Dr. habil. Nicolai Lehnert

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EDUCATION

Jan. 1996 – Feb. 1999 **Ph.D. of natural sciences (Dr. rer. nat.)**
Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University Mainz, Germany
Supervisors: Priv.-Doz. Dr. F. Tuczek & Prof. Dr. P. Gütlich
Topic: '*Spectroscopic and Theoretical Studies on the Reduction and Protonation of Dinitrogen with Relevance to the Nitrogenase Problem*'

Feb. 1996 Minor Degree in Philosophy
Heinrich-Heine-University Düsseldorf, Germany

Nov. 1995 **Diploma in Chemistry**
Heinrich-Heine-University Düsseldorf, Germany
Diploma Thesis: Institute of Theoretical Chemistry
Supervisor: Prof. Dr. H.-H. Schmidtke
Topic: '*Optical Spectra of six-coordinate Osmium(IV)-Complexes with Halogeno Ligands*'

RESEARCH EXPERIENCE

May 20th, 2016 **Promotion to Professor with Tenure**
College of Literature, Science, and the Arts, University of Michigan, Ann Arbor, USA

May 18th, 2012 **Promotion to Associate Professor with Tenure**
College of Literature, Science, and the Arts, University of Michigan, Ann Arbor, USA

since Oct. 2007 **Assistant Professor of Biophysics**
Biophysics Research Division, The University of Michigan, Ann Arbor, USA

since Sept. 2006 **Assistant Professor of Chemistry**
Department of Chemistry, The University of Michigan, Ann Arbor, USA

Nov. 2001 – July 2006	**Habilitation** (senior research assistant, includes the conduction of independent research) Institute of Inorganic Chemistry, Christian-Albrechts-University Kiel, Germany Advisor: Prof. Dr. F. Tuczek Focus: *Synthesis, Spectroscopic Properties and Electronic Structure of Model Complexes for Nitrite and Nitric Oxide Reductases*
May 24th, 2006	Receipt of the Habilitation (qualification for permanent faculty positions at German Universities)
April 1999 – Aug. 2001	**Postdoctoral Fellow** Stanford University, Stanford, California, USA Supervisor: Prof. Dr. E. I. Solomon Focus: *Oxygen Activation by Non-Heme Iron Enzymes*

HONORS AND AWARDS

April 2018	Harold R. Johnson Diversity Service Award, University of Michigan
June 2016	John Dewey Teaching Award, College of Literature, Science, and the Arts, University of Michigan
June 2014	Individual Award for Outstanding Contributions to Undergraduate Education, College of Literature, Science, and the Arts, University of Michigan
2013-2017	Editorial Board Member, *Journal of Biological Inorganic Chemistry (JBIC)*
Aug. 2011	Keynote Lecture at the *International Conference on Biological Inorganic Chemistry* (*ICBIC 15*), August 7 - 12, 2011, Vancouver, Canada
Mar. 2011	3M Non-Tenured Faculty Award
Feb. 2009	National Science Foundation (NSF) CAREER Award
June 2008	Japan Society for the Promotion of Science (JSPS) Invitation Fellowship to visit Japan in June 2008
Sept. 2007 – Aug. 2010	Dow Corning Assistant Professor of Chemistry
since Sept. 2007	Michigan Memorial Phoenix Energy Institute (MMPEI) Faculty Fellow

2001	SBIC grant to attend the *International Conference on Biological Inorganic Chemistry* (*ICBIC 10*), August 2001, Florence, Italy
1997	ACS Bioinorganic Spectroscopy Symposium Travel Award for the *213th American Chemical Society Meeting*, April 1997, San Francisco, CA, USA

RESEARCH FELLOWSHIPS

1999 - 2001	Postdoctoral fellowship of the Deutscher Akademischer Austausch Dienst (DAAD; German Academic Exchange Agency)
1996 - 1998	Kekulé research fellowship of the Fonds des Verbandes der Chemischen Industrie (FCI; German Chemical Industry Association Fund)

TEACHING EXPERIENCE: COURSES TAUGHT AT THE UNIVERSITY OF KIEL

Semester Courses (Laboratory and Lectures)

- **'Spectroscopic Methods'**: lab course covering important spectroscopic techniques applied to coordination chemistry. The lab is accompanied by a seminar. Mandatory for advanced chemistry majors.
- **'Quantitative Analysis'**: a lecture for educational students accompanied by a lab course. Mandatory class for students in the second semester.

Lectures

- **'Coordination Chemistry'**: introductory lecture
- **'Organometallics'**; newly developed course
- **'Chemistry for medical students'**: introductory lecture
- **'Quantum-Chemical Methods in Inorganic Chemistry I'**: lecture plus exercises (the Hartree-Fock method), newly developed course
- **'Quantum-Chemical Methods in Inorganic Chemistry II'**: lecture plus exercises (electron correlation plus density functional theory), newly developed course

TEACHING EXPERIENCE: COURSES TAUGHT AT THE UNIVERSITY OF MICHIGAN

Fall 2006: CHEM 507

- **'Introduction to Inorganic Chemistry'**; graduate course (3 credits)
- Repeat: Fall 2007

Winter 2008: CHEM 616

- **'Physical Inorganic Chemistry: Electronic Structure and Spectroscopy'**; graduate course (3 credits)
- Repeat: Winter 2009 - Winter 2013, Winter 2016 - Winter 2018

Fall 2008: CHEM 130	▪ **'General Chemistry'**; undergraduate course (3 credits) ▪ Repeat: Fall 2009
Fall 2010: CHEM 303	▪ **'The Role of Metals in Life: Introduction to Bioinorganic Chemistry'**; undergraduate course (3 credits) ▪ Repeat: Fall 2011 – Fall 2017
Winter 2015: CHEM 508	▪ **'Advanced Bioinorganic Chemistry'**; graduate course (3 credits)

RESEARCH SUPERVISION (current coworkers are listed in bold face)

Postdoctoral Fellows and Senior Scientists (total currently: 0)

- Dr. Huayang Lee (May 2007 – July 2008)
- Dr. Mary Grace I. Galinato (Oct. 2007 – June 2011)
- Dr. Lili Arabuli (visiting research fellow, Sept. – Dec. 2010 and Fulbright Scholar, Nov. 2011 – Aug. 2012)
- Prof. Timothy Machonkin (Whitman College, sabbatical visit Sept. 2013 – Jan. 2014)
- Prof. Robert Scarrow (Haverford College, sabbatical visit May 2015 – July 2015)
- Dr. Subhra Samanta (Nov. 2015 – Oct. 2017)

Ph.D. Students (total currently: 7)

