" at the concurrent poster session: we had ~80 posters up during the entire meeting and, in addition, one afternoon was reserved for a formal 2-h poster session and a social event in a nearby park. However, most participants were so enthusiastic about the experimental program that they sought 10th, 11th, or even 12th units in their "open" slots!

The third part of the 2012 workshop consisted of 12 lectures presented by the attendees on their own research; the speakers were selected from submitted abstracts. In 2014 this component was replaced with the Frontiers in Metallobiochemistry Symposium in 2014. The previous two Frontiers in Metallobiochemistry symposia featured ~25 faculty speakers. For 2014, we included talks by students and postdocs. The 2014 Symposium featured 9 sessions and 3 plenary talks. Each session began with a faculty talk, followed by a student/postdoc talk, and another faculty talk. We felt that this arrangement gives students/postdocs a maximum exposure. The student and postdoc talks were selected from submitted abstracts. One of the talks was given by Mr. Martin McLaughlin, an undergraduate student from MIT and an alumnus of our 2012 workshop!

For the duration of the workshop and symposium, participants met informally in the evenings. The "bioinorganic bar of the day" was announced each morning on the meeting bulletin board to ensure that the participants met predominantly in one place, thus facilitating informal networking. It was amazing to witness the energy and

commitment of the future generation of bioinorganic chemists: they worked hard, they worked together, they partied hard, and they partied together! Overall, the workshop had an outstanding dynamic among all participants. Jeff Agar (Brandeis University), who had helped organize some of the UGA bioinorganic workshops in the late 1990s as a graduate student in Michael Johnson's group and taught the mass spectrometry section at our event, judged the Penn State workshop to be at least the equal of the classic UGA events!

Our significant success in raising funds for the 2014 workshop is yet another sign of its perceived value to the community. We were able to reimburse all costs to the visiting faculty and most of the costs of the visiting student and postdoc "teachers" (some had received funds from their institutions to attend the meeting). Moreover, we were able to waive the registration fee and provide assistance with travel costs for participants from research groups without external funding. See the unsolicited letter we received from Prof. Michael Machczynski (SUNY New Paltz).

Perhaps the ultimate long-term benefit of the "classic workshops" at UGA and Louvain-la-Neuve has been the many successful long-term collaborations that they gave birth to. In the 2012 progress report we stated that it was at the time too early to assess the long-term success of this and future Penn State bioinorganic workshops. In 2014, we can see the gradual build-up of this collaborative infrastructure. We will just give a few examples. (1) Two of the 36 participants of the 2010 workshop were Kyle Lancaster and Jonathan Caranto (graduate students at Caltech and UT San Antonio at the time). They met for the first time at our workshop. Jon Caranto also attended our 2012 workshop. Kyle Lancaster is now Assistant Professor at Cornell University. Jon Caranto decided to join Kyle Lancaster's group as a postdoctoral scholar. They both attended the 2014 symposium and met many of their class mates from the 2010 and 2012 workshops. (2) Hannah Shafaat attended the 2012 workshop when she was a postdoctoral scholar. She is now Assistant Professor at Ohio State University and sent two of her students to the 2014 workshop. She also attended the 2014 symposium and met other alumni of the 2012 workshop. There are more examples to tell, but for the sake of brevity we will stop here. We are confident that the participants of our workshops and symposia will continue to network for many years, hopefully decades, to come.

As in 2012, feedback from the participants was very positive in 2014 and is provided in the appendix.

The planning of the 2016 workshop has now begun.

3rd Bioinorganic Workshop & 3rd Frontiers in Metallobiochemistry Symposium

Tuesday May 27

4:00 – 6:00	Registration desk	Chemistry Building, Willaman Bridge
6:00 – ...	<i>First social get-together & beer</i>	<i>Champs, 1611 N Atherton St</i>
	<i>Shuttles are running from the Chemistry Building starting at 5:30; last return run to Eastview Terraces (on campus housing) and Atherton will be around 10 pm from Champs</i>	

Wednesday May 28

9:00 – 10:30	Introduction to coordination chemistry (Frank Neese)	100 Berg Auditorium
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	Introduction to computational chemistry (Frank Neese)	100 Berg Auditorium
12:30 – 2:00	<i>Lunch break</i>	
2:00 – 3:30	X-ray spectroscopy (Serena DeBeer)	100 Berg Auditorium
3:30 – 4:00	<i>Coffee break</i>	
4:00 – 5:30	Biological electron transfer (P. Leslie Dutton)	100 Berg Auditorium

Thursday May 29

9:00 – 10:30	Resonance Raman spectroscopy (Frank Neese)	100 Berg Auditorium
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	EPR spectroscopy (Art van der Est)	100 Berg Auditorium
12:30 – 2:00	<i>Lunch break</i>	
2:00 – 3:30	Pulse EPR: ENDOR/ESEEM/DEER (Stefan Stoll)	100 Berg Auditorium
3:30 – 4:00	<i>Coffee break</i>	
4:00 – 5:30	Mössbauer spectroscopy (Eckard Münck)	100 Berg Auditorium

Friday May 30

9:00 – 10:30	MCD spectroscopy (Nicolai Lehnert)	100 Berg Auditorium
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	Protein electrochemistry (Fraser A. Armstrong)	100 Berg Auditorium
12:30 – 2:00	<i>Lunch break</i>	
2:00 – 4:00	Poster session	Willaman Bridge
4:00 – 6:00	<i>Social get-together</i>	<i>Sunset Park (see map)</i>
	<i>[Clems BBQ & softball game]</i>	<i>15 min walking distance</i>

Saturday – May 31

9:00 – 10:30	Isothermal titration calorimetry (Dean E. Wilcox)	100 Berg Auditorium
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	Transient state methods (J. Martin Bollinger, Jr.)	100 Berg Auditorium
12:30 – 2:00	<i>Lunch break</i>	
2:00 – 3:30	X-ray crystallography (Amie K. Boal)	100 Berg Auditorium
3:30 – 4:00	<i>Coffee break</i>	
4:00 – 5:30	Small-angle X-ray scattering (Nozomi Ando)	100 Berg Auditorium

Sunday June 1

9:00 – 10:30	Mass spectrometry (Jeffrey N. Agar)	100 Berg Auditorium
10:30 – 11:00	<i>Coffee break</i>	
11:00 – 12:30	Bioinformatics methods (Patricia S. Babbitt)	100 Berg Auditorium
12:30 – 2:00	<i>Lunch break</i>	
2:00 – 4:00	Experiments in small groups 1	(see personal schedule and map)
4:15 – 6:15	Experiments in small groups 2	(see personal schedule and map)

Monday – June 2

8:30 – 10:30	Experiments in small groups 3	(see personal schedule and map)
10:45 – 12:45	Experiments in small groups 4	(see personal schedule and map)
12:45 – 2:00	<i>Lunch break</i>	
12:45 – 2:00	Brown-Bag-Lunch 1	110 Wartik
	<i>This event is optional – pizza and water/soda will be provided</i>	
	Vera Krewald (Max Planck Institute of Chemical Energy Conversion) Spectroscopically consistent Mn oxidation state assignments for the natural water splitting catalyst	
2:00 – 4:00	Experiments in small groups 5	(see personal schedule and map)
4:15 – 6:15	Experiments in small groups 6	(see personal schedule and map)

Tuesday – June 3

8:30 – 10:30	Experiments in small groups 7	(see personal schedule and map)
10:45 – 12:45	Experiments in small groups 8	(see personal schedule and map)
12:45 – 2:00	<i>Lunch break</i>	
2:00 – 4:00	Experiments in small groups 9	(see personal schedule and map)
4:15 – 6:15	Experiments in small groups 10	(see personal schedule and map)

Wednesday – June 4

8:30 – 10:30	Experiments in small groups 11	(see personal schedule and map)
10:45 – 12:45	Experiments in small groups 12	(see personal schedule and map)
12:45 – 6:00	<i>Lunch and free time</i>	
6:00 – 9:00	<i>Reception in the Arboretum</i>	<i>Arboretum (see map)</i> <i>15 min walking distance</i>
9:00 - ...	<i>Post-reception “social get together”</i>	<i>downtown State College</i> <i>listen to the grapevine for location(s)</i>

