

LIST OF PUBLICATIONS

Wolfgang Lubitz

1. W. Lubitz, K.P. Dinse, K. Möbius and R. Biehl
Fluorine and Proton ENDOR of Aromatic Radicals in Solution
Chem. Phys. 8, 371-383 (1975)
2. R. Biehl, W. Lubitz, K. Möbius and M. Plato
Observation of Deuterium Quadrupole Splittings of Aromatic Free Radicals in Liquid Crystals by ENDOR and TRIPLE Resonance
J. Chem. Phys. 66, 2074-2078 (1977)
3. R. Biehl, K. Hinrichs, H. Kurreck, W. Lubitz, U. Mennenga and K. Roth
ESR, NMR and ENDOR Studies of Partially Deuterated Phenyl Substituted Anthracenes. π - σ Delocalization
J. Am. Chem. Soc. 99, 4278-4286 (1977)
4. W. Lubitz, R. Biehl and K. Möbius
Sodium and Proton ENDOR and TRIPLE-Resonance Experiments on Biphenyl and Fluorenone Ion Pairs in Solution
J. Magn. Reson. 27, 411-417 (1977)
5. R. Biehl, Ch. Hass, H. Kurreck, W. Lubitz and S. Oestreich
ESR and ENDOR Studies of Partially Deuterated and Chlorinated Phenalenyls
Tetrahedron 34, 419-424 (1978)
6. B. Kirste, H. Kurreck, W. Lubitz and K. Schubert
 ^{13}C ENDOR Studies of Organic Doublet and Triplet State Molecules
J. Am. Chem. Soc. 100, 2292-2299 (1978)
7. H.-J. Fey, W. Lubitz, H. Zimmermann, M. Plato, K. Möbius and R. Biehl
 ^{13}C - and Proton-ENDOR Studies of ^{13}C -labelled Organic Radicals
Z. Naturforsch. 33a, 514-522 (1978)
8. W. Lubitz, W. Broser, B. Kirste, H. Kurreck and K. Schubert
 ^{13}C - and ^1H -ENDOR Studies of a Phenoxy Type Radical
Z. Naturforsch. 33a, 1072-1076 (1978)
9. H. J. Fey, H. Kurreck and W. Lubitz
ENDOR Studies of [6] Helicene Anion Radical
Tetrahedron 35, 905-907 (1979)

10. W. Lubitz, M. Plato, K. Möbius and R. Biehl
Alkali and H ENDOR on Aromatic Ion Pairs in Solution. An INDO Approach
J. Phys. Chem. 83, 3402-3413 (1979)
11. B. Kirste, H. Kurreck, W. Lubitz and H. Zimmermann
 ^1H , ^2H and ^{13}C ENDOR Studies of Labeled Bis(biphenyl)propenyl Type Radicals in Isotropic Solution and in Liquid Crystals
J. Am. Chem. Soc. 102, 817-825 (1980)
12. W. Lubitz and T. Nyrönen
 ^{14}N and ^1H ENDOR and TRIPLE Resonance on Azaaromatic Radicals Produced by Sodium Reduction in Liquid Ammonia
J. Magn. Reson. 41, 17-29 (1980)
13. M. Plato, W. Lubitz and K. Möbius
A Solution ENDOR Sensitivity Study of Various Nuclei in Organic Radicals
J. Phys. Chem. 85, 1202-1219 (1981)
14. W. Lubitz, F. Lendzian and K. Möbius
 ^{14}N and ^1H Electron Nuclear Multiple Resonance Experiments on Bacteriochlorophyll *a* Anion Radicals in Solution
Chem. Phys. Lett. 81, 235-241 (1981)
15. F. Lendzian, W. Lubitz, H. Scheer, C. Bubenzer and K. Möbius
In Vivo Liquid Solution ENDOR and TRIPLE Resonance of Bacterial Photosynthetic Reaction Centers of *Rhodospseudomonas Sphaeroides* R-26
J. Am. Chem. Soc. 103, 4635-4637 (1981)
16. M. Bock, W. Lubitz, H. Kurreck, H. Fenner and R. Grauert
 ^{14}N and ^1H ENDOR and TRIPLE Resonance Experiments of Flavin and Thiaflavin Radical Cations in Liquid Solution
J. Am. Chem. Soc. 103, 5567-5568 (1981)
17. W. Lubitz, F. Lendzian and K. Möbius
The Bacteriopheophytin *a* Anion Radical. A Solution ENDOR and TRIPLE Resonance Study
Chem. Phys. Lett. 84, 33-38 (1981)
18. W. Möhl, C.J. Winscom, M. Plato, K. Möbius and W. Lubitz
Examination of the Conditions for ENDOR-in-Solution on Transition Metal Complexes
J. Phys. Chem. 86, 149-152 (1982)