- V. Koombil Kummaya Praneeth (Aug. 2003 – Feb. 2008)
  Thesis: "*Model Complexes of Heme Protein NO Adducts: Syntheses, Spectroscopy, Electronic Structures, and Reactivity*"
- Florian Paulat (Aug. 2004 – April 2008)
  Thesis: "*Synthesis, MCD- and Raman-Spectroscopic, and Quantum Chemical Investigation of Ferric Heme Model Complexes and their Reaction with NO*"
- Anna Merkle (May 2007 – Dec. 2011)
  Thesis: "*Investigation of the Electronic Structure and Photolability of Copper-, Manganese-, and Ruthenium-Nitrosyl Complexes*"
- Timothy Berto (May 2008 – Dec. 2012)
  Thesis: "*Synthetic, Spectroscopic, and Theoretical Investigations into the Interactions and Detoxification of Nitric Oxide in Biology*"
- Lauren Goodrich (May 2008 – Dec. 2012)
  Thesis: "*Model Complexes of Cytochrome P450 Nitric Oxide Reductase*"
- Deidra Gerlach (May 2008 – June 2013; joint student with the Coucouvanis group)
  Thesis: "*Synthesis and Characterization of Functionalized [4Fe-4S] Cubane Clusters and Linkage to Metalloporphyrins as Catalytic Sites*"
- Shawn Eady (May 2011 – Jan. 2016)
  Thesis: "*Design of Catalyst Interfaces for Heterogeneous Dihydrogen Production Manifolds and Incorporation into Photocathode Systems*"
- Amy Speelman (May 2011 – April 2016)
  Thesis: "*Investigation of the Electronic Structure and Reactivity of Non-Heme Iron Nitrosyl and Nitroxyl Complexes*"

- Ashley McQuarters (May 2012 – Jan. 2017)
  Thesis: "*Model Complexes for Reactive Intermediates in Cytochrome P450 Nitric Oxide Reductase (P450nor)*"
- Matthew Wolf (May 2013 – April 2018)
  Thesis: "*Heme Protein Engineering and Mechanistic Investigations*"
- **Andrew Hunt** (since May 2014)
- **Molly MacInnes** (since May 2016; joint student with the Maldonado group)
- **Corey White** (since May 2016)
- **Hai Dong** (since May 2017)
- **Brad Musselman** (since May 2017)
- **Jill Harland** (since May 2018)
- **Victor Sosa Alfaro** (since May 2018)

Diploma and Masters Students
(total currently: 0)

Felix Studt (with Prof. Dr. F. Tuczek, University of Kiel, Germany); Klaus Mersmann (with Prof. Dr. F. Tuczek, University of Kiel, Germany); Florian Paulat (University of Kiel, Germany); Corinne Sulok (July 2007 – Dec. 2009); Josh Skodack (July 2009 – April 2011); Nicholas Roe (May 2011 – April 2012); Kathryn Craigo (May 2012 – Dec. 2012), Jacques Kumutima (May 2015 – Dec. 2016), Max Bilodeau (May 2016 – Dec. 2016)

Undergraduate Research Students
(total currently: 4)

Torben Kuschel (Bachelor Thesis, University of Kiel, Germany)**;** Susie Chen (2006); Yuki Murata (2007); Jonathan L. Bauer (2007); Corey J. Lager (2007-2008); Alex Navarro (2008); Sherri Martin (2008-2009); Brandon M. Knope (2008-2009); Melissa B. Hoffman (2009-2011); Breana R. Siljander (2009-2010); Thomas Seong-Soo Chae (2010-2011); Ashley McQuarters (2010-2011); Qi N. Zhang (2010); Matthew Forster (2010-2012); Sheng Zheng (2011-2012); Claire Goodrich (2011); Joseph Gurrentz (2013-2015); Nathaniel Wirgau (2013); Sarah Neville (2013); Jamal Mohamud (2013-2014); Alison Zachritz (2014); Claire Kozemchak (2014-2016); Christian Ramsland (2014); Desmond Madu (2014-2016); **Diamond Thomas** (since 2014); Karina Gomez (2015), Richard Wan (2015-2016), David Vargas (2016-2017), Gabriel Ang (2016), Paul Yousif (2016-2018), **Allison Batka** (since 2016), **Ronnie Alvarez** (since 2017), **Stephanie Camarena** (since 2017)

GRANT FUNDING

07/01/2018 – 06/30/2022	National Institutes of Health (NIH) - The National Institute of General Medical Sciences; Award: R01GM124174 Title: 'Biochemical Mechanism of Mercury Methylation' Role: Co-PI (PI: Prof. Steve Ragsdale, University of Michigan)
09/01/2017 – 08/31/2019	Department of Energy, Office of Basic Energy Science: 0000229455 Title: 'DNRA: Catalyzing Multi-Electron Reductions Using a Pentaheme Scaffold'
01/01/2017 – 12/31/2020	National Institutes of Health (NIH) - The National Heart Lung, and Blood Institute; Award: R01HL132037 Title: 'Advanced Thromboresistant/Bactericidal Catheters via Electromodulated NO Release' Role: Co-PI (PI: Prof. Mark Meyerhoff, University of Michigan)
01/01/2017 – 12/31/2020	National Institutes of Health (NIH) - The National Institute of General Medical Sciences; Award: R01GM110390 Title: 'Structure, Function and Diversity in the Bacterial Cytochrome *c* Peroxidase Family' Role: Co-PI (PI: Prof. Sean Elliott, Boston University)
08/01/2016 – 07/31/2019	National Science Foundation (NSF) Award: CHE-1608331 Title: 'Non-Heme Iron(II)-Nitroxyl Complexes: Modeling Key Intermediates in Nitric Oxide Reductases'
11/24/2015 – 11/23/2017	University of Michigan M-Cubed Title: 'Chemical mechanism of the 17,20-lyase reaction' Role: Co-PI (with Prof.s Richard Auchus and Lucy Waskell)
09/01/2015 – 08/31/2016	National Science Foundation (NSF) Award: CHE-1550842 Title: 'Workshop: Feeding the World in the 21st Century: Grand Challenges in the Nitrogen Cycle'
07/01/2015 – 08/31/2018	National Science Foundation (NSF) Award: CHE-1464696 Title: 'Modeling the Active Site and Reactivity of Cyt. P450 Enzymes: A New Beginning'
05/01/2014 – 04/30/2015	Office of the Vice President for Research (OVPR) Small Scale and Preliminary Projects Faculty Grant Title: 'Nuclear resonance vibrational spectroscopy study on the aging-related human enzyme CLK-1'
06/01/2013 – 05/31/2016	National Science Foundation (NSF) Award: CHE-1305777 Title: 'Non-Heme Iron(II)-Nitrosyl and -Nitroxyl Complexes: Key Intermediates in Nitric Oxide Reductases'
07/01/2013 – 04/30/2016	Associate Professor Support Fund (APSF), College of Literature, Science and the Arts, University of Michigan Title: 'Engineering Heme Proteins for Organometallic Catalysis'

