

## ***Summary of the 4<sup>th</sup> Penn State Bioinorganic Workshop***

The 4<sup>th</sup> Penn State Bioinorganic Workshop took place June 2-10 2016. The workshop was comparable in scope to those offered in 2012 and 2014. Like the previous workshops, the 2016 workshop consisted of three parts. The first part consisted of 9 90-min lectures and 8 45-min lectures presented by faculty experts on the topic of their expertise (see below). As for the 2014 workshop, we have recorded the lectures professionally and make them available to the entire bioinorganic community via streaming from the workshop website (<https://sites.psu.edu/bioinorganic/workshops/>). In addition, hard copies of the recordings are available as backup.

Introduction to coordination chemistry (Serena DeBeer)  
Protein electrochemistry (Sean Elliott)  
EPR spectroscopy (Art van der Est)  
X-ray spectroscopy (Serena DeBeer)  
Isothermal titration calorimetry (Dean Wilcox)  
NMR spectroscopy of paramagnetic molecules (Kara Bren)  
Mössbauer spectroscopy (Carsten Krebs)  
Survey of typical EPR spectra (Stefan Stoll)  
Bioinformatics methods (Patsy Babbitt)  
Pulse EPR spectroscopy (Stefan Stoll)  
Continuous-flow resonance Raman spectroscopy (Denis Proshlyakov)  
Biological electron transfer (David Beratan)  
Mass spectrometry (Jeff Agar)  
Nuclear resonance vibrational spectroscopy (Nicolai Lehnert)  
MCD spectroscopy (Frank Neese)  
X-ray crystallography (Oliver Einsle)  
Transient kinetics (Marty Bollinger)

The second part (the center piece of the workshop) provided hands-on training in 20 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. Regular participants thus had the opportunity to learn up to 12 new methods. 80 of the 154 total participants were teachers. In other words, more than half of the participants served as teachers. The “teachers” included 16 faculty, 17 postdocs, 39 graduate students, 2 undergraduate students, and even one high-school student. The following 20 sections were offered:

1. Anaerobic protein purification (Squire Booker, Patrick Corrigan, Jackson Ho, Hayley Knox, Erin McCarthy, and Matt Radle)
2. Bioinformatics methods (Patsy Babbitt and Shoshana Brown)
3. Cryoreduction (Marty Bollinger, Candace Davison, and Jovan Livada)

4. DFT calculations with the ORCA software package (Agisilaos Chantzis, Vijay Chilkuri, and Casey Van Stappen)
5. Electrochemistry (Pierre Ceccaldi, Sean Elliott, Zhong Fang, Bin Li, and Kim Rizzolo)
6. EPR1 – continuous wave EPR (John Golbeck, Mike Gorka, Vasily Kurashov, Alexey Silakov, and Karim Walters)
7. EPR2 – pulse EPR (Ellen Hayes and Stefan Stoll)
8. EPR3 – transient state EPR (Bryan Ferlez and Art van der Est)
9. EPR4 – EPR data analysis (Eckhard Bill, Maria Pandelia, and Alexey Silakov)
10. Freeze-Quench method (Marty Bollinger, Susan Butch, Chris Pollock, Erica Schwalm, and Jarett Wilcoxon)
11. High-resolution mass spectrometry (Jeff Agar, Tatiana Laremore, and Catie Rawlins)
12. Isothermal titration calorimetry (Edward Badding, Michael Cukan, Rachel Johnson, Michael Stevenson, and Dean Wilcox)
13. MCD spectroscopy (Andrew Hunt, Nicolai Lehnert, and Matt Wolf)
14. Mössbauer spectroscopy (Yisong Guo, Carsten Krebs, and Ryan Martinie)
15. NMR of paramagnetic molecules (Kara Bren, Emmanuel Hatzakis, Jesse Kleingardner, Carlos Pacheco, and Frances Pong)
16. QQQ mass spectrometry for analysis of small molecules (Matt Bauerle, Anthony Blasczyk, and Nicholas Lanz)
17. Resonance Raman spectroscopy (Beth Blaesi, Denis Proshlyakov, Yegor Proshlyakov, and Bo Zhang)
18. Stopped-flow absorption spectroscopy (Ellis Beardsley, Marty Bollinger, Rachelle Copeland, Manas Ghosh, Juan Pan, Lauren Rajakovich, and Bennett Streit)
19. X-ray crystallography (Amie Boal, Noah Dunham, Oliver Einsle, Ailiena Maggiolo, Andrew Mitchell, and Hannah Rose)
20. X-ray spectroscopy (Serena DeBeer, Stefan Hugenbruch, and Julian Rees)

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 because even a high-school student served as “teacher” and faculty enrolled in hands-on tutorials as “students”.