19. K. Möbius, M. Plato and W. Lubitz
Radicals in Solution Studied by ENDOR and TRIPLE Resonance Spectroscopy
Phys. Rep. 87, 171-208 (1982)
20. A.J. Hoff, F. Lenzian, K. Möbius and W. Lubitz
Proton and Nitrogen Electron Nuclear Double and Triple Resonance of the Chlorophyll a Anion in Liquid Solution
Chem. Phys. Lett. 85, 3-8 (1982)
21. F. Lenzian, K. Möbius and W. Lubitz
The Pheophytin a Anion Radical. ¹⁴N- and ¹H-ENDOR and TRIPLE Resonance in Liquid Solution
Chem. Phys. Lett. 90, 375-381 (1982)
22. K. Möbius, W. Fröhling, F. Lenzian, W. Lubitz, M. Plato and C.J. Winscom
Multiple Magnetic Resonance Studies on Organic Molecules in their Ground and Excited States
J. Phys. Chem. 86, 4491-4507 (1982)
23. C.J. Winscom, W. Lubitz, H. Diegruber and R. Mösel
EPR Studies of Co(II)-Bis(dimethylglyoximato)-Complexes and their Oxygen Adducts in a Zeolite X Matrix
Studies in Surface Science and Catalysis 12, 15-21 (1982), Elsevier, Amsterdam
24. W. Lubitz, F. Lenzian, H. Scheer, M. Plato and K. Möbius
Electron-Nuclear Multiple Resonance Studies on Primary Products of Bacterial Photosynthesis
in: Photochemistry and Photobiology, Proceedings of the International Conference, University of Alexandria, Egypt, ed. Zewail, A.H. (Harwood Academic Publishers, New York), 1983, pp. 1057-1069
25. W. Kaim and W. Lubitz
Radical Products in Single Electron Transfer Reactions of Lithium Triethylhydridoborate as Detected by ESR and Multinuclear (¹H, ¹⁰B, ¹¹B, ¹⁴N) ENDOR Spectroscopy
Angew. Chem. 95, 915-916 (1983)
Angew. Chem. Int. Ed. Engl. 22, 892 (1983)
Angew. Chem. Suppl. 1209-1220 (1983)
26. H. Bock, B. Hierholzer, H. Kurreck and W. Lubitz
²⁹Si-E(lectron) N(uclear) DO(uble) R(esonance)
Angew. Chem. 95, 817-819 (1983)
Angew. Chem. Int. Ed. Engl. 22, 787-788 (1983)
Angew. Chem. Suppl. 1088-1105 (1983)

27. W. Lubitz, F. Lendzian, H. Scheer, J. Gottstein, M. Plato and K. Möbius
Structural Studies of the Primary Donor Cation Radical P_{870}^{+} in Reaction Centers of *Rhodospirillum rubrum* by Electron-Nuclear Double Resonance in Solution
Proc. Natl. Acad. Sci. USA 81, 1401-1405 (1984)
28. H. Kurreck, B. Kirste and W. Lubitz
ENDOR Spectroscopy - A Promising Technique for Investigating the Structure of Organic Radicals
Angew. Chem. 96, 171-193 (1984)
Angew. Chem. Int. Ed. Engl. 23, 173-194 (1984)
29. H. Kurreck, M. Bock, N. Bretz, M. Elsner, H. Kraus, W. Lubitz, F. Müller, J. Geissler and P.M.H. Kroneck
Fluid Solution and Solid-State Electron Nuclear Double Resonance Studies of Flavin Model Compounds and Flavoenzymes
J. Am. Chem. Soc. 106, 737-746 (1984)
30. I.M. Smith, L.H. Sutcliffe, S. Wiesner, W. Lubitz and H. Kurreck
Magnetic Resonance Studies of Cation Radicals from Chromans. Part 2. Nuclear Magnetic Resonance, Electron Spin Resonance, ENDOR and TRIPLE Spectroscopy of Some Tricyclic Chromans
J. Chem. Soc., Farad. I, 80, 3021-3036 (1984)
31. F. Lendzian, K. Möbius, M. Plato, U.H. Smith, M.C. Thurnauer and W. Lubitz
 ^{25}Mg ENDOR and TRIPLE Resonance in Liquid Solution of the Bacteriochlorophyll a Cation and Anion Radicals
Chem. Phys. Lett. 111, 583-588 (1984)
32. W. Lubitz, R.A. Isaacson, E.C. Abresch and G. Feher
 ^{15}N Electron Nuclear Double Resonance of the Primary Donor Cation Radical P_{865}^{+} in Reaction Centers of *Rhodopseudomonas sphaeroides*: Additional Evidence for the Dimer Model
Proc. Natl. Acad. Sci. USA 81, 7792-7796 (1984)
33. W. Lubitz, F. Lendzian and H. Scheer
Characterization of 10-Hydroxybacteriochlorophyll a by ENDOR and TRIPLE Resonance Spectroscopy
J. Am. Chem. Soc. 107, 3341-3343 (1985)
34. W. Lubitz, E.C. Abresch, R.J. Debus, R.A. Isaacson, M.Y. Okamura and G. Feher
Electron Nuclear Double Resonance of Semiquinones in Reaction Centers of *Rhodopseudomonas sphaeroides*
Biochim. Biophys. Acta 808, 464-469 (1985)