04/2012	Rackham Spring/Summer Research Grant Title: 'Mono- and Dinuclear Catalysts for the Oxidation of Dihydrogen'
06/07/2011 – 06/06/2012	Office of the Vice President for Research (OVPR) Small Scale and Preliminary Projects Faculty Grant Title: 'Nitric Oxide Reductases: Bacterial Defense Machinery against Nitrosative Stress'
06/02/2011	IBM Equipment Grant Title: 'Hybrid Quantum-Chemical/Molecular Mechanics Calculations on whole Proteins'
03/17/2011 – 03/16/2013	3M Non-Tenured Faculty Grant: NTFG#5286067 Title: 'Bioinspired Catalysts for the Generation of Hydrogen in Fuel Cells: Bridging Homogeneous and Heterogeneous Catalysis'
09/01/2010 – 08/31/2013	National Science Foundation (NSF) MRI Award: CHE-1040008 Title: 'MRI: Acquisition of a Superconducting Quantum Interference Device (SQUID)'; Role: Co-PI
02/01/2009 – 01/31/2014	National Science Foundation (NSF) CAREER Award: CHE-0846235 Title: 'The Interaction of Nitric Oxide with Cytochrome P450'
04/2008	Rackham Spring/Summer Research Grant 2008: Title: 'Detoxification of Nitric Oxide in Biological Systems: Development of cofacial Porphyrins as efficient Catalysts for the Reduction of Nitric Oxide'
03/01/2008 – 08/31/2009	Rackham Faculty Grant: Title: 'The Detoxification of Nitric Oxide *in vivo* by Flavorubredoxin NO Reductase from *Escherichia coli* and its Role in Chronic Diseases'
09/01/2007 - 12/31/2008	Office of the Vice President for Research (OVPR) Faculty Grant and OVPR Energy Initiative: OVPR#5805 Title: 'Design, Synthesis and Spectroscopic Investigation of Model Systems for Fe-Only Hydrogenases'
07/01/2007 - 08/31/2009	American Chemical Society Petroleum Research Fund (ACS-PRF), PRF-G grant: PRF#47013-G3 Title: 'Molecular Mechanism of Hydrogen-Formation in Fe-Only Hydrogenases'

2005	Grant from the University of Kiel for excellence in obtaining external funding
2005	Grant from the Deutsche Forschungsgemeinschaft (DFG; German Science Foundation) for 1 year including one Ph.D. student position
2005	Chemiefonds fellowship for one Ph.D. student position granted by the Fonds des Verbandes der Chemischen Industrie (FCI; National Chemical Industry Foundation Fund) for 2 years

2004 Grant from the Fonds des Verbandes der Chemischen Industrie (FCI; National Chemical Industry Foundation Fund) for young scientists (Habilitandenförderung)

2003 Grant from the Deutsche Forschungsgemeinschaft (DFG; German Science Foundation) for 2 years including one Ph.D. student position

PROFESSIONAL ACTIVITIES & MEMBERSHIPS

- Co-organizer (with Prof. K. Lancaster, Cornell University) of the symposium 'Nitrogen Un-Fixation: Mechanisms and Models in Nitrification and Denitrification', consisting of three oral sessions plus one poster session; *255th American Chemical Society National Meeting*, New Orleans, LA, USA, March 18 - 22, 2018
- Organizer, NextProf Science Workshop 2017 and 2018, University of Michigan. I organized the activities for the Chemistry participants of the NextProf Workshop in May 2017 and May 2018.
- Invited contributor: 2nd - 5th '*Bioinorganic Training Workshop*', Penn State University, June 2012, 2014, 2016 and 2018. I taught Magnetic Circular Dichroism (MCD) Spectroscopy at the workshop (both theory and practical training sessions for data analysis) and Nuclear Resonance Vibrational Spectroscopy (NRVS, theoretical background).
- Co-organizer (with Prof. Fabio Doctorovich, Ciudad University, Argentina, Prof. Kiyoshi Fujisawa, Ibaraki University, Japan and Prof. G. B. Richter-Addo, University of Oklahoma) of the symposium 'The Bio-Coordination Chemistry of Nitric Oxide and Its Derivatives: Mechanisms of NO_x Generation, Signaling and Reduction in Biological Systems'; *Pacifichem 2015*, Honolulu, HI, Dec. 15 – 20, 2015.
- Organizer/PI (with co-organizers Prof. Gloria Coruzzi, New York University, Prof. Eric Hegg, Michigan State University, and Prof. Lance Seefeldt, Utah State University) of the NSF-sponsored workshop 'Feeding the World in the 21st Century: Grand Challenges in the Nitrogen Cycle'. This workshop was held Nov. 09 – 10, 2015 at the NSF headquarters (Arlington, VA). The major goal of the workshop was to identify the BIG scientific challenges in the nitrogen cycle and possible solutions (with a focus on the contributions that (bio)chemistry can make).
- Guest editor (with Prof. Jonas Peters, CalTech) of the *Inorganic Chemistry* FORUM 'Small Molecule Activation: From Biological Principles to Energy Applications', published in October 2015 (issue: 19).
- Director and founder, University of Michigan D-RISE (Detroit Research Internship Summer Experience) Program with Detroit High Schools. Raised funds from the NSF, the University of Michigan College of Literature, Science, and the Arts, and Cass Technical High School in Detroit to bring Cass Tech students (juniors and seniors) into the Chemistry Department for a 7 weeks summer research internship (since Summer 2014).
- Co-organizer (with Prof. G. B. Richter-Addo, University of Oklahoma) of the symposium 'Small Molecule Activation by Heme Active Sites in Proteins and Model complexes'; *International Conference on Porphyrins and Phthalocyanins (ICPP 7)*, Jeju Island, South Korea, July 01 – 06, 2012
- Guest editor (with Prof. W. R. Scheidt, University of Notre Dame) of the *Inorganic Chemistry* FORUM 'The Coordination Chemistry of Nitric Oxide and its Significance for Metabolism, Signaling and Toxicity', published in July 2010 (issue 14)

- Co-organizer (with Prof. W. R. Scheidt, University of Notre Dame) of the symposium 'Coordination Chemistry of Nitric Oxide and its Implication for Metabolism, Imaging and Toxicity', consisting of four oral sessions plus one poster session; *237th American Chemical Society National Meeting*, Salt Lake City, UT, USA, March 22 - 26, 2009
- Reviewer for proposals: NIH, NSF, ACS-PRF, DOE, Research Corporation
- Reviewer for: *Nat. Chem.*, *Proc. Nat. Acad. Sci. U.S.A.*, *J. Am. Chem. Soc.*, *Angew. Chem.*, *Chem. Rev.*, *Chem. Commun.*, *Inorg. Chem.*, *Chem. Europ. J.*, *J. Phys. Chem.*, *Europ. J. Inorg. Chem.*, *J. Biol. Inorg. Chem. (JBIC), J. Inorg. Biochem. (JIB)*
- Member of: American Chemical Society (ACS, since 2000), Society of Porphyrins & Phthalocyanins (SPP, since 2006), Society of Biological Inorganic Chemistry (SBIC, since 2007)

INVITED SEMINAR AND CONFERENCE PRESENTATIONS

1. "Spectroscopic Properties and Electronic Structure of Alkyl- and Hydroperoxo Intermediates", University of Tsukuba, Japan, September 12, 2000
2. "Vibrational and Electronic Spectroscopy of Metalloporphyrins correlated to DFT calculations", Physikalisches Kolloquium, University of Lübeck, Germany, January 21, 2005
3. "Electronic Structure and Reactivity of Heme-Nitrosyl Complexes", University of Michigan, Ann Arbor, MI, USA, December 13, 2005
4. "Electronic Structure and Reactivity of Heme-Nitrosyl Complexes", Texas A&M University, College Station, TX, USA, January 23, 2006
5. "Electronic Structure of Ferrous Heme-Nitrosyls", University of Göttingen, Germany, May 02, 2006
6. "Electronic Structure and Reactivity of Heme-Nitrosyl Complexes", *International Conference on Porphyrins and Phthalocyanines (ICPP 4)*, Rome, Italy, July 2 - 7, 2006
7. "Detoxification of Nitric Oxide in Biological Systems: Mechanisms and Model Systems", Andrews University, MI, USA, February 15, 2007
8. "Detoxification of Nitric Oxide in Biological Systems: Mechanisms and Model Systems", Biophysics Division, University of Michigan, MI, USA, February 23, 2007
9. "Detoxification of NO in Bacterial Denitrification: Electronic Structure and Spectroscopic Properties of five- vs. six-coordinate ferrous Heme Nitrosyls", University of Notre Dame, Notre Dame, IN, USA, May 4, 2007
10. "Detoxification of NO in Bacterial Denitrification: Electronic Structure and Spectroscopic Properties of ferrous Heme Nitrosyls", Bowling Green State University, Bowling Green, OH, USA, January 23, 2008
11. "Electronic Structure and Spectroscopic Properties of Ferric Heme-Nitrosyls: the elusive Fe(III)-NO(Radical) State", Marquette University, Milwaukee, WI, USA, April 04, 2008
12. "Development of Synthetic Catalysts inspired by Nature for Application in Metal-based Drug Design and Alternative Energies", Dow Corning, Midland, MI, USA, May 05, 2008
13. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", University of Tsukuba, Tsukuba, Japan, June 06, 2008
14. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", Kanazawa University, Kanazawa, Japan, June 10, 2008