8:30 – 10:40 Session 1 - Non-heme-iron enzymes

Chair: J. Martin Bollinger, Jr. (*Pennsylvania State University*)

8:30 – 9:10 **Chuan He** (*University of Chicago*)

Oxidative Demethylation of RNA and DNA in Biological Regulation

9:10 – 9:30 **Nitai C. Giri** (*University of Texas, San Antonio*)

Distinguishing Reactivities of the Individual Iron Centers in Flavo-Diiron Proteins (FDPs)

9:30 – 10:10 **Lana Saleh** (*New England Biolabs*)

Biochemical and structural insight into the *modus operandi* of NgTET1, a 5-methylpyrimidine oxygenase from *Naegleria gruberi*

10:10 – 10:40 *Coffee break*

10:10 – 12:20 Session 2 - X-ray techniques

Chair: Yisong (Alex) Guo (*Carnegie Mellon University*)

10:40 – 11:20 **Serena DeBeer** (*Max Planck Institute for Chemical Energy Conversion*)

X-ray Spectroscopic Studies of Biological Catalysis

11:20 – 11:40 **Kelly N. Chacón** (*Oregon Health & Science University*)

A “sensor-switch” has control: Using multi-edge x-ray absorption spectroscopy to solve the mechanism of the CusCFBA Cu⁺/Ag⁺ efflux pump in *E. coli*

11:40 – 12:20 **Oliver Einsle** (*University of Freiburg*)

A Really Close Look at Bioinorganic Metal Centers

12:20 – 2:30 *Lunch break*

Thursday – June 5 – Afternoon Session

100 Berg Auditorium

- 2:30 – 4:10** **Session 3 - Maintenance and homeostasis of metallocofactors**
Chair: Kathryn L. Haas (*Saint Mary's College*)
- 2:30 – 3:10** **Celia W. Goulding** (*University of California, Irvine*)
Insights into how *Mycobacterium tuberculosis* acquires iron from heme
- 3:10 – 3:30** **Grace E. Kenney** (*Northwestern University*)
Dismantling copper homeostasis in methanotrophs
- 3:30 – 4:10** **Michael K. Johnson** (*University of Georgia*)
Iron-Sulfur Cluster Assembly and Repair
- 4:10 – 7:30** *Free time / dinner*

Thursday – June 5 – Evening Session

- 7:30 – 8:30** **Plenary lecture 1** 100 Berg Auditorium
Chair: Amie K. Boal (*Pennsylvania State University*)
Jacqueline K. Barton (*California Institute of Technology*)
DNA-mediated Signaling
- 8:30 – 10:30** **Poster session 1** Willaman Bridge

8:30 – 10:40 Session 4 – Detailed insight into biological long-range redox reactions

Chair: John H. Golbeck (*Pennsylvania State University*)

8:30 – 9:10 **Aimin Liu** (*Georgia State University*)

Bis-Fe(IV): Nature's Sniper for Long-range Oxidation

9:10 – 9:30 **Lisa Olshansky** (*Massachusetts Institute of Technology*)

Kinetics of Hydrogen Atom Abstraction from Substrate by an Active Site Thiyl Radical in the *E. coli* Class Ia Ribonucleotide Reductase

9:30 – 10:10 **Brian M. Hoffman** (*Northwestern University*)

Nitrogenase: Mechanism of New Substrates and Old

10:10 – 10:40 *Coffee break*

10:10 – 12:20 Session 5 - Controlling reactivity in transition metal complexes

Chair: Kyle Lancaster (*Cornell University*)

10:40 – 11:20 **Wonwoo Nam** (*Ewha Womans University, Seoul*)

Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry

11:20 – 11:40 **Isaac Garcia-Bosch** (*Johns Hopkins University*)

A Different Approach to the Synthesis of CcO Model Systems: A “Naked” Heme-Peroxo-Copper Complex Leads to the Stepwise Formation of Low-Spin Cores with Tunable Structure and Reactivity

11:40 – 12:20 **David P. Goldberg** (*Johns Hopkins University*)

Tuning the First and Second-Coordination Sphere in Biologically Relevant Mn and Fe Complexes

12:20 – 2:30 *Lunch break*

Friday – June 6 – Afternoon Session

100 Berg Auditorium

2:30 – 4:10 **Session 6 - Radical SAM enzymes**

Chair: Squire J. Booker (*Pennsylvania State University*)

2:30 – 3:10 **Vahe Bandarian** (*University of Arizona*)

Tales from the mines: Prospecting for novel transformations in secondary metabolism and tRNA modification

3:10 – 3:30 **Martin I. McLaughlin** (*Massachusetts Institute of Technology*)

Caught in the Act: Snapshots of Sulfur Insertion by Lipoyl Synthase

3:30 – 4:10 **Catherine L. Drennan** (*Massachusetts Institute of Technology*)

SPASMs and twitches in the AdoMet radical superfamily

4:10 – 7:30 *Free time / dinner*

Friday – June 6 – Evening Session

7:30 – 8:30 **Plenary lecture 2**

100 Berg Auditorium

Chair: Partha Basu (*Duquesne University*)

Markus W. Ribbe (*University of California, Irvine*)

Hydrocarbon Formation by Nitrogenase

8:30 – 10:30 **Poster session 2**

Willaman Bridge

8:30 – 10:40 Session 7 - Hydrogenases

Chair: Hannah Shafaat (*Ohio State University*)

8:30 – 9:10 **R. David Britt** (*University of California, Davis*)

Assembling the H-Cluster of [FeFe] Hydrogenase

9:10 – 9:30 **Daniel L. M. Suess** (*University of California, Davis*)

Mechanistic Investigations into [FeFe]-Hydrogenase H-Cluster Bioassembly

9:30 – 10:10 **Rudolf K. Thauer** (*Max Planck Institute of Terrestrial Microbiology*)

Electron-Bifurcating Hydrogenase Complexes

10:10 – 10:40 *Coffee break*

10:10 – 12:20 Session 8 - Controlling reactivity in transition metal complexes II

Chair: Matthew Kieber-Emmons (*University of Utah*)

10:40 – 11:20 **Jonas C. Peters** (*California Institute of Technology*)

Catalytic Reduction of Nitrogen to Ammonia by Mononuclear Iron Complexes

11:20 – 11:40 **Ashley B. McQuarters** (*University of Michigan*)

Modeling the Key Intermediate in Cytochrome P450 Nitric Oxide Reductase:
Electronic Structure and Reactivity

11:40 – 12:20 **Kenneth D. Karlin** (*Johns Hopkins University*)

Copper Dioxygen Coordination Chemistry in Relationship to Copper Proteins

12:20 – 2:30 *Lunch break*

Saturday – June 7– Afternoon Session

100 Berg Auditorium

2:30 – 4:10 Session 9 – Design and control of reaction outcomes in metalloproteins

Chair: Ben Allen (*Pennsylvania State University*)

2:30 – 3:10 **Amie K. Boal** (*Pennsylvania State University*)

The essential stereoinversion in carbapenem antibiotic biosynthesis (1): Structure

3:10 – 3:30 **Wei-chen Chang** (*Pennsylvania State University*)

The essential stereoinversion in carbapenem antibiotic biosynthesis (2): Mechanism

3:30 – 4:10 **F. Akif Tezcan** (*University of California, San Diego*)

Evolution of Inorganic Reactivity in Biological Scaffolds

4:10 – 7:30 *Free time / dinner*

Saturday – June 7 – Evening Session

7:30 – 8:30 Plenary lecture 3

100 Berg Auditorium

Chair: Michael T. Green (*Pennsylvania State University*)

Andrew S. Borovik (*University of California, Irvine*)

Synthetic Chemistry as a Window into Metallobiochemistry

8:30 – ... *Final social get-together & beer*

Champs, 1611 N Atherton St

Shuttles to Champs will leave from the Chemistry Building starting at 8:30; last return shuttles from Champs to Eastview Terraces (on-campus housing) and the Atherton hotel will leave at midnight