35. W. Lubitz, F. Lendzian, M. Plato, K. Möbius and E. Tränkle
ENDOR Studies of the Primary Donor in Bacterial Reaction Centers
Springer Series in Chemical Physics (Springer Verlag, Berlin) 42,
164-173 (1985)
36. G. Feher, R.A. Isaacson, M.Y. Okamura and W. Lubitz
ENDOR of Semiquinones in RC's from *Rhodopseudomonas sphaeroides*
Springer Series in Chemical Physics (Springer Verlag, Berlin) 42,
174-189 (1985)
37. F. Lendzian, W. Lubitz, R. Steiner, E. Tränkle, M. Plato, H. Scheer
and K. Möbius
**The Radical Cation of Bacteriochlorophyll b. A Liquid-Phase
ENDOR and TRIPLE Resonance Study**
Chem. Phys. Lett. 126, 290-296 (1986)
38. M. Plato, E. Tränkle, W. Lubitz, F. Lendzian and K. Möbius
**Molecular Orbital Investigation of Dimer Formations of
Bacteriochlorophyll a. Model Configurations for the Primary Donor
of Photosynthesis**
Chem. Phys. 107, 185-196 (1986)
39. M. Huber, F. Lendzian, W. Lubitz, E. Tränkle, K. Möbius
and M.R. Wasielewski
**ENDOR and TRIPLE Resonance in Solutions of the Chlorophyll a
and Bis(chlorophyll)cyclophane Radical Cations**
Chem. Phys. Lett. 132, 467-473 (1986)
40. K. Möbius and W. Lubitz
ENDOR Spectroscopy in Photobiology and Biochemistry
in: Biological Magnetic Resonance, eds. L.J. Berliner and J. Reuben
(Plenum Press, New York), Vol. 7, pp. 129-247 (1987)
41. W. Lubitz and G.T. Babcock
ENDOR Spectroscopy
Trends Biochem. Sci. 12, 96-100 (1987)
42. M. Baumgarten, W. Lubitz and C.J. Winscom
EPR and ENDOR Studies of Cobaloximee(II)
Chem. Phys. Lett. 133, 102-108 (1987)
43. W. Lubitz, C.J. Winscom, H. Diegruber and R. Mösele
**EPR Characterization of Bis(dimethylglyoximato) Cobalt(II)
Complexes and their Oxygen Adducts Synthesised in an X-Zeolite
Matrix**
Z. Naturforsch. 42a, 970-986 (1987)

44. H. Kurreck, B. Kirste and W. Lubitz
Electron Nuclear Double Resonance Spectroscopy of Radicals in Solution - Applications to Organic and Biological Chemistry
Monograph: Methods in Stereochemical Analysis, ed. A.P. Marchand (VCH Publishers, Inc., Deerfield Beach, Florida)(1988), 374 pages with 770 references and 139 figures

45. G. Feher, R.A. Isaacson, M.Y. Okamura and W. Lubitz
ENDOR of Exchangeable Protons of the Reduced Intermediate Acceptor in Reaction Centers from *Rhodobacter sphaeroides* R-26
in: The Photosynthetic Bacterial Reaction Center, Structure and Dynamics, J. Breton and A. Vermeglio (eds.), Plenum Press (1988), pp. 229-235

46. M. Plato, F. Lenzian, W. Lubitz, E. Tränkle and K. Möbius
Molecular Orbital Studies on the Primary Donor P₉₆₀ in Reaction Centers of *Rps. viridis*
in: The Photosynthetic Bacterial Reaction Center, Structure and Dynamics, J. Breton and A. Vermeglio (eds.), Plenum Press (1988), pp. 379-388

47. F. Lenzian, W. Lubitz, H. Scheer, A.J. Hoff, M. Plato, E. Tränkle and K. Möbius
ESR, ENDOR and TRIPLE Resonance Studies of the Primary Donor Radical Cation P₉₆₀⁺ in the Photosynthetic Bacterium *Rhodopseudomonas. viridis*
Chem. Phys. Lett. 148, 377-385 (1988)

48. M. Plato, W. Lubitz, F. Lenzian and K. Möbius
Magnetic Resonance and Molecular Orbital Studies of the Primary Donor Cation Radical P₉₆₀⁺ in the Photosynthetic Bacterium *Rhodopseudomonas viridis*
Isr. J. Chem. 28, 109-119 (1988)

49. K. Möbius, M. Plato, W. Lubitz and F. Lenzian
Electron-Nuclear Multiple Resonance on Stable and Transient Radicals
Isr. J. Chem. 28, 239-248 (1988)

50. K. Möbius, M. Plato and W. Lubitz
Bacteriochlorophyll Dimers in Photosynthesis: ENDOR and MO Studies
24th Ampere Congress, Magnetic Resonance and Related Phenomena, Posen, 1988, pp. 517-527