15. "Detoxification of NO in Bacterial Denitrification: Electronic Structure and Spectroscopic Properties of Ferrous Heme Nitrosyls", *Plenary Lecture*, Global COE Annual Meeting, University of Nagoya, Nagoya, Japan, June 11, 2008
16. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", Nagoya Institute of Technology (NIT), Nagoya, Japan, June 12, 2008
17. "Electronic Structure and Spectroscopic Properties of Ferric Heme-Nitrosyls: the elusive Fe(III)-NO(Radical) State", PIO Meeting, Rikkyo University, Tokyo, Japan, June 14, 2008
18. "Detoxification of NO in Bacterial Denitrification: Electronic Structure and Spectroscopic Properties of Ferrous Heme Nitrosyls", Tohoku University, Sendai, Japan, June 16, 2008
19. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", FIBER Institute International Lecture, Konan University, Kobe, Japan, June 18, 2008
20. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", Osaka University, Osaka, Japan, June 19, 2008
21. "Detoxification of NO in Bacterial Denitrification: Electronic Structure and Spectroscopic Properties of Ferrous Heme Nitrosyls", Osaka University, Osaka, Japan, June 20, 2008
22. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", Kyoto University, Kyoto, Japan, June 24, 2008
23. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", Nara Women's University, Nara, Japan, June 25, 2008
24. "The Copper(I)-NO Intermediate of Copper Nitrite Reductase", Tokyo University of Agriculture and Technology, Tokyo, Japan, June 27, 2008
25. "Electronic Structure and Spectroscopic Properties of Ferric Heme-Nitrosyls: the elusive Fe(III)-NO(Radical) State", Tokyo University of Agriculture and Technology, Tokyo, Japan, June 27, 2008
26. "The Electronic Structure of Five-Coordinate High-Spin Ferrous Hemes and corresponding Adducts with Nitric Oxide", *2nd International Symposium on Bioinorganic Chemistry of the New Era*, Takayama, Japan, July 31 – August 2, 2009
27. "Binding of Nitric Oxide to High-spin Ferrous Heme Protein Active Sites: Electronic Structures and Reactivities of the Coordinated NO", Wayne State University, Detroit, MI, USA, October 15, 2009
28. "Binding of Nitric Oxide to High-spin Ferrous Heme Protein Active Sites: Electronic Structures and Reactivities of the Coordinated NO", University of Minnesota at Duluth, Duluth, MN, USA, November 06, 2009
29. "Binding of Nitric Oxide to High-spin Ferrous Heme Protein Active Sites: Electronic Structures and Reactivities of the Coordinated NO", Kalamazoo College, Kalamazoo, MI, USA, November 16, 2009
30. "Binding of Nitric Oxide to High-spin Ferrous Heme Protein Active Sites: Electronic Structures and Reactivities of the Coordinated NO", *Gordon Research Conference: Metals in Biology*, Ventura, CA, USA, January 31 – February 5, 2010
31. "Electronic Structure and Spectroscopic Properties of Ferric Heme-Nitrosyls: the elusive Fe(III)-NO(Radical) State", University of Michigan at Flint, Flint, MI, USA, February 15, 2010

32. "Ferric Heme-Nitrosyls in Nitric Oxide Transport and Catalysis", California Institute of Technology, Pasadena, CA, USA, March 08, 2010
33. "The Fundamental Chemistry of Nitric Oxide with Ferric Heme-Thiolate Active Sites", *International Conference on Porphyrins and Phthalocyanines (ICPP 6)*, Santa Ana Pueblo, NM, USA, July 4 - 9, 2010
34. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Johns Hopkins University, Baltimore, MD, USA, September 21, 2010
35. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Rochester, Rochester, NY, USA, October 04, 2010
36. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Cornell University, Ithaca, NY, USA, October 05, 2010
37. "Modeling the Active Site of Bacterial Nitric Oxide Reductase", Oakland University, Rochester, MI, USA, October 13, 2010
38. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Oklahoma, Norman, OK, USA, October 18, 2010
39. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Oklahoma State University, Stillwater, OK, USA, October 19, 2010
40. "Modeling the Active Site of Bacterial Nitric Oxide Reductase", University of Michigan at Flint, Flint, MI, USA, November 11, 2010
41. "Modeling the Active Site of Bacterial Nitric Oxide Reductase", Society of Physics Students, University of Michigan, Ann Arbor, MI, USA, January 11, 2011
42. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", UC San Diego, CA, USA, February 04, 2011
43. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Southern California, Los Angeles, CA, USA, February 07, 2011
44. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", UC Santa Barbara, CA, USA, February 09, 2011
45. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Minnesota, Minneapolis, MN, USA, March 01, 2011
46. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Wisconsin, Madison, WI, USA, March 02, 2011
47. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Illinois at Urbana-Champaign, Urbana, IL, USA, March 08, 2011
48. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", UC Davis, CA, USA, March 31, 2011
49. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", UC Berkeley, CA, USA, April 01, 2011
50. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Stanford University, Stanford, CA, USA, April 05, 2011
51. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", UC Santa Cruz, CA, USA, April 06, 2011

52. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Penn State University, University Park, PA, USA, April 26, 2011
53. "Modeling the Active Site of Bacterial Nitric Oxide Reductase", invited Keynote Lecture, *International Conference on Biological Inorganic Chemistry (ICBIC 15)*, Vancouver, Canada, August 7 - 12, 2011
54. "Nitric Oxide Function and Detoxification in Biological Systems", University of Michigan at Dearborn, Dearborn, MI, USA, November 10, 2011
55. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Dartmouth College, Hanover, NH, USA, November 17, 2011
56. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Middlebury College, Middlebury, VT, USA, November 18, 2011
57. "Non-Heme Iron-Nitrosyl Complexes as Models for the Active Sites of Bacterial Nitric Oxide Reductases", *Zing Coordination Chemistry Conference*, Cancun, Mexico, December 9 - 13, 2011
58. "Nitric Oxide Function and Detoxification in Biological Systems", Reed College, Portland, OR, USA, February 09, 2012
59. "Nitric Oxide Function and Detoxification in Biological Systems", Whitman College, Walla Walla, WA, USA, February 10, 2012
60. "Iron-Nitroxyl Complexes as Intermediates in Nitric Oxide Reductases", *Sixteenth Mesilla Chemistry Workshop*, Mesilla, NM, USA, February 11 - 15, 2012
61. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Akron, Akron, OH, February 29, 2012
62. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Kent State University, Kent, OH, March 01, 2012
63. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", Cleveland State University, Cleveland, OH, March 02, 2012
64. "Mono- and Dinuclear Non-Heme Iron-Nitrosyl Complexes: Models for the Active Sites of Bacterial Nitric Oxide Reductases", *243rd American Chemical Society National Meeting*, San Diego, CA, USA, March 25 - 29, 2012
65. "The many Faces of the Coordination Chemistry of Nitric Oxide and its Biological Significance", University of Washington, Seattle, WA, USA, April 24, 2012
66. "Magnetic Circular Dichroism Spectroscopy", 2nd *Bioinorganic Workshop*, Penn State University, University Park, PA, USA, May 31 – June 08, 2012
67. "Ferrous Heme-Nitroxyl Complexes as Intermediates of Fungal Nitric Oxide Reductase (Cytochrome P450nor)", *2nd International Bioinorganic Chemistry Conference on Small Molecule Activation by Heme and Nonheme Enzymes and Models*, Ewha Womens University, Seoul, South Korea, June 30, 2012
68. "Ferrous Heme-Nitroxyl Complexes as Intermediates of Fungal Nitric Oxide Reductase (Cytochrome P450nor)", *International Conference on Porphyrins and Phthalocyanines (ICPP 7)*, Jeju Island, South Korea, July 01 – 06, 2012
69. "Non-Heme Iron Nitrosyls as Intermediates in Bacterial Nitric Oxide Reductases", Boston University, Boston, MA, USA, October 17, 2012

70. "Non-Heme Iron Nitrosyls as Intermediates in Bacterial Nitric Oxide Reductases", Brown University, Providence, RI, USA, October 18, 2012
71. "Non-Heme Iron Nitrosyls as Intermediates in Bacterial Nitric Oxide Reductases", Kenyon College, Gambier, OH, USA, April 10, 2013
72. "Magnetic Circular Dichroism Spectroscopy provides Insight into the Fe-S(Cys) Interaction in Heme-Thiolate Protein Active Sites", *4th Georgian Bay International Conference on Bioinorganic Chemistry (CanBIC-4)*, Parry Sound, Canada, May 21 – 25, 2013
73. "Iron Nitroxyl Complexes as Central Intermediates in Nitric Oxide Reductases", Yale University, New Haven, CT, USA, October 08, 2013
74. "Iron Nitroxyl Complexes as Central Intermediates in Nitric Oxide Reductases", University of Nevada, Reno, NV, USA, November 08, 2013
75. "The first Functional Model System for Flavodiiron Nitric Oxide Reductases", *The 1st International Symposium for Young Chemists on Stimuli-Responsive Chemical Species for the Creation of Functional Molecules*, Tokyo, Japan, December 02 – 03, 2013
76. "Iron Nitroxyl Complexes as Central Intermediates in Nitric Oxide Reductases", Ibaraki University, Mito, Japan, December 05, 2013
77. "Iron Nitroxyl Complexes as Central Intermediates in Nitric Oxide Reductases", Tokyo University of Agriculture and Technology, Tokyo, Japan, December 06, 2013
78. "The first Functional Model System for Flavodiiron Nitric Oxide Reductases", *T-BIC Seminar* (Bryn Mawr College, Haverford College, Swarthmore College), Haverford, PA, USA, February 05, 2014
79. "The first Functional Model System for Flavodiiron Nitric Oxide Reductases", Drexel University, Philadelphia, PA, USA, February 06, 2014
80. "The first Functional Model System for Flavodiiron Nitric Oxide Reductases", Ursinus College, Collegeville, PA, USA, February 07, 2014
81. "Iron Nitroxyl Complexes as Central Intermediates in Nitric Oxide Reductases", University of Alabama, Tuscaloosa, AL, USA, February 20, 2014
82. "Magnetic Circular Dichroism Spectroscopy", 3rd *Bioinorganic Workshop*, Penn State University, University Park, PA, USA, May 28 – June 04, 2014
83. "Reactivity of {[Fe(OEP)]$_2$(μ-N_2O_2)} as a Model for the Proposed Hyponitrite-Bridged Intermediate of Bacterial Nitric Oxide Reductase (NorBC)", *International Conference on Porphyrins and Phthalocyanines (ICPP 8)*, Istanbul, Turkey, June 22 – 27, 2014
84. "The first Functional Model System for Flavodiiron Nitric Oxide Reductases", *Fusion Conference on Small Molecule Activation*, Chicago, IL, USA, July 15 – 18, 2014
85. "Nitroxyl Complexes of Non-Heme Iron Centers: Properties and Reactivity", invited Keynote Lecture, *Latin American Meeting on Biological Inorganic Chemistry (LABIC 4)*, Chascomus, Argentina, Aug. 05 – 08, 2014
86. "Modeling Key Intermediates in Cytochrome P450 Nitric Oxide Reductase: Electronic Structure and Reactivity", University of Michigan at Flint, Flint, MI, USA, October 13, 2014
87. "The Mechanism of Flavodiiron Nitric Oxide Reductases and their Role in Bacterial Pathogenesis", Muhlenberg College, Allentown, PA, USA, November 21, 2014

88. "Iron-Nitroxyl Complexes: Properties and Biologically Relevant Reactivity", Emory University, Atlanta, GA, USA, December 01, 2014
89. "The Mechanism of Flavodiiron Nitric Oxide Reductases: Electronic Structure and Reactivity of Iron-Nitroxyl Complexes", Miami University, Oxford, OH, USA, April 09, 2015
90. "Nitroxyl Complexes of Non-Heme Iron Centers: Properties and Reactivity", IRTG Symposium, University of Göttingen, Göttingen, Germany, August 27, 2015
91. "Going Heterogeneous: Bringing Proton Reduction Catalysts to Electrode Surfaces", University of Texas at Austin, Austin, TX, USA, October 21, 2015
92. "Nitroxyl Complexes of Non-Heme Iron Centers: Properties and Reactivity", *Pacifichem 2015*, Honolulu, Hawaii, Dec. 15 – 20, 2015
93. "Novel Methods for Electrode Surface Functionalization and Applications in (Photo)Electrocatalysis", *Fusion Conference on Molecules and Materials for Artificial Photosynthesis*, Cancun, Mexico, February 25-28, 2016
94. "From Non-Heme $\{FeNO\}^6$ to $\{FeNO\}^8$ to Fe(II)-HNO Complexes: One Ligand Platform can Do it All", *251st American Chemical Society National Meeting*, San Diego, CA, USA, March 13 – 17, 2016
95. "Second Coordination Sphere Effects in Cytochrome P450s and Mechanism of NO Reduction", Michigan State University, East Lansing, MI, USA, April 12, 2016
96. "Nuclear Resonance Vibrational Spectroscopy", 4th *Bioinorganic Workshop*, Penn State University, University Park, PA, USA, June 02 – 10, 2016
97. "Non-Heme Iron-Nitroxyl Complexes: Properties and Biologically Relevant Reactivity", Marquette University, Milwaukee, WI, USA, Nov. 11, 2016
98. "Non-Heme Iron-Nitroxyl Complexes: Properties and Biologically Relevant Reactivity", Sonoma State University, Sonoma, CA, Dec. 02, 2016
99. "Modeling the Key "Intermediate I" in Cytochrome P450 Nitric Oxide Reductase", *Symposium on Advanced Biological Inorganic Chemistry (SABIC) 2017*, Kolkata, India, Jan. 07 – 11, 2017
100. "Non-Heme Iron-Nitroxyl Complexes: Properties and Biologically Relevant Reactivity", St. Xavier's College, Kolkata, India, Jan. 12, 2017
101. "Novel Methods for Electrode Surface Functionalization and Applications in (Photo)Electrocatalysis", College of William and Mary, Williamsburg, VA, March 17, 2017
102. "Modeling the Key Intermediate in Cytochrome P450 NO Reductase: Electronic Structure and Reactivity", *6th Georgian Bay International Conference on Bioinorganic Chemistry (CanBIC-6)*, Parry Sound, Canada, May 23 – 27, 2017
103. "Modeling the active site and reactivity of flavodiiron nitric oxide reductases", *254th American Chemical Society National Meeting*, Washington, DC, USA, Aug. 20 – 24, 2017
104. "Nature to the Rescue: Understanding Enzyme Mechanism and Building Synthetic Catalysts", BASF, Wyandotte, MI, Dec. 12, 2017
105. "The Activation of Nitric Oxide by Non-Heme Iron Centers. Modeling Flavodiiron Nitric Oxide Reductases", plenary lecture, *E-COST BIO Meeting*, Berlin, Germany, April 09 – 11, 2018