Bioinorganic Workshop and III Frontiers in Metallobiochemistry Symposium
2014 Survey Results

259 Attendees Surveyed
104 Responses

1. EVALUATION OF OVERALL MEETING

Course Reservation Procedure

50- Excellent
34- V. Good
8- Good
0- Poor
12- No Response

Breaks

53- Excellent
36- V. Good
11- Good
2- Poor
2- No Response

Facilities (lecture halls)

77- Excellent
22- V. Good
4- Good
0- Poor
1- No Response

Facilities [lab (workshop only)]

50- Excellent
19- V. Good
4- Good
0- Poor
31- No Response

Lodging

43- Excellent
34- V. Good
11- Good
0- Poor
14 No Response

Networking Opportunities

59- Excellent
32- V. Good
9- Good
1- Poor
10 – No Response

Lecture Topics

63- Excellent
28- V. Good
6- Good
1- Poor
6 – No Response

Lab Exercises [workshop only]

42- Excellent

28- V. Good

2- Good

0- Poor

32- No Response

Staff

81- Excellent

19- V. Good

1- Good

1- Poor

2- No Response

Please answer the following questions if you attended the bioinorganic workshop. If you attended only the symposium, please go to question 22.

2. Did this workshop provide valuable professional development for you?

68- Yes

3- No

3. Would you recommend this training session to a colleague?

69- Yes

3- Maybe

0- No

4. Where did you learn about this training program?

1- Website

46- Supervisor

21- Colleague

3- Other (please specify)

- at the Metals in Biology GRC

- Already knew about it from attending the past two times.

- A seminar speaker at my University told me about it when we went out to lunch.

-oops - I accidentally answered these questions about the workshop - I sent students but did not attend myself

5. What area of research/work do you do?

1- Biocatalysis

4 - Biochemistry

1- Biochemistry and Biophysical Chemistry

1- Biochemistry/Bioinorganic

1- Biogeochemistry

12- Bioinorganic Chemistry

1- Bioinorganic/Biophysical work on Photosynthesis

1- Biological Chemistry, FeS Clusters

2- Biophysics

1- Carbohydrate degradation

1- Chemistry

1- Chlorite Dismutase Proteins and other heme binding proteins

2- Computational Chemistry

3- Enzymology

1- EPR on Photosynthesis

1- EPR spectroscopy

5. Continued: What area of research/work do you do?

- 1- Fe enzymes
- 1- Fe Fe Hydrogenase
- 1- Fe-S proteins and Fe homeostasis
- 1- Heme Biochemistry
- 1- heme protein spectroscopy
- 2- Hydrogenase
- 2- Inorganic chemistry
- 1- ITC Zn binding
- 2- Metalloprotein design
- 1- Metalloprotein engineering
- 1- Mononuclear and dinuclear non-heme iron mechanistic studies
- 1- peptide metal coordination
- 1- Protein Biochemistry
- 1- Protein Crystallography and Kinetics
- 1- Pulse EPR
- 2- Radical SAM enzymes
- 1- Redox enzymology
- 1- Redox protein enzymology
- 1- RnR
- 1- Structural bioinorganic chemistry
- 1- Structural biology
- 1- Structural biology, bioinformatics
- 1- Syntheses of model complexes for hemoglobin, myoglobin, p450, and intermediates of related reactions
- 1- Synthetic analogues for active sites in metalloenzymes
- 1- Synthetic Models of Metalloenzymes
- 1- x-ray absorption spectroscopy, metallobiochemistry
- 1- X-ray Crystallography
- 1- X-ray Spectroscopy
- 1- X-ray spectroscopy / biochemistry

6. Why did you participate in this training program?

- a teacher
- acquire a broader knowledge in areas related to my work
- all topics are essential for my professional development
- caught up on current research/learn more techniques
- exposure to new techniques, training in several techniques i would like to use in my own research
- first real international-level symposium/workshop i decided to attend during my phd. was a great experience to see, meet, and network with the best in the world regarding bioinorganic chemistry.
- for learning more techniques
- gain expertise in certain biophysical techniques
- gain knowledge on other techniques
- group convention and personal interest
- hands on practice.
- i participated as a teacher in the workshop
- i taught in the hands-on portion
- i was asked to participate
- i was invited to give a lecture
- i was teaching the itc section. i go to psu
- i work for carsten
- i've always wanted to learn more about spectroscopic techniques but find it hard to learn so many so quickly. this course was a great overview.
- improve bioinorganic skills
- instructor for epr i
- learn bioinorganic techniques
- learn new methods

- learn new methods, networking
- learn new techniques and instrumentation from experts in the field
- mass spec
- my advisor wanted me to
- networking
- networking, gaining fundamental understanding in many areas of bioinorganic chemistry
- opportunity to learn new techniques
- professional development and networking
- psu third floor resident
- recent shift in focus towards corrinoid proteins and ferredoxins
- recommendation of my advisor
- referred by pi
- suggested by my pi.
- taught a section.
- teaching & training
- teaching and networking
- to become familiar with collaborator techniques
- to become more familiar with a variety of techniques in this field
- to discover techniques available to me and network with colleagues
- to enhance my knowledge
- to further my general knowledge of techniques used in bioinorganic research
- to gain experience
- to gain hands on introductions to multiple technique we may decide to pursue at a later date
- to gain knowledge about things and techniques we do not do in our lab.
- to get an overview of the methods used in the field
- to get exposure to the field and research methods used in this field
- to get more experience and learn more
- to get updated with the field and networking
- to help teach a workshop and gain understanding of other spectroscopic methods not available on our campus
- to learn
- to learn about basic spectroscopic methods that i will use for my research
- to learn about new techniques
- to learn about the techniques available to my research project
- to learn many important spectroscopic technique in my research field as well as also it will help me in my carrier development.
- to learn many new techniques.
- to learn more about available experimental techniques
- to learn more about experimental techniques
- to learn more about spectroscopy and its applications
- to learn new spectroscopic techniques
- to learn new techniques
- to learn spectroscopies covered
- to learn techniques that we do in our lab
- to teach
- to understand thermodynamic, kinetic, spectroscopic and theoretical aspects of protein sciences.

7. Which lectures, if any, did not live up to their educational merit?

Please elaborate and suggest improvements.

- protein electrochem
- biological electron transfer
- ..not on target. needs to be more instructive and not geared to an audience that knows a lot about that subdiscipline
- All were exceptional
- Bioinformatics
- Bioinformatics
- Bioinformatics - The talked seemed to miss the audience in that it was hard to find relevance to the work I'm doing.
- Biological electron transfer - This talk was more of an overview of the presenter's work instead of a pedagogical review of the topic; it was hard for someone unfamiliar with the topic to be engaged. Perhaps this talk would have been more

appropriate for the symposium.