51. M. Möbius, W. Lubitz and M. Plato
Liquid-State ENDOR and TRIPLE Resonance
in: Advanced EPR, Applications in Biology and Biochemistry, A.J. Hoff (ed.), Elsevier (1989), pp. 441-499
52. A.M.L. Krebber, L.H. Sutcliffe, W. Lubitz and H. Kurreck
Structural Effects on ESR Hyperfine Coupling Constants of Some Dithiazolidinyl Free Radicals
Magn. Reson. Chem. 27, 288-294 (1989)
53. W. Lubitz, R.A. Isaacson, M.Y. Okamura, E.C. Abresch, M. Plato and G. Feher
ENDOR Studies of the Intermediate Electron Acceptor Radical Anion I^- in Photosystem II Reaction Centers
Biochim. Biophys. Acta 977, 227-232 (1989)
54. W. Lubitz, B. Bönigk, M. Plato, R.A. Isaacson, M.Y. Okamura and G. Feher
ENDOR Studies of the Intermediate Electron Acceptor Radical Anion I^- in Reaction Centers of *Rps. viridis*
in: Current Research in Photosynthesis, M. Baltscheffsky (ed.), Kluwer (1990), Vol. I, pp. 141-144
55. F. MacMillan, H. Gleiter, G. Renger and W. Lubitz
EPR/ENDOR Studies of Plastoquinone Anion Radical in Photosystem II (Q_A^-) and in Organic Solvents
in: Current Research in Photosynthesis, M. Baltscheffsky (ed.), Kluwer (1990), Vol. I, pp. 531-534
56. M. Plato, K. Möbius, W. Lubitz, J.P. Allen and G. Feher
Magnetic Resonance and Molecular Orbital Studies of the Primary Donor States in Bacterial Reaction Centers
Perspectives in Photosynthesis, Vol. 22, Proceedings of the 22nd Jerusalem Symposium in Quantum Chemistry and Biochemistry, J. Jortner and B. Pullmann (Eds.), Kluwer (1990), pp. 423-434
57. F. Lendzian, B. Endeward, M. Plato, D. Bumann, W. Lubitz and K. Möbius
ENDOR and TRIPLE Resonance Investigation of the Primary Donor Cation Radical $P_{865}^{+\cdot}$ in Single Crystals of *Rhodobacter sphaeroides* R-26 Reaction Centers
Springer Series in Biophysics, Vol. 6, Reaction Centers of Photosynthetic Bacteria, M.-E. Michel-Beyerle (ed.), Springer Verlag (1990), pp. 57-68

58. W. Lubitz
EPR and ENDOR Studies of Chlorophyll Cation and Anion Radicals
in: Chlorophylls, H. Scheer (ed.), CRC Press, Inc., Boca Raton, Florida
(1991), pp. 903-944
59. M. Plato, K. Möbius and W. Lubitz
Molecular Orbital Calculations on Chlorophyll Radical Ions
in: Chlorophylls, H. Scheer (ed.), CRC Press, Inc., Boca Raton, Florida
(1991), pp. 1015-1046
60. O. Burghaus, M. Plato, D. Bumann, B. Neumann, W. Lubitz and K.
Möbius
3 mm EPR Investigation of the Primary Donor Cation Radical $P_{865}^{+\cdot}$
in Single Crystals of *Rb. sphaeroides* R-26 Reaction Centers
Chem. Phys. Lett. 185, 381-386 (1991)
61. Ch. Geßner, F. Lenzian, B. Bönigk, M. Plato, K. Möbius and W. Lubitz
Proton ENDOR and TRIPLE Resonance Investigation of $P_{865}^{+\cdot}$ in
Photosynthetic Reaction Center Single Crystals of *Rb.*
***Sphaeroides* Wild Type 2.4.1**
Appl. Magn. Res. 3, 763-777 (1992)
62. J. Rautter, Ch. Geßner, F. Lenzian, W. Lubitz, J.C. Williams, H.A.
Murchison, S. Wang, N.W. Woodbury and J.P. Allen
EPR and ENDOR Studies of the Primary Donor Cation Radical in
Native and Genetically Modified Bacterial Reaction Centers
in: "The Photosynthetic Bacterial Reaction Center II", J. Breton and A.
Verméglio (eds.), Plenum Press, New York (1992), pp. 99-108
63. F. Lenzian, B. Bönigk, M. Plato, K. Möbius and W. Lubitz
 ^{15}N ENDOR Experiments on the Primary Donor Cation Radical $D^{+\cdot}$
in Bacterial Reaction Center Single Crystals of *Rb. sphaeroides* R-
26
in: "The Photosynthetic Bacterial Reaction Center II", J. Breton and A.
Verméglio (eds.), Plenum Press, New York (1992), pp. 89-97
64. M. Plato, F. Lenzian, W. Lubitz and K. Möbius
Molecular Orbital Study of Electronic Asymmetry in Primary
Donors of Bacterial Reaction Centers
in: "The Photosynthetic Bacterial Reaction Center II", J. Breton and A.
Verméglio (eds.), Plenum Press, New York (1992), pp. 109-118
65. W. Zwegart, T. Weyhermüller, G. Renger, K. Wieghardt and W. Lubitz
EPR and ENDOR Studies of Manganese Clusters in the Water-
Oxidizing Complex and Related Model Compounds
in: Research in Photosynthesis (N. Murata, ed.), Kluwer, 1992, Vol. II,
pp. 289-292