106. "The Activation of Nitric Oxide by Non-Heme Iron Centers: The Mechanism of Flavodiiron Nitric Oxide Reductases", University of Göttingen, Göttingen, Germany, April 13, 2018
107. "The Activation of Nitric Oxide by Non-Heme Iron Centers: The Mechanism of Flavodiiron Nitric Oxide Reductases", University of Aachen, Aachen, Germany, April 16, 2018
108. "Fungal Denitrification and N_2O Production", *Gordon Research Conference: Metallocofactors*, Mount Holyoke College, South Hadley, MA, USA, June 10 – 15, 2018
109. "Modeling Key Intermediates in Cytochrome P450 Nitric Oxide Reductase: Electronic Structure and Reactivity", *International Conference on Porphyrins and Phthalocyanines (ICPP 10)*, Munich, Germany, July 01 – 06, 2018
110. "The Reactivity Landscape of Non-Heme Iron and Nitric Oxide: Fundamental Chemistry and Biological Relevance", University of Erlangen-Nürnberg, Erlangen, Germany, Nov. 06, 2018
111. "The Reactivity Landscape of Non-Heme Iron and Nitric Oxide: Fundamental Chemistry and Biological Relevance", University of Bayreuth, Bayreuth, Germany, Nov. 07, 2018

ADDITIONAL ORAL PRESENTATIONS

1. "Alkylperoxo Intermediates in Non-Heme Iron Enzymes", *219th American Chemical Society National Meeting*, San Francisco, CA, USA, March 26 – 30, 2000
2. "Synthesis and Spectroscopic Investigation of Iron-Porphyrin Adducts of Nitric Oxide: Effect of the trans Ligand on the coordinated NO", *Chemiedozententagung 2005*, LMU München, Germany, March 06 – 09, 2005
3. "Electronic Structure and Reactivity of Thiolate-Coordinated Iron-Porphyrin Nitrosyls: Molecular Mechanism of P450nor", *Chemiedozententagung 2006*, University of Hamburg, Germany, March 19 – 22, 2006
4. "Iron-Porphyrin NO Complexes with Covalently Attached Proximal N-Donor Ligands", *International Conference on Biological Inorganic Chemistry (ICBIC 13)*, Vienna, Austria, July 15 – 20, 2007
5. "Electronic Structure of Six-Coordinate Iron(III)-Porphyrin NO Adducts: the Elusive Iron(III)-NO(radical) State", *237th American Chemical Society National Meeting*, Salt Lake City, UT, USA, March 22 – 26, 2009
6. "The Spectroscopic Properties and Electronic Structures of Ferric-Heme Nitrosyls: Significance for Nitric Oxide Transport and Catalysis", *International Conference on Biological Inorganic Chemistry (ICBIC 14)*, Nagoya, Japan, July 25 – 30, 2009
7. "The first Functional Model System for Flavodiiron Nitric Oxide Reductases", *International Conference on Biological Inorganic Chemistry (ICBIC 16)*, Grenoble, France, July 22 – 26, 2013

UNIVERSITY SERVICE

Since Oct. 2017	Member of the Growing STEM/NCID Knowledge Community Steering Committee (UM)
Since Sept. 2017	Member of the UROP Director Search Committee (UM)
Since Jan. 2017	Member of the Research Administration Advisory Council (RAAC) Faculty Advisory Council (FAC) at UM
Since Jan. 2017	Chair, Diversity Committee (UM) and Department of Chemistry liaison for the NextProf Science Workshop
Since Sept. 2016	Member of the Admissions Committee (UM)
Since Sept. 2016	Member of the Faculty Search Committee (UM)
Sept. 2014 – Dec. 2016	Member of the Diversity Committee (UM)
Sept. 2014 – August 2016	Chair of the Graduate Committee (UM)
Sept. 2013 – Aug. 2014	Member of the Executive Committee of the Department of Chemistry (UM)
June 2008 – August 2016	Faculty Advisor for UM's annual graduate student symposium (Karle Symposium; former: V. Vaughan Symposium)
Feb. 2007 – Aug. 2014	Member of the Graduate Committee (UM)
Sept. 2006 – Aug. 2012	Member of the Recruiting Committee and Member of the Gomberg Committee (UM)
Sept. 2006 – Aug. 2009	Coordinator of the Inorganic Cluster Seminars (UM)
April 2004 – July 2006	Member of the Budget Committee for the Faculty of Science (Haushalts- und Planungsausschuß) at the University of Kiel, Germany
Oct. 2002 – July 2006	Member of the Executive Committee for the Chemistry Department (Sektionsausschuß Chemie) at the University of Kiel, Germany. Responsibilities include: budget, curriculum, administration, etc.

REFERENCES Available upon request.

