

Dr. habil. Nicolai Lehnert

Dow Corning Assistant Professor of Chemistry
Assistant Professor of Biophysics
Department of Chemistry
The University of Michigan
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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. Gütllich
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

- 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

Feb. 2009 National Science Foundation (NSF) CAREER Award

Nov. 2007 Japan Society for the Promotion of Science (JSPS)
Invitation Fellowship to visit Japan in June 2008

since Sept. 2007 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 IN GERMANY

- 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 UM

- Fall 2006: CHEM 507
- **‘Introduction to Inorganic Chemistry’**; graduate course (3 credits), newly developed course
- Fall 2007: CHEM 507
- **‘Introduction to Inorganic Chemistry’**; graduate course (3 credits)
- Winter 2008: CHEM 616
- **‘Physical Inorganic Chemistry: Electronic Structure and Spectroscopy’**; graduate course (3 credits), newly developed course
- Fall 2008: CHEM 130
- **‘General Chemistry’**; undergraduate course (3 credits), newly developed course
- Winter 2009: CHEM 616
- **‘Physical Inorganic Chemistry: Electronic Structure and Spectroscopy’**; graduate course (3 credits)

RESEARCH SUPERVISION

- Postdoctoral Fellows (total currently: 1)
- Huayang Lee (May 2007 – July 2008)
 - Mary Grace I. Galinato (since October 2007)
- Ph.D. Students (total currently: 5)
- 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 (since May, 2007)
 - Corinne Sulok (since July, 2007)
 - Timothy Berto (since May 2008)
 - Lauren Goodrich (since May 2008)
 - Deidra Gerlach (since May 2008; joint student with Coucouvanis group)
- Diploma and Master Students (total currently: 0)
- Felix Studt (together with Prof. Dr. F. Tucek)
 - Klaus Mersmann (together with Prof. Dr. F. Tucek)
 - Florian Paulat
- Rotations (CHEM 597) (total currently: 0)
- Anna Merkle, Khoi Nguyen (Winter 2007)
 - Corinne Sulok (Spring 2007)
 - Timothy Berto, Austin Kizzie (Fall 2007)
 - Lauren Goodrich, Amanda Hickman, Aireen Romu (Winter 2008)
 - Melissa Zastrow (Winter 2009)
- Undergraduate Research (total currently: 3)
- Torben Kuschel, Bachelor Thesis
 - Susie Chen (CHEM 398: Fall 2006)
 - Yuki Murata (CHEM 399: Winter/Fall 2007; Summer Undergraduate Research Award, 2007)
 - Timothy C. Berto (Summer Research Internship, 2007)
 - Jonathan L. Bauer (CHEM 399: Fall 2007)
 - Corey J. Lager (CHEM 399: Fall 2007, Winter/Fall 2008; Summer Undergraduate Research Award, 2008)
 - Melissa Zastrow (Summer Research Internship, 2008)
 - Joey Braymer (Summer Research Internship, 2008)
 - Alex Navarro (SROP 2008)
 - Sherri Martin (CHEM 398: Fall 2008, Winter 2009)
 - Brandon M. Knope (UROP: Fall 2008, Winter 2009)

GRANT FUNDING

02/01/2009 – 01/31/2014	National Science Foundation (NSF) CAREER Award: 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’
03/2008 – 12/31/2009	Rackham Faculty Grant: Title: ‘The Detoxification of Nitric Oxide <i>in vivo</i> by Flavorubredoxin NO Reductase from <i>Escherichia coli</i> 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 researchers (Habilitationenförderung)
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. W. R. Scheidt, University of Notre Dame) of the symposium ‘Coordination Chemistry of NO 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, USA, March 22 - 26, 2009

- Reviewer for proposals: NSF, ACS-PRF
- Reviewer for: *J. Am. Chem. Soc.*, *Angew. Chem.*, *Inorg. Chem.*, *Chem. Europ. J.*, *J. Inorg. Biochem.*, *J. Phys. Chem.*, *Europ. J. Inorg. Chem.*, *Inorg. Chim. Acta*, *Vibrational Spectroscopy*
- Member of: American Chemical Society (ACS, since 2000), Society of Porphyrins & Phthalocyanins (SPP, since 2006), Society of Biological Inorganic Chemistry (SBIC, since 2007)

SEMINAR PRESENTATIONS: INVITED

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 Phthalocyanins (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