66. F. Lendzian, C. Geßner, B. Bönigk, M. Plato, K. Möbius and W. Lubitz
 ^{15}N - and ^1H -ENDOR/TRIPLE Resonance of the Primary Donor Cation Radical $\text{D}^{\bullet+}$ in Isotopically Labeled Reaction Centers of *Rhodobacter sphaeroides*
in: Research in Photosynthesis (N. Murata, ed.), Kluwer, 1992, Vol. I, pp. 433-436
67. R. Bittl, A. van der Est, G. Fücksle, W. Lubitz and D. Stehlik
Transient EPR of Photosynthetic Reaction Centers: Structural Information on the Radical Pair P^+Q^- in Zn-Substituted *Rb. sphaeroides* and Photosystem I
in: Research in Photosynthesis (N. Murata, ed.), Kluwer, 1992, Vol. I, pp. 461-464
68. R. Klette, J.T. Törring, M. Plato, K. Möbius, B. Bönigk and W. Lubitz
Determination of the g Tensor of the Primary Donor Cation Radical in Single Crystals of *Rhodobacter sphaeroides* R-26 Reaction Centers by 3-mm High-Field EPR
J. Phys. Chem. 97, 2015-2020 (1993)
69. G. Fücksle, R. Bittl, A. van der Est, W. Lubitz and D. Stehlik
Transient EPR Spectroscopy of the Charge Separated State P^+Q^- in Photosynthetic Reaction Centers. Comparison of Zn-Substituted *Rhodobacter sphaeroides* R-26 and Photosystem I
Biochim. Biophys. Acta 1142, 23-35 (1993)
70. O. Burghaus, M. Plato, M. Rohrer, K. Möbius, F. MacMillan and W. Lubitz
3 mm High-Field EPR on Semiquinone Radical Anions Q^- Related to Photosynthesis and on the Primary Donor $\text{P}^{\bullet+}$ and Acceptor Q_A^- in Reaction Centers of *Rhodobacter sphaeroides* R-26
J. Phys. Chem. 97, 7639-7647 (1993)
71. A. van der Est, R. Bittl, E.C. Abresch, W. Lubitz and D. Stehlik
Transient EPR Spectroscopy of Perdeuterated Zn-Substituted Reaction Centers of *Rhodobacter sphaeroides* R-26
Chem. Phys. Lett. 212, 561-568 (1993)
72. F. Lendzian, M. Huber, R.A. Isaacson, B. Endeward, M. Plato, B. Bönigk, K. Möbius, W. Lubitz and G. Feher
The Electronic Structure of the Primary Donor Cation Radical in *Rhodobacter sphaeroides* R-26: ENDOR and TRIPLE Resonance Studies in Single Crystals of Reaction Centers
Biochim. Biophys. Acta 1183, 139-160 (1993)

73. H. Käss, J. Rautter, W. Zweggart, A. Struck, H. Scheer and W. Lubitz
EPR, ENDOR and TRIPLE Resonance Studies of Modified Bacteriochlorophyll Cation Radicals
J. Phys. Chem. 98, 354-363 (1994)
74. W. Zweggart, R. Thanner and W. Lubitz
An Improved TM₁₁₀ ENDOR Cavity for the Investigation of Transition Metal Complexes
J. Magn. Reson. Ser. A 109, 172-176 (1994)
75. R. Bittl, A. van der Est, A. Kamlowski, W. Lubitz and D. Stehlik
Time-Resolved EPR of the Radical Pair P₈₆₅⁺ Q_A⁻ in Bacterial Reaction Centers. Observation of Transient Nutations, Quantum Beats and Envelope Modulation Effects
Chem Phys. Lett. 226, 349-358 (1994)
76. J. Rautter, F. Lenzian, W. Lubitz, S. Wang and J.P. Allen
Comparative Study of Reaction Centers from Photosynthetic Purple Bacteria: Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Spectroscopy
Biochemistry 33, 12077-12084 (1994)
77. H. Käss, J. Rautter, B. Bönigk, P. Höfer and W. Lubitz
2D ESEEM on the ¹⁵N-labeled Radical Cations of Bacteriochlorophyll a and of the Primary Donor in Reaction Centers of *Rhodobacter sphaeroides*
J. Phys. Chem. 99, 436-448 (1995)
78. W. Lubitz, J. Rautter, H. Käß and F. Lenzian
Light-Induced Charge Separation in Photosynthetic Reaction Centers - Magnetic Resonance Studies
Sol. Energ. Mat. Sol. C. 38, 77-89 (1995)
79. V.A. Shuvalov, R. Fiege, U. Schreiber, F. Lenzian and W. Lubitz
EPR Study of Cytochrome in the D1D2 Cyt b-559 Complex
Biochim. Biophys. Acta 1228, 175-180 (1995)
80. L. Cui, S.E. Bingham, M. Kuhn, H. Käss, W. Lubitz and A.N. Webber
Site-directed Mutagenesis of Conserved Histidines in the Helix VIII Domain of PsaB Impairs Assembly of the Photosystem I Reaction Center without Altering Spectroscopic Characteristics of P₇₀₀
Biochemistry 34, 1549-1558 (1995)
81. A. van der Est, I. Sieckmann, W. Lubitz and D. Stehlik
Differences in the Binding of the Primary Quinone Acceptor in Photosystem I and Reaction Centers of *Rb. sphaeroides* R-26 Studied with Transient EPR Spectroscopy
Chem. Phys. 194, 349-359 (1995)