- Protein electrochemistry - Again, this talk was not very pedagogical and would have benefited from an overview of the topic.
- Bioinformatics I was good in familiarizing us with online resources but not how to use them; I heard this was addressed in the second part, so it may have been more helpful to consolidate parts I and II or have some overlap for those who only enrolled in I.
- Bioinformatics.
- Computational chemistry - good overall and emphasized the imperfection of DFT, but it would have been nice to go into more detail regarding what DFT is good for, and what areas are weak
- Electron transfer - this felt more like a plenary on Dutton's career, rather than a lecture on the theory of electron transfer or the tools used to study it
- Mossbauer Spectroscopy - provided lots of very interesting exceptions to the usual rules, but I don't think Eckard spent enough time on the basics; a novice would have been overwhelmed
- Protein Electrochem - as with Les Dutton's talk, it would have been nice to get more into the technique itself, how it works, and what you can learn from it
- Mass spec - I thought the focus was awfully narrow. I'm not sure what I would've done differently, but I don't feel like - I will use what he talked about in my work.
- crystallography, I don't think the basics were taught/explained well enough to follow
- DFT/ORCA: I think this would have benefitted from a guided tutorial as opposed to giving the class free range to work on their own.
- Bioinformatics II: The task was quickly completed and not entirely fulfilling.
- Electron transfer: I did not learn much about the technique itself or the necessary controls/procedures we should take in case we are interested in applying these methods to our research. The lecturer was difficult to understand. It would be great if the lecture emphasized methodology more.
- X-ray crystallography: The lecturer was clear, but the content of the lecture was very basic. I think most people did not learn much new. Oliver Einsler's lecture during the symposium really captured what can be done with X-ray crystallography, and I wish the workshop talk was more like that.
- Mossbauer: Speaker was not engaging.
- I felt like I learned a lot from each lecture.
- I really enjoyed the MCD lecture but I expect it was too advanced for many of the students.
- I struggled with the Mossbauer lecture. Found it hard to follow. Perhaps just another set of eyes during preparation of the lecture slides.
- I think the mass spectrometry lecture was interesting, but it could be related a more to the bioinorganic chemistry
- Mossbauer spectroscopy (Eckard Munck)
- EPR spectroscopy (Art van der Est)
- Frank Neese set-up such beautiful lectures teaching us about theory and then applying it, it felt really easy to follow and understand his examples. I think a few times these professors mentioned above may have missed a few steps when going from theory to applying that knowledge. While going through some of the examples, I was not able to understand the point they were trying to make and specifically how one goes about interpreting the raw data.
- Magnetic Circular Dichroism, Mossbauer. They were more of a talk about the professors current projects than a lecture to teach students about the theory and technique.
- Markus W. Ribbe, Kenneth D. Karlin, Bioinformatics, Wonwoo Nam
- Mass Spectrometry, X-ray crystallography, Bioinformatics
- Mossbauer was disorganized
- Electrochemistry was more of a research summary than educational on the technique
- most
- N/A.
- no
- no problems! all of the lectures were very good!
- No.
- none
- None
- None in particular
- Protein electrochemistry skipped how interpretation of the data is performed. Explaining what the signals mean.
- protein electrochemistry was a great lecture, but did not introduce many concepts of the method
- Some lectures on the techniques and method in Bio-inorganic were maybe too specific and not enough general.
- Some lectures were difficult to understand without a good background in physics or spectroscopy. I think when understanding and learning about techniques there has to be a good balance of what knowledge is necessary to be able to

use the technique in an experiment and understand the experiment versus knowing all the mathematical derivations.

- The following speaker's lecture was well-intentioned, but presented in a confusing manner (the speaker was a brilliant scientist but not good at presenting the material to a non-specialized audience): Eckard Munck
- The following speakers' lectures could have more instructive content: Fraser Armstrong, Leslie Dutton
- The missing talk. I was very much looking forward to the talk by Catherine Drennan on SAM enzymes.
- The Mossbauer lecture was basically at a level for Mossbauer experts, i.e., a too high level for the audience. The electrochemistry lecture was a lecture about hydrogenases, not about electrochemistry. I am certain that Sean Elliot would have given a much better lecture, because the tutorial was excellent. The crystallography lecture was a bit confused, I think (I am a crystallographer). It would benefit from a clearer structure, following the organization of textbooks.
- those that focused on the lecturer's own research rather than the method itself
- X-ray crystallography, electrochemistry

8. Which lectures did you like best?

List as many as you wish to mention.

- EPR 1 and 2
- all of Frank's lectures
- all
- All lectures by Frank Neese were A-M-A-Z-I-N-G,
- Stefan Stoll lecture was great (pulse EPR)
- Nicolai Lehnert (MCD)
- Serena DeBeer (Xray Spec)
- Nozomi Ando (SAXS)
- Jeff Agar (MS)
- Dean Wilcox (ITC)
- All lectures were good. My favorite was Introduction to coordination chemistry, EPR, pulse EPR, Magnetic circular dichroism spectroscopy, X-ray spectroscopy
- all lectures were great
- All of the lectures by Frank Neese. Jeff Agar's lecture was both educational and entertaining.
- All of the lectures were great but I particularly enjoyed Stefan Stoll's pulse EPR talk.
- As the content of the lectures were all very good, the only thing separating the different lectures would be the quality of the lecturer. Frank Neese, Serena DeBeer, Amie Boal and Nozomi Ando were the best. Honourable mention must go to Nicolai Lehnert whose ability to party every night and still give a good lecture is impressive.
- computational chemistry
- ligand theory
- pulsed EPR
- MCD
- Resonance Raman
- small angle x-ray scattering
- Dean Wilcox, ITC
- Pulse EPR, Stefan Stoll
- EPR
- EPR
- Pulse EPR
- SAXS
- EPR (both), X-ray spectroscopy, rRaman, Mossbauer, and kinetics
- EPR by Dr. van der Est
- X-ray absorption spectroscopy
- EPR I and II lectures, Raman
- EPR I and Mossbauer
- EPR, ENDOR, ITC, x-ray spectroscopy
- EPR, X-ray spectroscopy, ITC, SAXS
- EPR, XAS, Dr. Bollingers lecture, ITC.
- EPR!
- F. Neese
- O. Einsle
- S. DeBeer

- B. Hoffman
- Frank Neese's lectures were very useful during the workshop. Also I enjoyed learning about SAXS. Marty Bollinger's kinetics talk was also helpful.
- Frank Neese's talks were not only extremely informative, but exquisitely paced
- high resolution mass spec
- High Resolution Mass Spec
- Isothermal titration calorimetry
- Pulse EPR
- Transient Kinetics
- I think one of the best lectures were stefan Stoll's Pulse EPR, and Dean Wilcox's ITC one.
- Intro to Coordination chem - very good
- X-ray spectroscopy - excellent
- Resonance Raman - very good
- EPR - simply phenomenal
- Pulse EPR - excellent
- SAXS - very good
- Intro to coordination chemistry, Intro to comp chemistry, Biological electron transfer, resonance Raman spectroscopy, - Both EPR lectures, Mossbauer, small angle x-ray scattering,
- Introduction to Coordination Chemistry, Introduction to Computational Chemistry, Pulse EPR ENDOR ESEEM DEER, - - - Mossbauer Spectroscopy, Small angle X-ray scattering
- ITC
- EPR
- SAXS
- Biological electron transfer
- ITC, among others
- ITC: I learned a lot, and Professor Wilcox was really engaging. It was neat that there was a lot of emphasis on the methodology as well as a variety of scientific problems.
- SAXS: The lecture was very succinct and covered theory, instrumentation, and application very well. The speaker was very engaging.
- Lectures by: Frank Neese, Stefan Stoll, Dean Wilcox, Nozomi Ando. Great speakers with very relevant information to present!
- Les Dutton
- Michael Johnson
- Ligand field theory, Computational Chemistry, EPR, Pulse EPR, MCD, Transient State Methods, Mossbauer
- Neese's talks (especially the first one)
- Stoll's EPR
- Pulse EPR, ITC, SAXS
- Pulse EPR, X-ray spectroscopy
- pulsed epr, exafs, mcd, coordinaion chem, computational chem, itc, sax, transient methods
- Raman/IR, MCD
- SAXS
- SAXS - Very well explained the theory and pratical examples (and I had no previous knowledge of SAXS)
- SAXS,
- SAXS, PULSE EPR, and ITC
- Serena DeBeer, Dean Wilcox, Oliver Einsle, Jonas C. Peters, David P. Goldberg
- Stefan Stoll
- Stefan's pulse EPR even though I already do pulse EPR. Neese's intro lecture was very good too.
- The EPR lectures were fantastic, as was the quantum lecture
- The lecture (transient kinetics) by Prof. Bollinger
- The lecture on EPR given by Art van der Est was by far the best lecture, even with the limited amount of time given he still managed to cover everything that was important for the workshop, while still maintaining an even keel pace.
- The Neese lectures were excellent, but you already knew that.
- transient state kinetics; biological ET; Intro to QChem; Ligand field theory; SAXS; EPR (both).
- Transient-state kinetics (Prof. J. Martin Bollinger, The Pennsylvania State University)
- X-ray crystallography,
- X-ray spectroscopy
- X-ray spectroscopy, differential scanning calorimetry, protein film voltammetry
- XAS, both EPR lectures, MCD, ITC, SAXS

9. What topics, if any, did not live up to their educational merit?

Please elaborate and suggest improvements.