SEMINAR PRESENTATIONS: CONFERENCES

1. "Alkylperoxo Intermediates in Non-Heme Iron Enzymes", 219th *American Chemical Society National Meeting*, San Francisco, 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", *Chemiedozentagung 2005*, LMU München, Germany, March 06 - 09, 2005
3. "Electronic Structure and Reactivity of Thiolate-Coordinated Iron-Porphyrin Nitrosyls: Molecular Mechanism of P450nor", *Chemiedozentagung 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, USA, March 22 - 26, 2009

UNIVERSITY SERVICE

- Since June 2008 Faculty Advisor for UM's annual student symposium PECRUM
(Perspectives on Chemistry Research at the University of Michigan)
- Since Feb. 2007 Member of the Graduate Committee (UM)
- Since Sept. 2006 Member of the Recruiting Committee (UM)
Coordinator of the Inorganic Cluster Seminars (UM)
Member of the Gomberg Committee (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.

MILITARY SERVICE

June 1989 – Aug. 1990 Served in the German Army in Wuppertal, Germany

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 N₂ Bonding in Iron(II)-Phosphane Complexes: Structure, Synthesis and Properties of the Monomeric Adducts trans-[FeX(N₂)(depe)₂]BPh₄, X=Cl, Br"
Angew. Chem. **1998**, (*Int. Ed.*), *37*, 815-817
6. F. Tuczek, N. Lehnert
Highlight: "New Developments in Nitrogen Fixation"
Angew. Chem. **1998**, (*Int. Ed.*), *37*, 2636-2638
7. N. Lehnert, F. Tuczek
"The Reduction Pathway of End-on Coordinated Dinitrogen:
I. Vibrational Properties of Mo/W-N₂, -NNH and -NNH₂ 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-N₂, -NNH and -NNH₂ 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]BPh₄, X=Cl, Br: Electronic Structure and Spin-Forbidden Reaction with N₂"
Inorg. Chem. **2002**, *41*, 3491-3499
10. C. M. Habeck, N. Lehnert, C. Näther, F. Tuczek
"Mo/W-N₂ and -N₂H₂ 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. Tucek
 "Vibrational Properties of $[\text{FeH}(\text{N}_2)(\text{depe})_2]^+$ and $[\text{FeCl}(\text{N}_2)(\text{depe})_2]^+$: 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. Tucek
 "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. Tucek
 "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. Tucek, 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. Tucek
 "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. Tucek
 "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. Tucek
 "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. Tucek
 "The Iron Hydrido Complex $[\text{FeH}(\text{dppe})_2]^+$: 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. Tucek
 "Spectroscopic Comparison of Dinuclear Ti^+ and Ti^{2+} $\mu\text{-}\eta^1\text{:}\eta^1$ Dinitrogen Complexes with $\text{Cp}^*/\text{Pentafulvene}$ 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 Lipoygenase"
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
32. K. Fujisawa, N. Lehnert, Y. Ishikawa, K. Okamoto
"Diazeno Complexes of Copper: Synthesis, Spectroscopic Analysis, and Electronic Structure"
Angew. Chem. **2004**, (*Int. Ed.*), *43*, 4944-4947
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 N₂O and Reactivity"
Inorg. Chem. **2004**, *43*, 6979-6994
34. Y. Wu, C. Näther, N. Lehnert, W. Bensch
"Synthesis, crystal structure and properties of K₄Ba₂(Nb₂S₁₁)₂"
Solid State Sci. **2005**, *7*, 1062-1069
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
36. V. K. K. Praneeth, E. Haupt, N. Lehnert
"Thiolate Coordination to Fe(II)-Porphyrin NO Centers"
J. Inorg. Biochem. **2005**, *99*, 940-948 (special issue: Heme-Diatomic Interactions, Part 2)
Erratum: *J. Inorg. Biochem.* **2005**, *99*, 1744
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
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
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

40. N. Lehnert, V. K. K. Praneeth, F. Paulat
"Electronic Structure of Fe(II)-Porphyrin Nitroxyl Complexes: Molecular Mechanism of fungal Nitric Oxide Reductase (P450nor)"
J. Comput. Chem. **2006**, *27*, 1338-1351 (special issue: Theoretical Bioinorganic Chemistry)
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
43. F. Paulat, N. Lehnert
"Electronic Structure of Ferric Heme Nitrosyl Complexes with Thiolate Coordination"
Inorg. Chem. **2007**, *46*, 1547-1549
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
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"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"
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