82. T.F. Prisner, A. van der Est, R. Bittl, W. Lubitz, D. Stehlik and K. Möbius
Time-Resolved W-Band (95 GHz) EPR Spectroscopy of Zn-Substituted Reaction Centers of *Rb. sphaeroides* R-26
Chem. Phys. 194, 361-370 (1995)
83. H. Käß. E. Bittermann-Weidlich, L.-E. Andréasson, B. Bönigk and W. Lubitz
ENDOR and ESEEM of the ^{15}N Labelled Radical Cations of Chlorophyll *a* and the Primary Donor P_{700} in Photosystem I
Chem. Phys. 194, 419-432 (1995)
84. F. MacMillan, F. Lenzian, G. Renger and W. Lubitz
EPR and ENDOR Investigation of the Primary Electron Acceptor Radical Anion Q_A^- in Iron-Depleted Photosystem II Membrane Fragments
Biochemistry 34, 8144-8156 (1995)
85. J. Rautter, F. Lenzian, C. Schulz, A. Fetsch, M. Kuhn, X. Lin, J.C. Williams, J.P. Allen and W. Lubitz
ENDOR-Studies of the Primary Donor Cation Radical in Mutant Reaction Centers of *Rhodobacter sphaeroides* with Altered Hydrogen-Bond Interactions
Biochemistry 34, 8130-8143 (1995)
86. R.A. Isaacson, F. Lenzian, E.C. Abresch, W. Lubitz and G. Feher
Electronic Structure of Q_A^- in Reaction Centers from *Rb. sphaeroides*: I. EPR in Single Crystals
Biophys. J. 69, 311-322 (1995)
87. M. Rohrer, M. Plato, F. MacMillan, Y. Grishin, W. Lubitz and K. Möbius
Orientation-Selected 95 GHz High-Field ENDOR Spectroscopy of Randomly Oriented Plastoquinone Anion Radicals
J. Magn. Reson. A 116, 59-66 (1995)
88. F. MacMillan, F. Lenzian and W. Lubitz
EPR and ENDOR Characterization of Semiquinone Anion Radicals Related to Photosynthesis
Magn. Reson. Chem. 33, S81-S93 (1995)
89. A.T. Gardiner, F. Lenzian, F. MacMillan, S.G. Zech, R. Bittl, M. Kuhn and W. Lubitz
EPR Characterization of Q_A^- from Biosynthetically and Chemically Substituted Zn(II) Reaction Centers from *Rhodobacter sphaeroides* and *Rhodopseudomonas viridis*
in: Photosynthesis: From Light to Biosphere (P. Mathis, ed.), Vol. I, pp. 655-658, Kluwer Academic Publishers, Dordrecht (1995)

90. F. MacMillan, J. Kurreck, N. Adir, F. Lenzian, H. Käß, F. Reifarth, G. Renger and W. Lubitz
EPR, ENDOR and ESEEM Investigation of the Electron Acceptor Radical Anion Q_A^- in Photosystem II (PS II) Reaction Centers
in: Photosynthesis: From Light to Biosphere (P. Mathis, ed.), Vol. I, pp. 659-662, Kluwer Academic Publishers, Dordrecht (1995)
91. L. Krabben, H. Käß, E. Schlodder, M. Kuhn, W. Lubitz, H. Xu, S. Bingham and A. Webber
Site-Directed Mutations of *PsaB* for the Study of Cofactor-Protein and Protein-Protein Interactions of Photosystem I
in: Photosynthesis: From Light to Biosphere (P. Mathis, ed.), Vol. II, pp. 123-126, Kluwer Academic Publishers, Dordrecht (1995)
92. W. Lubitz, F. Müh, J. Rautter, F. Lenzian, J.P. Allen and J.C. Williams
Magnetic Resonance Studies of Bacterial Reaction Centers: Effects of Hydrogen Bonds on the Electronic Structure of P^{+} and I^-
in: Photosynthesis: From Light to Biosphere (P. Mathis, ed.), Vol. I pp. 413-418, Kluwer Academic Publishers, Dordrecht (1995)
93. R. Fiege, W. Zwegart, K.-D. Irrgang, N. Adir, B. Geiken, G. Renger and W. Lubitz
EPR/ENDOR Studies of the Water Oxidizing Complex in Photosystem II
in: Photosynthesis: From Light to Biosphere (P. Mathis, ed.), Vol. II, pp. 369-372, Kluwer Academic Publishers, Dordrecht (1995)
94. M. Huber, J.T. Törring, M. Plato, U. Fink, W. Lubitz, R. Feick, C.C. Schenck and K. Möbius
Investigation of the Electronic Structure of the Primary Electron Donor in Bacterial Photosynthesis - Measurements of the Anisotropy of the Electronic G -Tensor using High-Field/High-Frequency EPR
Sol. Energ. Mat. Sol. C. 38, 119-126 (1995)
95. A. van der Est, I. Sieckmann, W. Lubitz and D. Stehlik
Quinone Binding in *Rb. sphaeroides* and Photosystem I Studied by Transient EPR
in: Photosynthesis: From Light to Biosphere (P. Mathis, ed.), Vol. II, pp. 143-146, Kluwer Academic Publishers, Dordrecht (1995)
96. R. Fiege, U. Schreiber, G. Renger, W. Lubitz and V.A. Shuvalov
Study of Heme Fe(III) Ligated by OH^- in Cytochrome *b*-559 and its Low Temperature Photochemistry in Intact Chloroplasts
FEBS Lett. 377, 325-329 (1995)

