

## **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            |

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|--------------|-----------|---|
| 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                               |

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| 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                                |

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| 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                               |