- bioinformatics 2
- Anaerobic protein purification was basically the same protein purification methods I'm used to, but in a glove box. I did not learn much from that session, but my research has involved a great deal of aerobic protein purification. EPR II with Alexey Silakov was not very informative. He talked at us the whole time without any notes or figures, and just confused everyone. I'm told the sessions run by Professor Stoll were much better. Bioinformatics I was not very helpful (just another powerpoint presentation), but bioinformatics II was presented in a very useful format (a self-guided series of tasks that the course instructors could assist with as needed).
- Bioinformatics
- Bioinformatics
- Bioinformatics: the motivation was not clear to me initially, and for a general audience the common aspects of all databases introduces could be highlighted before going into details.
- biological electron transfer, protein electrochemistry
- DFT with orca. Overall the hands-on topic was interesting and helpful, but I could not get much out of the experience solely due to computing power. If there were just a few computers with sufficient processing power and we worked in small groups, the experience would have been more rewarding.
- DFT/ORCA - all they did was give us a .pdf of exercises and let us loose for 4 hrs. This was nice if you have one thing you want to learn how to do. But, it would have been nice to get some sort of overview of how to use the program and what sorts of things it is good at telling you. Also, what can ORCA do that gaussian or other DFT suites cannot?
- For most of the talks, we ran out of time, and I wish we got to see actual examples or applications that the technique or approach helped us to understand the science.
- I enjoyed all the topics I choose. Although I learned a lot from the anaerobic protein purification and the technique is obviously indispensable, the layout of the demonstration was rather dull.
- I think I had a little trouble understanding the MCD portion in the workshops. It was good to work through the data, but I feel like all I really learned was how to use Origin and I didn't further my understanding of the MCD method.
- Isn't this the same as question 7?
- MCD Hands on
- Mossbauer, Electrochemistry
- n/a
- no
- no problems! all of the lectures were very good!
- No.
- none
- none
- None
- None
- None
- None
- Protein electrochemistry. There was a lot of hype about this topic, but the lecture was sort of dry. The information was ok, but it could have been prepared a little better.
- Resonance Raman
- they were all educational
- They were all fine!
- X-ray spectroscopy. I think some work on the soft-wares needed to be done before the workshop.

10. Which lab topics did you like best?

List as many as you wish to mention.

- all I attended
- all I attended were good and effective
- Anaerobic Protein Purification, Resonance Raman, Protein Electrochemistry, Stopped-Flow,
- Anaerobic protein purification, stopped-flow kinetics, bioinformatics, resonance Raman spectroscopy
- anaerobic protein purification
- Because I was teaching I did not attend any of the other labs.
- DFT with ORCA, Mossbauer spectroscopy, Small-molecule QQQ mass spectrometry and EPR I

- Ditto.
- Electrochemistry, Resonance Raman, Bioinformatics II and III, Pulse EPR
- Electrochemistry, ITC, stopped-flow, freeze-quench, resonance Raman
- EPR
- EPR, Protein electrochemistry, Raman spectroscopy
- EPR 1 was by far the most illuminating lab section I attended. Dr. Golbeck's explanation of EPR fundamentals was the first to finally "click" for me.
- EPR I and EPR II X-Ray Crystallography, X-Ray Absorption, DFT
- EPR I, EPR II, Electrochemistry, Stopped-flow
- EPR I; Mossbauer; ORCA; FQ; stopped-flow
- EPR II - Pulsed EPR techniques
- EPR III, SAXS, X-ray spec
- EPR III, Protein electrochemistry, Raman Spectroscopy.
- EPR1 by Prof. Golbeck.
- EPRI, Freeze-quench, Anaerobic protein purification, ITC
- Freeze quench
- Freeze quench
- Freeze quench, ITC!!!!
- High Res Mass Spec, Small Molecule Mass Spec, X-Ray Spectroscopy, Freeze Quench
- I enjoyed the ITC and EPR workshops
- I liked all the lab sections I took: Cryoreduction, EPR I, Mossbauer spectroscopy, and anaerobic protein purification
- I loved the x-ray crystallography section, I also thought the bioinformatics session was easily applicable to my own work (I took 1 and 2)
- ITC, Freeze Quench, EPR, and Stopped Flow
- ITC; Pulse EPR and introductory EPR were really good.
- John Goldbeck's EPR I class was phenomenal!
- MCD spectroscopy, protein electrochemistry, stopped-flow, freeze quench
- MCD, X-ray crystallography
- Mossbauer, cryoreduction
- Mossbauer, EPR, and ITC
- Mossbauer, EPR1
- Mossbauer; Bioinformatics I, II, III; Stopped-Flow Absorption; X-ray Spectroscopy, Isothermal Titration Calorimetry.
- Protein Electrochemistry
- Protein electrochemistry, EPRI, Freeze-quench method
- Protein purification
- Pulse EPR
- Pulse EPR, stopped flow, Mossbauer
- pulsed epr, transient epr, resonance raman
- Raman, epr 2, cryoreduction, stopped flow
- Raman, MÅssbauer, MCD
- Raman, X-ray Crystallography, EPR I and II, Steady State
- rapid freeze quench, electrochemistry
- Rapid freeze quench, anaerobic protein purification, DFT with orca.
- Resonance Raman, EPR I, and freeze quench
- rRaman, ITC, EPR1 and EPR3 were great.
- rRaman was very hands on. There was in depth explanation of how the instrument works as well issues that one might encounter.
- ITC was taught by one of Dean's students. She was very thorough and anticipated/answered all of the questions that I had before I even asked them. Getting to explore the software was also nice.
- EPR1 was good in that it started on a very fundamental level (considering the short time frame). We got to look at the inner workings of the instrument (such as the resonant cavity). We went over what has to be done to collect good data, such as saturation curves, a point that I think is often overlooked. The prof seemed a bit bothered that I had run EPR before; I think he was worried that I would be bored. However, I found it both interesting and informative!
- EPR3 was also very hands on. Stephan packed a lot of information into the session. He asked us a lot of questions and kept us engaged and thinking. I feel like this is the session that I learned the most in.
- I heard varied opinions about these sessions. It seems that it depended on who taught the session.
- stop flow
- Stopped flow and freeze quench were great because they were hands on.

- Stopped-flow
- Stopped-flow kinetics
- The ITC workshop was very informative, and the stop flow was extremely helpful. Raman was also very interesting.
- The more interactive ones were the best, such as: resonance raman, stopped-flow and EPR3.
- X-ray Spec, MCD, MS, Protein Electrochemistry
- X-ray Crystallography, cryoreduction, anaerobic purification, epr

11. What lecture topics, if any would you like to see covered in future bioinorganic workshops?

- bioinformatics
- cryo-EM
- Determining of Equilibrium Binding constants using fitting software like Hyperquad, Specfit.
- Electron microscopy
- I thought the topics were perfect.
- I would like to see some sort of fluorescence microscopy
- Flow cytometry"
- Microscopy methods (Cryo-EM, fluorescence, TEM, SEM, AFM, etc.)
- Model complexes - seeing how big a role it plays in the field, and how many organic chemists come to the workshop to learn more about bio(inorganic)chemistry, I think the biochemists would benefit from learning more about (metallo)organic chemistry as well.
- More about inorganic synthesis and ligand design for model complexes
- More copper-related things. (I agree with Kenneth Karlin, too much iron (-sulphur clusters)).
- n/a
- NMR spectroscopy with respect to metalloproteins (or model complexes) that includes 2D NMR
- NMR, SPR (Surface Plasmon Resonance), Fluorescence
- none
- NRVS
- NRVS, Marcus theory (got mentioned probably a dozen times in the week, but was never fully explained), Tunneling/Kinetic isotope effects?
- Nuclear Magnetic Resonance (NMR) Spectroscopy, Fluorescence spectroscopy, Circular Dichroism (CD) spectroscopy, - - Infrared (IR) spectroscopy, Terahertz Spectroscopy and Laser Flash Photolysis.
- Nuclear Resonance Vibrational Spectroscopy
- Nuclear resonance vibrational spectroscopy is something that is starting to appear a bit more in the literature. It would be nice if it were mentioned/explained in one of the lecture talks.
- Sensing (calcium, zinc, hydrogen peroxide, etc.) and application to metal-ion homeostasis
- The current selection is just right.
- transient optical spectroscopy