97. W. Lubitz and F. Lendzian
ENDOR Spectroscopy
in: Advances in Photosynthesis. "Biophysical Techniques in Photosynthesis", Kluwer, Dordrecht, 1996, pp. 255-275
98. J. Rautter, F. Lendzian, X. Lin, J.C. Williams, J.P. Allen and W. Lubitz
Effect of Orbital Asymmetry in P^{*+} on Electron Transfer in Reaction Centers of *Rb. sphaeroides*
in: The Reaction Center of Photosynthetic Bacteria - Structure and Dynamics (M.-E. Michel-Beyerle, ed.), Springer, Berlin (1996), pp. 37-50
99. R. Isaacson, E. Abresch, F. Lendzian, C. Boullais, M. Paddock, C. Mioskowski, W. Lubitz, G. Feher
Asymmetry of the Binding Sites of $Q_A^{-\bullet}$ and $Q_B^{-\bullet}$ in Reaction Centers of *Rb. sphaeroides* Probed by Q-Band EPR with ^{13}C -labeled Quinones
in: The Reaction Center of Photosynthetic Bacteria, Structure and Dynamics (M.-E. Michel-Beyerle, ed.), Springer, Berlin (1996), pp. 353-367
100. H. Käß and W. Lubitz
Evaluation of 2D-ESEEM of the ^{15}N -Labeled Radical Cations of the Primary Donor P_{700} in Photosystem I and Chlorophyll a
Chem. Phys. Lett., 251, 193-203 (1996)
101. R. Bittl, S. Zech and W. Lubitz
Light-Induced Changes in Transient EPR Spectra of $P_{865}^{+\bullet} Q_A^{-\bullet}$
in: The Reaction Center of Photosynthetic Bacteria, Structure and Dynamics (M.-E. Michel-Beyerle, ed.), Springer, Berlin (1996), pp. 333-339
102. I. Muegge, J. Apostolakis, U. Ermler, G. Fritzsche, W. Lubitz and E.W. Knapp
Shift of the Special Pair Redox Potential: Electrostatic Energy Computations of Mutants of the Reaction Center of *Rhodobacter sphaeroides*
Biochemistry 35, 8359-8370 (1996)
103. J.P. Allen, K. Artz, X. Lin, J.C. Williams, A. Ivancich, D. Albouy, T.A. Mattioli, A. Fetsch, M. Kuhn and W. Lubitz
Effects of Hydrogen Bonding to a Bacteriochlorophyll-Bacteriopheophytin Dimer in Reaction Centers from *Rhodobacter sphaeroides*
Biochemistry 35, 6612-6619 (1996)

104. W. Zweggart, R. Bittl, K. Wieghardt and W. Lubitz
EPR and ^{55}Mn cw-ENDOR Study of an Antiferromagnetically Coupled Dinuclear Manganese ($\text{Mn}^{\text{III}} \text{Mn}^{\text{IV}}$) Complex
Chem. Phys. Lett. 261, 272-276 (1996)
105. R. Fiege, W. Zweggart, R. Bittl, N. Adir, G. Renger and W. Lubitz
EPR and ENDOR Studies of the Water Oxidizing Complex of Photosystem II
Photosyn. Research 48, 227-237 (1996)
106. A.N. Webber, H. Su, S.E. Bingham, H. Käß, L. Krabben, M. Kuhn, R. Jordan, E. Schlodder and W. Lubitz
Site-Directed Mutations Affecting the Spectroscopic Characteristics and Mid-Point Potential of the Primary Donor in Photosystem I
Biochemistry 35, 12857-12863 (1996)
107. Ch. Geßner, O. Trofanchuk, K. Kawagoe, Y. Higuchi, N. Yasuoka and W. Lubitz
Single Crystal EPR Study of the Ni Center of [NiFe] Hydrogenase
Chem. Phys. Lett. 256, 518-524 (1996)
108. H. Käß, P. Fromme and W. Lubitz
Quadrupole Parameters of Nitrogen Nuclei in the Cation Radical P_{700}^+ Determined by ESEEM of Single Crystals of Photosystem I
Chem. Phys. Lett. 257, 197-206 (1996)
109. F. Lendzian, M. Sahlin, F. MacMillan, R. Bittl, R. Fiege, St. Pötsch, B.-M. Sjöberg, A. Gräslund, W. Lubitz and G. Lassmann
Electronic Structure of Neutral Tryptophan Radicals in Ribonucleotide Reductase Studied by EPR and ENDOR Spectroscopy
J. Am. Chem. Soc. 118, 8111-8120 (1996)
110. S. Zech, W. Lubitz and R. Bittl
Pulsed EPR Experiments on Radical Pairs in Photosynthesis: Comparison of the Donor-Acceptor Distances in Photosystem I and Bacterial Reaction Centers
Ber. Bunsenges. Phys. Chem. 100, 2041-2044 (1996)
111. F. Müh, J. Rautter and W. Lubitz
Effects of Zwitterionic Detergents on the Primary Donor of Bacterial Reaction Centers
Ber. Bunsenges. Phys. Chem. 100, 1974-1977 (1996)
112. F. Lendzian, J. Rautter, H. Käß, A. Gardiner and W. Lubitz
ENDOR and Pulsed EPR Studies of Photosynthetic Reaction Centers: Protein-Cofactor Interactions
Ber. Bunsenges. Phys. Chem. 100, 2036-2040 (1996)