JOURNAL PUBLICATIONS

(a) Diploma and Graduate Research

1. H.-H. Schmidtke, N. Lehnert, M. Giesbers, "The vibronic structure of mixed ligand Os(IV) complexes III: Low temperature absorption spectra in high resolution". *Spectrochim. Acta Part A* **1997**, *53*, 789-803

2. H.-H. Schmidtke, N. Lehnert, "Charge Transfer Band Splittings in Electronic Spectra of Mixed Ligand Halogeno Os(IV) Complexes". *Inorg. Chem.* **1998**, *37*, 6373-6381

3. N. Lehnert, B. E. Wiesler, F. Tuczek, A. Hennige, D. Sellmann, "Activation of Diazene and the Nitrogenase Problem: An Investigation of Diazene-Bridged Fe(II) Centers with Sulfur Ligand Sphere. 1. Electronic Structure". *J. Am. Chem. Soc.* **1997**, *119*, 8869-8878

4. N. Lehnert, B. E. Wiesler, F. Tuczek, A. Hennige, D. Sellmann, "Activation of Diazene and the Nitrogenase Problem: An Investigation of Diazene-Bridged Fe(II) Centers with Sulfur Ligand Sphere. 2. Vibrational Properties". *J. Am. Chem. Soc.* **1997**, *119*, 8879-8888

5. B. E. Wiesler, N. Lehnert, J. Neuhausen, W. Tremel, F. Tuczek, "Influence of the trans Substituent on N_2 Bonding in Iron(II)-Phosphane Complexes: Structure, Synthesis and Properties of the Monomeric Adducts trans-[$FeX(N_2)(depe)_2$]BPh_4, X=Cl, Br". *Angew. Chem. Int. Ed.* **1998**, *37*, 815-817

6. F. Tuczek, N. Lehnert, Highlight: "New Developments in Nitrogen Fixation". *Angew. Chem. Int. Ed.* **1998**, *37*, 2636-2638

7. N. Lehnert, F. Tuczek, "The Reduction Pathway of End-on Coordinated Dinitrogen: I. Vibrational Properties of Mo/W-N_2, -NNH and -NNH_2 Complexes and Quantum Chemistry Assisted Normal Coordinate Analysis". *Inorg. Chem.* **1999**, *38*, 1659-1670

8. N. Lehnert, F. Tuczek, "The Reduction Pathway of End-on Coordinated Dinitrogen: II. Electronic Structure of Mo/W-N_2, -NNH and -NNH_2 Complexes and Relevance to Nitrogenase". *Inorg. Chem.* **1999**, *38*, 1671-1682

9. O. Franke, B. E. Wiesler, N. Lehnert, C. Näther, V. Ksenofontov, J. Neuhausen, F. Tuczek, "The Five-Coordinate Complexes [$FeX(depe)_2$]BPh_4, X=Cl, Br: Electronic Structure and Spin-Forbidden Reaction with N_2". *Inorg. Chem.* **2002**, *41*, 3491-3499

10. C. M. Habeck, N. Lehnert, C. Näther, F. Tuczek, "Mo/W-N_2 and -N_2H_2 Complexes with *trans* Nitrile Ligands: Electronic Structure, Spectroscopic Properties and Relevance to Nitrogen Fixation". *Inorg. Chim. Acta* **2002**, *337C*, 11-31

11. O. Franke, B. E. Wiesler, N. Lehnert, F. Tuczek, "Vibrational Properties of $[FeH(N_2)(depe)_2]^+$ and $[FeCl(N_2)(depe)_2]^+$: Dinitrogen Bonding in the Low Activation Limit". *Z. Anorg. Allg. Chemie* **2002**, *628*, 2395-2402

12. F. Studt, L. Morello, N. Lehnert, M. D. Fryzuk, F. Tuczek, "Side-on Bridging Coordination of N_2: Spectroscopic Characterization of the Planar Zr_2N_2 Core and Theoretical Investigation of the Butterfly Distortion". *Chem. Eur. J.* **2003**, *9*, 520-530

13. K. H. Horn, N. Lehnert, F. Tuczek, "The Reduction Pathway of End-on Coordinated Dinitrogen: III. Electronic Structure and Spectroscopic Properties of Mo/W Hydrazidium Complexes". *Inorg. Chem.* **2003**, *42*, 1076-1086

14. F. Tuczek, K. H. Horn, N. Lehnert, "Vibrational spectroscopic properties of molybdenum and tungsten N_2 and N_2H_x complexes with depe coligands: comparison to dppe systems and influence of H-bridges".
Coord. Chem. Rev. **2003**, *245*, 107-120

15. G. C. Stephan, G. Peters, N. Lehnert, C. M. Habeck, F. Tuczek, "Bonding, Activation and Protonation of Dinitrogen in a Molybdenum Pentaphosphine Complex: Comparison to Tetraphosphine Systems with *trans*-Bis(dinitrogen) and Nitrile/Dinitrogen Ligands". *Can. J. Chem.* **2005**, *83*, 385-402

16. K. H. Horn, N. Böres , N. Lehnert, K. Mersmann, C. Näther, G. Peters, F. Tuczek, "Reduction Pathway of End-on Terminally Coordinated Dinitrogen. IV. Geometric, Electronic and Vibrational Structure of a W(IV) Dialkylhydrazido Complex and Its Two-Electron Reduced Derivative Undergoing N-N Cleavage upon Protonation". *Inorg. Chem.* **2005**, *44*, 3016-3030

17. K. Mersmann, K. H. Horn, N. Böres, N. Lehnert, F. Studt, F. Paulat, G. Peters, I. Ivanovic-Burmazovic, R. van Eldik, F. Tuczek, "Reduction Pathway of End-on Terminally Coordinated Dinitrogen.
V. N-N Bond Cleavage in Mo/W Hydrazidium Complexes with Diphosphine Coligands. Comparison with Triamidoamine Systems". *Inorg. Chem.* **2005**, *44*, 3031-3045

18. O. Franke, B. E. Wiesler, N. Lehnert, G. Peters, P. Burger, F. Tuczek, "The Iron Hydrido Complex $[FeH(dppe)_2]^+$: Singlet and Triplet State Reactivity with Dinitrogen". *Z. Anorg. Allg. Chemie* **2006**, *632*, 1247-1256

19. F. Studt, N. Lehnert, B. E. Wiesler, A. Scherer, R. Beckhaus, F. Tuczek, "Spectroscopic Comparison of Dinuclear Ti^+ and Ti^{2+} μ-η^1:η^1 Dinitrogen Complexes with Cp*/Pentafulvene and Amine/Amide Ligation: Moderate vs. High Activation of N_2". *Europ. J. Inorg. Chem.* **2006**, 291-297

(b) Postdoctoral Research

20. E. I. Solomon, T. Brunold, M. I. Davis, J. N. Kemsley, S.-K. Lee, N. Lehnert, F. Neese, A. J. Skulan, Y.-S. Yang, J. Zhou, "Geometric and Electronic Structure/Function Correlations in Non-Heme Iron Enzymes". *Chem. Rev.* **2000**, *100*, 235-349

21. N. Lehnert, S. DeBeer George, E. I. Solomon, "Recent advances in bioinorganic spectroscopy". *Curr. Op. Chem. Biol.* **2001**, *5*, 173-184

22. N. Lehnert, R. Y. N. Ho, L. Que, Jr., E. I. Solomon, "Spectroscopic Properties and Electronic Structure of Low-Spin Fe(III)-Alkylperoxo Complexes: Homolytic Cleavage of the O-O Bond". *J. Am. Chem. Soc.* **2001**, *123*, 8271-8290

23. N. Lehnert, R. Y. N. Ho, L. Que, Jr., E. I. Solomon, "Electronic Structure of High-Spin Fe(III)-Alkylperoxo Complexes and Its Relation to Low-Spin Analogues: Reaction Coordinate of O-O Bond Homolysis". *J. Am. Chem. Soc.* **2001**, *123*, 12802-12816

24. N. Lehnert, F. Neese, R. Y. N. Ho, L. Que, Jr., E. I. Solomon, "Electronic Structure and Reactivity of Low-Spin Fe(III)-Hydroperoxo Complexes: Comparison to Activated Bleomycin", *J. Am. Chem. Soc.* **2002**, *124*, 10810-10822