In the hands-on section of the workshop, a total of ~1,150 2-h person-training-units were administered to “students” by the 80 “teachers”. 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 10<sup>th</sup>, 11<sup>th</sup>, or even 12<sup>th</sup> units in their “open” slots!

The third part of the 2016 workshop consisted of 12 lectures presented by the attendees on their own research; the speakers were selected from submitted abstracts. In addition, there were two 2-h poster sessions, where the participants shared the results of their research.

For the duration of the workshop and symposium, participants met informally in the evenings. It was amazing to witness the energy and commitment of the future generation of bioinorganic chemists. 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!

As in previous years, feedback from the participants was very positive in 2016 and is provided in the appendix.

The planning of the 2018 workshop and symposium has now begun.

List of participants:

Agar	Jeff	Northeastern University
Alcala-Torano	Rafael	Arizona State University
Ames	William	Juniata College
Arcinas	Arthur	Penn State University
Atkinson	Josh	Rice University
Babbitt	Patsy	University of California, San Francisco
Badding	Edward	Penn State University
Bahrama Dizicheh	Zahra	Arizona State University
Bauerle	Matt	Penn State University
Beardsley	Ellis	Penn State University
Beratan	David	Duke University
Bergman	Jonathan	Penn State University
Bhar	Somjit	University of Rochester
Bill	Eckhard	Max Planck Institute for Chemical Energy Conversion
Blaesi	Beth	Penn State University
Blaszcyk	Anthony	Penn State University
Boal	Amie	Penn State University
Bollinger	Marty	Penn State University
Booker	Squire	Penn State University
Bren	Kara	University of Rochester
Brown	Shoshana	University of California, San Francisco
Butch	Susan	Penn State University
Byer	Amanda	Montana State University
Campbell	Ian	Rice University
Ceccaldi	Pierre	Boston University
Chantzis	Agisilaos	Max Planck Institute for Chemical Energy Conversion
Chen	Yao	University of California, San Diego
Chilkuri	Vijay	Max Planck Institute for Chemical Energy Conversion
Chong	Grace	University of Southern California
Conklin	Steven	Duke University
Copeland	Rachelle	Penn State University
Corrigan	Patrick	Penn State University
Cory	Seth	Texas A&M University
Cukan	Michael	Dartmouth University
Davison	Candace	Penn State University
DeBeer	Serena	Max Planck Institute for Chemical Energy Conversion
Deng	Yunling	Dartmouth University
Dent	Matthew	University of Wisconsin, Madison
Dick	Benjamin	University of California, San Diego
Dunham	Noah	Penn State University
Dwaraknath	Sudharsan	University of Illinois, Urbana Champaign

Ealy	Julie	Penn State University, Lehigh
Ebersol	Lauren	Penn State University
Einsle	Oliver	University of Freiburg
Elliott	Sean	Boston University
Esakova	Olga	Penn State University
Fang	Zhong	Boston University
Fecko	Julia	Penn State University
Ferlez	Bryan	Penn State University
Fisher	Oriana	Northwestern University
Follmer	Alec	University of California, Irvine
Ghosh	Manas	Penn State University
Golbeck	John	Penn State University
Gorka	Michael	Penn State University
Gumkowski	James	Penn State University
Guo	Yisong	Carnegie Mellon University
Hahn	Anselm	Max Planck Institute for Chemical Energy Conversion
Harnden	Kevin	University of Illinois, Urbana Champaign
Hatzakis	Emmanuel	Penn State University
Hayes	Ellen	University of Washington
Henthorn	Justin	Max Planck Institute for Chemical Energy Conversion
Ho	Jackson	Penn State University
Hu	Kai	Penn State University
Hugenbruch	Stefan	Max Planck Institute for Chemical Energy Conversion
Hunt	Andrew	University of Michigan
Isaksen	Ingvild	Norwegian Institute of Life Sciences
James	Kimberly	University of Oklahoma
Johnson	Rachel	East Carolina University
Kim	Dongyoung	Yale University
Kincannon	William	University of Utah
Kleingardner	Jesse	Messiah College
Knox	Hayley	Penn State University
Krebs	Carsten	Penn State University
Kundu	Subrata	Georgetown University
Kurashov	Vasily	Penn State University
Landgraf	Brad	Penn State University
Lanz	Nicholas	Penn State University
Laremore	Tatiana	Penn State University
Le	Huynh	University of Oklahoma
Le	Jennifer	University of Rochester
Lehnert	Nicolai	University of Michigan
Li	Bin	Boston University
Li	Jikun	Carnegie Mellon University
Livada	Jovan	Penn State University