12. What topics of hands-on lab sections would you like to see offered at future bioinorganic workshops?

- Circular Dichroism
- Electrochemistry with respect to model complexes (in addition to the protein e-chem already offered)
- "fluorescence microscopy, Flow cytometry"
- Fluorescence, SPR
- Fluorimetry?
- Found the offer already quite broad
- freeze quench
- I thought the hands on sections were perfect.
- Just the ones that were offered this time.
- Maybe NMR, otherwise a large range of analytic tools and practical sessions are already provided which is great.
- Microscopy methods (Cryo-EM, fluorescence, TEM, SEM, AFM, etc.)
- Model complexes? If feasible.
- n/a
- NMR spectroscopy
- Nuclear Magnetic Resonance (NMR) Spectroscopy, Fluorescence spectroscopy, Circular Dichroism (CD) spectroscopy, - - Infrared (IR) spectroscopy, Terahertz Spectroscopy and Laser Flash Photolysis.
- "Oxygen electrode, Head space gas analysis"
- Spectroelectrochemistry

- The only thing I can think of is UV-vis or IR techniques, which the synthetic inorganic people use. However, this technique is rather basic.

13. Did you feel you had enough space to conduct the lab exercises?

67- Yes

2- No

14. Was the time allocated for the poster session adequate?

66- Yes

4- No

15. Did the on-campus housing (if applicable) live up to your expectations?

43- Yes

8- No (please comment)

- Shampoo would have been nice but not necessary.

- i did not use these services

- not applicable

- I didn't stay in the on-campus housing but my grad student did. We found it very difficult to find the residence where he was staying. Maybe we missed it but we didn't get any instructions on where to check-in. There was also a mix-up with payment. We were charged for the room although it was prepaid. This was sorted out and I got re-imbursed so it was not a huge problem. I also heard that there were problems with the hot water in the residence and my student had to have cold showers.

- we lived off-campus in a rented apartment, which costed us about half the price of the on-campus housing.

- not applicable

- The housing was fine, but dealing with any issues was a bit of a hassle. The kids in the Pollock Commons help desk did the best they could, but issues with parking passes, non-functioning meal cards and applying payments was kind of a headache.

- The rooms themselves were great. However, the staff did not seem to have a clue what was going on. They were very slow at checking us in. Also, they had us reserve a parking pass, but ran out of them. I ended up having to buy daily passes for a few days until they got the weekly, which ended up costing me more.

16. What services, if any, can the staff provide to make your stay more productive or pleasant?

- A list of activities one can do on campus during downtime, e.g. pool, swimming, table tennis, tennis, etc.

- Aspirin in the mornings would have been great... (just kidding, it was great!)

- Coffee breaks

- Everything was perfect.

- Getting access to the internet was really complicated and the instructions provided did not work. It would be good if this could be simplified.

- Getting internet access was very confusing.

- help finding campus services, dorm and parking when first arriving to campus

- I cannot think of anything!

- I had a lot of problems with the staff at Pollock Commons with getting my parking permit. They required me to purchase a parking permit even though I requested one through my registration.

- It was great that we had access to the buildings at any time and there was food and drink provided throughout all breaks. A recommendation for places/restaurants where to have lunch/dinner might be useful for people who haven't been to State College before. Bar of the day was a great way to interact with people in the evenings. For some nights it would have been equally good to know where to go after it closes/ have recommendations for places to stay out after midnight! However, all in all one has to really applaud the great organisation by staff and students involved!

- More coffee please

- None

- not applicable

- staff did a great job

- The hot water on our floor did not work very well. It would take 15-30 mins to get hot water.

- The PSU staff were awesome!

17. Additional comments and suggestions.

- An idea, although I don't know if its possible would be to organize lunch during the workshop.
- Both the workshop and symposium were fantastic! Many thanks to the faculty, staff, and students who organized it.
- Everything was awesome! I enjoyed the workshop and symposium!!
- I will definitely lobby for everyone from the group to participate in this workshop in the future!
- I would prefer some evening social activities that don't revolve around alcohol. The organizers were incredibly friendly, which I appreciated given how much stress and pressure they were under. Thanks for doing such a great job.
- if possible than, its good to get more time between hands on experiment.
- irving's catering was delicious.. stick with them for next time!
- It was a little difficult to sit through 1.5 hrs of lecture. I think that 1 hour lectures would be more efficient. Also, it - would be nice if the focus was less on theory and more on the potential applications of each technique.
- it was awesome - thank you!!
- Kudos to the faculty of the chemistry department for organizing such an excellent workshop!
- Less focus on drinking alcohol in social engagements and have more activities (bowling?) because it was difficult to - stay social if we were too tired/sick of drinking
- Nice social program :)
- no
- Organizes student/post doc with specific faculty social sessions
- Overall, this workshop and symposium were great. However, one comment/suggestion could be made: The cost of the workshop was a bit prohibitive. I guess that was due to travel fees of workshop teachers from aboard (i.e. Germany). I wonder if some more local workshop teachers could have been found in order to reduce the cost of the workshop.
- Some power outlets in the lecture hall did not work.
- Thank you for a great workshop and a wonderful symposium.
- Thank You for all of your hard work in putting this together! It was a wonderful experience.
- The ITC, Electrochem, and EPR I & III workshops were fantastic
- The on-campus housing was fantastic. I really wouldn't have expected it to be so good. Overall the Workshop and - Symposium were perfectly organized. Friendly staff, spacious facilities. Congratulations! If I must say something only vaguely "negative" that would only be too much AC in the Berg Auditorium!
- Unfortunately, a lot of the networking opportunities especially outside the workshop and symposia were at night at bars, so it was difficult for people who don't drink to get themselves involved in such activities. I think more diverse places for the night would be beneficial where everybody could attend.
- Well run workshop. All those who helped organize it did a wonderful job. It was clear they worked very hard.

18. Recommendations for improvement.

- Another caterer for the BBQ ;-)
 - One 5 minute break in the 1.5h lectures of the workshop
 - A group sporting evening like the hike/organized volleyball tournament known in advance (people very much enjoyed that!)
 - I was really overwhelmed by the amount of software I had to download for some of these workshops. Most of these downloads are programs I will never use again, and some of the recommended downloads are programs that aren't even compatible with my operating system. Could less burden be placed on participants' computers in the future? Also, Matlab doesn't offer a free trial version. Please, please, please give longer lunch breaks for the workshop. With travel time to restaurants / dorms , there was very little time to actually eat.
 - Improve communication and the flow of resources between the 'big-wigs' and the people actually running the Pollock Commons desk.
 - Also, improvement for question 21. Personally, I have no academic status, I am a research scientist, but that doesn't fit within your 4 choices.
 - Keep up the great work!
 - More breaks, or at least a break after 1 hour of lecture. 1.5 hours of sitting is too much and makes people restless.
 - More coffee during breaks especially post lunch.
 - More diverse socializing opportunities, like outing, or hiking.
 - more diversified topics for lecture
 - None whatsoever!
 - suggest airbnb to get combined, cheap housing off campus. worked well for a few of us
- The only complaint I have is that when we arrived to the housing front desk they told us that we had to pay for our lodging when in fact we were teaching a workshop...Eventually they figured out that we didn't have to pay. Upon

checkout the day we left they also tried to tell us we had to pay the balance remaining for our lodging. Again it worked out and they figured out that we didn't have to pay anything...I don't think this has anything to do with the PSU organizers, but rather the staff people at the front desk being unorganized!