25. N. Lehnert, E. I. Solomon, "Density Functional Investigation on the Mechanism of H-Atom Abstraction by Lipoxygenase". *J. Biol. Inorg. Chem. (JBIC)* **2003**, *8*, 294-305

26. N. Lehnert, K. Fujisawa, E. I. Solomon, "Electronic Structure and Reactivity of High-Spin Iron–Alkyl- and –Pterinperoxo Complexes". *Inorg. Chem.* **2003**, *42*, 469-481

27. E. I. Solomon, A. Decker, N. Lehnert, "Non-Heme Iron Enzymes: Contrast to Heme Catalysis". *Proc. Nat. Acad. Sci. U.S.A.* **2003**, *100*, 3589-3594

28. A. Decker, M. S. Chow, J. N. Kemsley, N. Lehnert, E. I. Solomon, "Direct Hydrogen-Atom Abstraction by Activated Bleomycin: An Experimental and Computational Study". *J. Am. Chem. Soc.* **2006**, *128*, 4719-4733

(c) Independent Research

29. C. L. Teske, N. Lehnert, W. Bensch, "On Polychalcogenides of Thallium with M_2Q_{11} Groups as a Structural Building Block. II. $Tl_4Ta_2Se_{11}$: Synthesis, Crystal Structure, Properties and Spectroscopic Investigations of the First Polyselenide being Composed of an Isolated $[Ta_2Se_{11}]^{4-}$ Anion". *Z. Anorg. Allg. Chemie* **2002**, *628*, 2651-2655

30. C. Näther, I. Jeß, N. Lehnert, D. Hinz-Hübner, "On the Thermal Decomposition Pathway of Coordination Compounds: Synthesis, Crystal Structures and Properties of New Polymorphic CuI(2-Ethylpyrazine) Coordination Compounds". *Solid State Sci.* **2003**, *5*, 1343-1357

31. M. Schäfer, C. Näther, N. Lehnert, W. Bensch, "Solvothermal Syntheses, Crystal Structures and Thermal Properties of new Manganese Thioantimonates(III): The First Example for the Thermal Transformation of an Amine-rich Thioantimonate into an Amine-poorer Thioantimonate". *Inorg. Chem.* **2004**, *43*, 2914-2921 [PMID: 15106979]

32. K. Fujisawa, N. Lehnert, Y. Ishikawa, K. Okamoto, "Diazene Complexes of Copper: Synthesis, Spectroscopic Analysis, and Electronic Structure". *Angew. Chem. Int. Ed.* **2004**, *43*, 4944-4947 [PMID: 15372560]

33. F. Paulat, T. Kuschel, C. Näther, V. K. K. Praneeth, O. Sander, N. Lehnert, "Spectroscopic Properties and Electronic Structure of Pentammineruthenium(II) Dinitrogen Oxide and corresponding Nitrosyl Complexes: Binding Mode of N_2O and Reactivity". *Inorg. Chem.* **2004**, *43*, 6979-6994 [PMID: 15500336]

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35. V. K. K. Praneeth, F. Neese, N. Lehnert, "Spin Density Distribution in Five- and Six-coordinate Iron(II)-Porphyrin NO Complexes evidenced by Magnetic Circular Dichroism Spectroscopy". *Inorg. Chem.* **2005**, *44*, 2570-2572 [PMID: 15819537]

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37. K. Fujisawa, T. Ono, Y. Ishikawa, N. Amir, Y. Miyashita, K. Okamoto, N. Lehnert, "Structural and Electronic Differences of Copper(I) Complexes with Tris(pyrazolyl)methane and Hydrotris(pyrazolyl)borate Ligands". *Inorg. Chem.* **2006**, *45*, 1698-1713 [PMID: 16471983]

38. V. K. K. Praneeth, C. Näther, G. Peters, N. Lehnert, "Spectroscopic Properties and Electronic Structure of Five- and Six-Coordinate Iron(II)-Porphyrin NO Complexes: Effect of the axial N-Donor Ligand". *Inorg. Chem.* **2006**, *45*, 2795-2811 [PMID: 16562937]

39. F. Paulat, V. K. K. Praneeth, C. Näther, N. Lehnert, "Quantum Chemistry-Based Analysis of the Vibrational Spectra of Five-Coordinate Metalloporphyrins [M(TPP)Cl]". *Inorg. Chem.* **2006**, *45*, 2835-2856 [PMID: 16562940]

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41. N. Lehnert, "Trendbericht: Bioanorganische Chemie 2005". *Nachrichten aus der Chemie* **2006**, *54*, 230-233

42. K. Mersmann, A. Hauser, N. Lehnert, F. Tuczek, "Electronic Structure, Spectroscopic Properties and Reactivity of Molybdenum and Tungsten Nitrido and Imido Complexes with Diphosphine Coligands: Influence of the *trans* Ligand". *Inorg. Chem.* **2006**, *45*, 5044-5056 [PMID: 16780326]

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44. N. Lehnert, U. Cornelissen, F. Neese, T. Ono, Y. Noguchi, K. Okamoto, K. Fujisawa, "Synthesis and Spectroscopic Characterization of Cu(II)-Nitrito Complexes with Hydrotris(pyrazolyl)borate and related Coligands". *Inorg. Chem.* **2007**, *46*, 3916-3933 [PMID: 17447754]

45. K. Fujisawa, Y. Noguchi, Y. Miyashita, K. Okamoto, N. Lehnert, "Mononuclear and Binuclear Copper(I) Complexes Ligated by Bis(3,5-diisopropyl-1-pyrazolyl)methane: Insight into the Fundamental Coordination Chemistry of Three-Coordinate Copper(I) Complexes with a Neutral Coligand". *Inorg. Chem.* **2007**, *46*, 10607-10623 [PMID: 17999490]

46. R. Meier, J. Maigut, B. Kallies, N. Lehnert, F. Paulat, F. W. Heinemann, G. Zahn, M. P. Feth, H. Krautscheid, K.-W. Brzezinka, R. van Eldik, "$[Fe^{III}(tmdta)]^-$ – *twist boat / half chair* conformer ratio reliably deduced from DFT calculated Raman spectra". *Chem. Commun.* **2007**, 3960-3962 [PMID: 17896046]

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48. K. Fujisawa, A. Tateda, T. Ono, Y. Miyashita, K. Okamoto, F. Paulat, V. K. K. Praneeth, A. Merkle, N. Lehnert, "Structural and Spectroscopic Characterization of Mononuclear Copper(I) Nitrosyl Complexes: End-on versus Side-on Coordination of NO to Copper(I)". *J. Am. Chem. Soc.* **2008**, *130*, 1205-1213 [PMID: 18179210]

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50. G. Bhosekar, I. Jeß, N. Lehnert, C. Näther, "Synthesis, Crystal Structure and Thermal Reactivity of $[ZnX_2$(2-chloropyrazine)] (X = Cl, Br, I) Coordination Compounds". *Eur. J. Inorg. Chem.* **2008**, 605-611

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55. T. C. Berto, V. K. K. Praneeth, L. E. Goodrich, N. Lehnert, "Iron-Porphyrin NO Complexes with Covalently Attached N-Donor Ligands: The Formation of a Stable Six-Coordinate Species in Solution".
J. Am. Chem. Soc. **2009**, *131*, 17116-17126 [PMID: 19891503]

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