Machi	Ursula	Penn State University
Maggiolo	Ailiena	Penn State University
Mannikko	Donald	University of Washington
Martinie	Ryan	Penn State University
McCarthy	Erin	Penn State University
Miller	Effie	Ohio State University
Mitchell	Andrew	Penn State University
Mukherjee	Arnab	Penn State University
Mukhopadhyay	Roma	New Mexico State University
Neese	Frank	Max Planck Institute for Chemical Energy Conversion
O'Hagan	Molly	Pacific Northwest National Laboratory
Onderko	Liz	Penn State University
Oswald	Victoria	University of California, Irvine
Oyugi	Mercy	University of Texas, Arlington
Pacheco	Carlos	Penn State University
Palmer	Elizabeth	SUNY New Paltz
Palowitch	Gavin	Penn State University
Pan	Juan	Penn State University
Pandelia	Maria	Brandeis University
Pirbadian	Sahand	University of Southern California
Poiana	Federica	University of Stockholm
Pollock	Chris	Penn State University
Pong	Frances	Penn State University
Prasser	Benedikt	University of Freiburg
Probst	Corinna	University of Braunschweig
Proshlyakov	Yegor	Michigan State University
Proshlyakov	Denis	Michigan State University
Purohit	Rahul	Northwestern University
Radle	Matt	Penn State University
Rajakovich	Lauren	Penn State University
Rawlins	Catherine	Northeastern University
Rees	Julian	University of Washington
Rivera	Shannon	Emory University
Rivera-Pomales	Pedro	Penn State University
Rizzolo	Kimberly	Boston University
Rose	Hannah	Penn State University
Ruetz	Markus	University of Michigan
Rush	Katherine	University of Michigan
Sanders	Brian	California Institute of Technology
Schäfer	Jacob	University of Stockholm
Schwalm	Erica	Penn State University
Sheetz	Stephen	Penn State University
Shin	Dong Woo	Dartmouth University

Silakov	Alexey	Penn State University
Stepanski	Brandon	University of Utah
Stevenson	Michael	Dartmouth University
Stoll	Stefan	University of Washington
Streit	Bennett	Montana State University
Sun	Chang	University of Illinois, Urbana Champaign
Tanner	Andrew	Rutgers University
Thirumurthy	Miyuki	Arizona State University
Van Cura	Devon	Penn State University
van der Est	Art	Brock University
van Stappen	Casey	Max Planck Institute for Chemical Energy Conversion
Walker	Tia Louise	Indiana Northwest University
Walters	Karim	Penn State University
Wandzilak	Aleksandra	Max Planck Institute for Chemical Energy Conversion
Wang	Roy	Penn State University
Wang	Yifan	University of Texas, San Antonio
Weaver	Brian	Valparaiso University, Indiana
Wilcox	Dean	Dartmouth University
Wilcoxon	Jarett	University of California, Davis
Williams	Garrett	Arizona State University
Wolf	Matt	University of Michigan
Wüst	Anja	University of Freiburg
Yang	Yu	University of Texas, San Antonio
Yazgi	Habib	Penn State University, Lehigh
Yennawar	Neela	Penn State University
Zhang	Bo	Penn State University
Zhou	Shengbin	Penn State University