- The topics for the plenary sessions are mostly biochemistry/bioorganic which makes sense considering the very title of the symposium. However little bit of more bioinorganic perspective I think would have been better. Also in even in biochem topics, the lectures were not much diversified, it was predominantly on Nitrogenase related stuff.

- There were a few hands on sections that could have been improved. Namely, the mossbauer and to a lesser degree, the resonance raman workshops.

19. Are you working at The Pennsylvania State University (University Park)?

14- Yes

58- No

20. Were you one of the workshop teachers (i.e. presented a lecture or taught one of the hands-on sections)?

25- Yes

47- No

21. What is your academic status?

50- Student

14- Postdoctoral Fellow

1- Research technician/assistant

8- Faculty

Please answer the following questions if you attended the Frontiers in Metallobiochemistry Symposium.

22. How do you view the selection of speakers and topics?

64- Excellent

27- Very Good

3- Good

1- Poor

23. What lectures did you like best?

Please list as many as you feel is appropriate.

- A Really Close Look at Bioinorganic Metal Center, Hydrocarbon Formation by Nitrogenase, The essential stereoinversion in carbapenem antibiotic synthesis, Evolution of Inorganic Reactivity in Biological Scaffolds, X-ray Spectroscopic Studies of Biological Catalysis.

- Really Close Look at Bioinorganic Metal Centers by Prof. Oliver Einsle

- Akif Tezcan always blows me away.

- Akif Tezcan, Martin McLaughlin

- All

- Already mentioned in Q8

- Andy Borovik

- Brain Hoffman

- Ceilia Goulding

- Andy Borovik

- Jacqueline Barton

- Serena DeBeer

- Chuan He

- Ken Karlin

- F. Akif Tezcan"

- Crystallography Model Systems

- D. Britt, S. DeBeer
- Einsle, Teczan
- Frank Nesse
- I really enjoyed the sessions on X-ray methods and controlling reactivity in metal complexes. Jackie Barton's talk on DNA-mediated signalling was outstanding. I really like the interpolation of student and post-doc talks into the program; the students and post docs gave excellent presentations and it's great to give them this opportunity.
- Insights into how Mycobacterium tuberculosis acquires iron from heme, Celia W. Goulding
- Jackie Barton, Andy Borovik, Serena DeBeer
- Jacqueline Barton, Oliver Einsle, Vahe Bandarian, Alexey Silakov (would have loved to hear Cathy Drennan, but Alexey did a great job filling in for her!), Akif Tezcan, Andrew Borovik, Martin McLaughlin, Daniel Suess
- Oliver Einsle because he pointed out the pitfalls to x-ray crystallography.
- Oliver Einsle, Serena DeBeer, Vera Krewald, Andy Borovik, Akif Tezcan, Dave Britt
- quality of all lectures was high
- Rolf Thauer
- Serena DeBeer, Oliver Einsle - phenomenal
- Lisa Olshansky
- Alexey Silakov
- Dave Britt, Daniel Suess
- Synthetic Chemistry as a Window into Metallobiochemistry, Evolution of Inorganic Reactivity in Biological Scaffolds
 - The ones on nitrogenases
 - X-ray Spectroscopic Studies of Biological Catalysis
- Burton
- I loved the student talks and Serena DeBeers. They were all really good though!
- all lectures in ""Controlling reactivity in transition metal complexes
- all lectures in ""Design and control of reaction outcomes in metalloproteins
- all lectures in ""Detailed insight into biological long-range redox reactions
- Martin Maclaughlin's
- Andy Borovik's, Aimin Liu's, Jacqueline Barton's, Oliver Einsle's, and Kenneth D. Karlin's
- Anne Boal, Dave Britt, Cathy Drennen, Oliver Einsle, Aimin Liu, Jonas Peters, Akif Tezcan, nearly all the student/postdoc talks
- Borovik, Peters, W. Nam, Aimin Liu, Britt
- All the plenary lectures
- All interesting
- I enjoyed the Tezcan lecture (I have an interest in protein engineering) and the lecture on DNA charge transfer.
- Mike Johnson, Lisa Olshansky, Serena DeBeer
- I liked all the lectures!
- Serena DeBeer, Oliver Einsle, Jacqueline K. Barton, F. Akif Tezcan and so many others... there were really only a small handful that I didn't enjoy. Many of the student/Post doc speakers were also top notch!
- Dr. Barton, Dr. Borovik, Dr. DeBeer, Dr. Einsle, Dr. Goulding, Dr. Tezcan, and Dr. Peters
- I enjoyed nearly all the lectures although some were definitely over my head. My very favorite was Jackie Barton's lecture about electron transfer in DNA. When Celia Goulding's computer stopped functioning in the middle of her talk and she made a joke and just kept going with every detail perfectly memorized, it was simply amazing. I wish that PSU had great female professors like these two!! Drs Hoffman, Johnson, and Thauer were all excellent as well. It was nice to have Lana come back from industry and give a talk & network too. Thank you!!
- All of the plenary lectures were very interesting and I think that the speakers were chosen well.
- I really liked all of them but especially the plenary ones were good.
- Jackie Barton, Andy Borovik and Akif Tezcan
- Evolution of Inorganic Reactivity in Biological Scaffolds - Akif Tezcan
- Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry - Wonwoo Nam
- DNA-mediated Signaling - Jacqueline K. Barton
- Prof. Andy Borovik
- the lecture by Oliver Einsle (A really close look at bioinorganic metal centers)
- Jacky Barton
- Chuan He, Oliver Einsle, Aimin Liu, Wonwoo Nam, Jonas Peters, Andrew Borovik
- A Really close Look at Bioinorganic Metal Centers (Oliver Einsle), DNA-mediated Signaling (Jaqueline Barton), Biomimetic Metal-Oxygen Intermediates in Dioxygen Activation Chemistry (Wonwoo Nam), Hydrocarbon Formation by Nitrogenase (Markus Ribbe), Copper Dioxygen Coordination Chemistry in Relationship to Copper Proteins (Kenneth Karlin)

- Jacqui Barton's lecture was great!!!
- Akif Tezcan's talk, Jacqueline Barton's talk on DNA-mediated signaling, and Markus Ribbe's talk
- Celia Goulding, Brian Hoffman, Akif Tezcan, Andrew Borovik
- Many of the lectures were very good
- Borovik, Tezcan, Karlin, Ribbe, Hoffman, Goulding
- Andy Borovick, Ken Karlin
- Brian Hoffman
- He, Einsle, Peters, Karlin, Tezcan, Borovik, Saleh, Chacon
- Oliver Einsle, Markus Ribbe, Aleksey Silakov, Celia Goulding, Michael Johnson
- Synthetic Chemistry as a Window into Metallobiochemistry by Andy Borovik

24. What other topics would you like to see covered in future bioinorganic symposia?

- Nuclear Magnetic Resonance (NMR) Spectroscopy, Fluorescence spectroscopy, Circular Dichroism (CD) spectroscopy, Infrared (IR) spectroscopy, Terahertz Spectroscopy and Laser Flash Photolysis.
- I'm very interested in the intersection(s) of bioinorganic chemistry with environmental science. Perhaps a session on geobiology / biogeochemistry would be interesting in the future.
- Something a bit out of the ordinary - perhaps someone less established in the community?
- metals in biology....?
- Metal trafficking and metal homeostasis; new methods for measuring metal content of tissues and cells; more co-factor biogenesis
- I think there was a good range of topics covered
- I think it was a well-balanced mix.
- More Mn, e.g. calprotectin.
- Structural biology, bioinformatics
- I thought it was perfect.
- Novel techniques in study metalloenzyme mechanisms and metalloprotein in redox signaling and transcription regulation
- Some variations to symposium one to the next would be expected. With the make-up of the Penn State bioinorganic research groups, O₂-activation must of course always be involved. But, of course there are many. Maybe something in the nitrogen oxide small molecule enzymes and models, bioinorganic would be good,
- More copper
- More on zinc fingers!
- Electron transfer, protein engineering, high level spectroscopy (EPR, MB, UVRR), membrane proteins
- Water Oxidation.
- more spectroscopy!
- More CHEMISTRY (model systems)
- Perhaps an attempt to include more biology & biochem researchers & grad students. There were lots of PSU grad students who didn't really think this applied to them (but it does/or will.)
- Transcriptional regulation
- More copper!
- Perhaps some more about metal homeostasis, i.e. where are metals in a cell, how much is there and what is it bound to.
- More copper chemistry!
- This year symposia, most of the lectures were on FeS cluster, topics like peroxidases, CcO, NOD, NOR, NiR, MMO, peptide chemistry etc was missing.
- disease related and drug screening related topics
- The bioinorganic symposia seemed very focus on metalloenzyme; I would be interested in seeing more medicinal applications of bioinorganic chemistry.
- Electron Transfer
- Less Fe, more Cu, more electron transfer. Metal sensor design, especially for in vivo applications. MRI reagents. - - Applications of bioinorganic (fuel cells, artificial oxygen carriers).
- MRI contrast agents, O₂ evolving complexes, Siderophores, etc.

25. How do you rate the ratio of faculty speakers to student/postdoc speakers?

- 48- Excellent
- 37- Very good
- 6- Good
- 2- Poor

26. Was the time allocated for the poster session adequate?

84- Yes

6- No

27. Did the on-campus housing (if applicable) live up to your expectations?

54- Yes

11- No (please comment)

- The housing itself was alright, but the staff were not organized and not very helpful.
- While the rooms themselves were very comfortable, I had a few complications with the set up and the staff that I would have preferred to have avoided. The staff responsible for the room registration were very disorganized, and they were checking people in very slowly. When I arrived at my room, the bed was lofted, such that it was located about 4 feet in the air. As an aging individual with a bad back, this was not an acceptable arrangement. I called to have the bed lowered. I was not able to reach anyone so I went back to the registration desk, where I stood in line again only to be told that nothing could be done that day but that a work order would be put in for the next day. Unfortunately, I fell hard onto the floor getting up in the night, which was what I was trying to avoid. Older people simply cannot be expected to stay in rooms with lofted beds - beds should all be at a normal height for your guests.
- Stayed in the hotel
- I forgot how loud and annoying dorms are (and how entitled to loudness and annoyingness other dorm denizens feel). - It was clearly a problem in my expectations, having enjoyed pleasant lodging for many years after undergrad.
- I was off-site.
- not applicable
- See above; rented apartment.
- See 15a.
- The housing was adequate, but the staff running the housing desk and check-in process were virtually clueless and not particularly knowledgeable. The maps provided did not indicate where parking was located; on those maps that did, the color-coded parking lots were on a black-and-white map (not particularly useful). The staff was not very helpful regarding parking, location of housing, duration of stay, whether payment was already provided. The key cards did not work. The experience checking in and been directed to housing and parking was probably the worst organized of any conference I have attended.
- not applicable
- The rooms themselves were great. However, the staff did not seem to have a clue what was going on. They were very slow at checking us in. Also, they had us reserve a parking pass, but ran out of them. I ended up having to buy daily passes for a few days until they got the weekly, which ended up costing me more.

28. What services, if any, can the staff provide to make your stay more productive or pleasant?

- More people at the front desk that know about the conference. Keys that are actually working. Information about internet access provided upon arrival. Maps of the area with signs where we are and where to go.
- More orderly registration process at the dorms and rooms set up for anyone of any age who attends the symposium.
- Not having a room right by the party lounge would be nice.
- N/A
- not applicable
- Please have better-informed staff members at the conference services desk when people check in.
- Perhaps some car-service (or golf cart) for faculty to go from hotel to the lecture areas.
- Make clear to us what the internet policy is and where the breakfast service is, along with what days the breakfast isn't open.
- see 16
- The catering during the workshop was much better, if less fancy looking. The ice water for the symposium came from dispensers that had clearly had coffee in them at one point. It was disgusting.
- The staff was excellent. Access to wifi could be streamlined, as I felt that the staff were forced to spend too much time repeating the answers to those questions.
- See above.
- Already mentioned in Q16
- Lectures too early in the morning.
- None
- "Free wi-fi. When I'm at a conference, I'm still conducting work via email. I was trying to publish a paper and files needed to be sent back and forth between authors. That's hard to do without internet, so I was forced to pay the \$5.99 for

each 24 hour period that I needed it.

- Possibly a regular shuttle service between the dorms and lecture hall.
- Coffee breaks
- staff did a great job
- None-- they did a great job!
- I might suggest providing a quick ref list of things to make people feel at home here. (I am local and people asked me "Where are the best wings?" "Where can I get a good bagel and a cup of coffee?") Other things would be, where to use a gym or go running, just basic things people need when they are far from home...

29. Additional comments and suggestions.

- Poster session was quite short, the numbers were mixed up and the setup of the boards made it difficult for people to walk by the posters near the windows.
- Excellent meeting.
- no
- The science part of the conference was great!
- Thank you for this great symposium!
- Q17
- I might be better to do a lecture then workshop instead of all the lectures at once. That way you can apply what you learn to workshop right away.
- None
- I think for the poster session it would have been better to put more people on the second floor and spread them out. It would have been good to also put a sign so that people knew there were some posters on the second floor. Also I was bummed that Catherine Drennan didn't end up giving her talk but I am very impressed by the impromptu speaker.
- Schedule morning talks a little later
- From a networking perspective, both the workshop and the symposium were a bust. Nearly all of the PIs congregated amongst themselves, making them completely unapproachable by students. This was exasperated by the host PIs that sought out other PIs at every function. The same was true for the poster session. Many of the PIs left or spoke only to each other instead of reading posters and interacting with the presenters.
- Wonderful conference-- one of the best I have attended!!
- Carsten did a fantastic job organizing the symposium, and Marty, Squire, Mike and Amie were wonderful as well!
- Loved the setup of lectures & breaks, although the plenary could have started a bit earlier so the poster sessions would get out earlier?
- Thank you very much for allowing me to attend the symposium for no charge. I am a wage payroll person at PSU and find it very difficult to afford additional, but so important, education. The workshop would have been really awesome, but that was full (and expensive.) Maybe consider finding funding opportunities for those who can't afford this? (Especially people like me who (B.S. level) are older and trying to keep skills & knowledge up to date when there really is no money.)
- Shorter lectures (1 hr vs 1.5 hrs), so can maybe add a few more to fill in the day.
- I couldn't stay for the symposium.

30. Recommendations for improvements.

- The poster session gets very crowded - I am not certain there's much to be done but it can be hard to navigate through to see everything. The lecture room is filled to capacity; at times there was little space and people were standing in the back.
- not applicable
- Please have better-informed staff members at the conference services desk when people check in.
- Keep up the great work!
- More coffee during breaks especially post lunch.
- The afternoon schedules were quite tight; a few times we had to rush back from lunch and/or be a little late to the afternoon sessions. As such, lunch was always kind of rushed and stressful. Also, because of the timing of the evening sessions, we had to eat dinner not that long after we'd finished lunch. I'm not sure of a great way to get around this, but maybe you can figure something out for next time.
- The spacing of the breaks in the symposium section should be changed. The lunch break was a good length, but then the dinner break started two hours after the lunch break and a early dinner was required to make it back in time for the night lecture.
- I would love to see the symposium every two years, and in a larger lecture hall. I also see an opportunity for PSU to

bring more undergraduates to the symposium; PSU is centrally located (<6 hour drive) with regards to many undergraduate colleges that are research active. The low registration and housing costs, relative to any other major conference, make the PSU conference highly accessible for undergraduate institutions.

- Thanks again, everything was fantastic!
- Everything was wonderfully organized!
- A longer lunch break to be able to walk into town.
- Dinner at the reception
- None
- Poster session was a little crowded, and I would have preferred that some posters were not tucked into back corners, facing the walls, etc. Those posters did not get as much attention.
- Great job-- not sure it could be improved!
- An excellent symposium that would be difficult to improve on
- Let people know about odd/even poster session in advance? Group posters by topic?
- Thank you!