113. W. Lubitz, R. Fiege, R. Bittl, K.-D. Irrgang and G. Renger
EPR and ENDOR Investigations of the Manganese Cluster in Photosystem II
in Bioinorganic Chemistry: Transition Metals in Biology and their Coordination Chemistry, (A.X. Trautwein, ed.), pp. 673-680, VCH Publishers, Weinheim (1996)
114. W. Lubitz, W. Zweggart, R. Bittl, K. Wieghardt, G. Haselhorst and Th. Weyhermüller
EPR and ENDOR Investigations of Dinuclear Manganese Complexes as Models for the Water Oxidizing Unit in Photosynthesis
in Bioinorganic Chemistry: Transition Metals in Biology and their Coordination Chemistry, (A.X. Trautwein, ed.), pp. 665-672, VCH Publishers, Weinheim (1996)
115. G. Renger, J. Kurreck, Haag, E., Reifarth, A. Bergmann, F. Parak, A. Garbers, F. MacMillan, F. Lenzian and W. Lubitz
The Non-Heme Iron Center of Photosystem II and Modulatory Effects of Exogenous Copper (II)
in Bioinorganic Chemistry: Transition Metals in Biology and their Coordination Chemistry, (A.X. Trautwein, ed.), pp. 260-276, VCH Publishers, Weinheim (1996)
116. A. van der Est, T. Prisner, R. Bittl, P. Fromme, W. Lubitz, K. Möbius and D. Stehlik
Time Resolved X-, K-, and W-Band EPR of the Radical Pair State $P_{700}^+ A_1^-$ in Photosystem I in a Comparison with $P_{865}^+ Q_A^-$ in Bacterial Reaction Centers
J. Phys. Chem. B 101, 1437-1443 (1997)
117. F. Müh, J. Rautter and W. Lubitz
Two Distinct Conformations of the Primary Electron Donor in Reaction Centers from *Rb. sphaeroides* Revealed by ENDOR/TRIPLE-Spectroscopy
Biochemistry 36, 4155-4162 (1997)
118. D. Albouy, M. Kuhn, J.C. Williams, J.P. Allen, W. Lubitz and T.A. Mattioli
Fourier Transform Raman Investigation of the Electronic Structure and Charge Localization in a Bacteriochlorophyll-Bacteriopheophytin Dimer of Reaction Centers from *Rb. sphaeroides*
Biochim. Biophys. Acta 1321, 137-148 (1997)

119. R. Bittl, S. Zech, P. Fromme, H.T. Witt and W. Lubitz
Pulsed EPR Structure Analysis of Photosystem I Single Crystals: Localization of the Phylloquinone Acceptor
Biochemistry 36, 12001-12004 (1997)
120. S.G. Zech, J. Kurreck, H.-J. Eckert, G. Renger, W. Lubitz and R. Bittl
Pulsed EPR Measurement of the Distance between $P_{865}^{+\cdot}$ and $Q_A^{-\cdot}$ in Photosystem II
FEBS Lett. 414, 454-456 (1997)
121. W. Lubitz, F. Lendzian, M. Plato, H. Scheer and K. Möbius
The Bacteriochlorophyll a Cation Radical Revisited. An ENDOR and TRIPLE Resonance Study
Appl. Magn. Res. 13, 531-551 (1997)
122. S. Zech, R. Bittl, A. Gardiner and W. Lubitz
Transient and Pulsed EPR Spectroscopy on the Radical Pair State $P_{865}^{+\cdot} Q_A^{-\cdot}$ to Study Light-Induced Structural Changes in Bacterial Reaction Centers
Appl. Magn. Reson. 13, 517-529 (1997)
123. K. Artz, J.C. Williams, J.P. Allen, F. Lendzian, J. Rautter and W. Lubitz
Relationship between the Oxidation Potential and Electron Spin Density of the Primary Electron Donor in Reaction Centers from *Rhodobacter sphaeroides*
Proc. Natl. Acad. Sci. USA 94, 13582-13587 (1997)
124. H. Käß, W. Lubitz, G. Hartwig, H. Scheer, D. Noy and A. Scherz
ENDOR Studies of Substituted Chlorophyll Cation Radicals
Spectrochim. Acta A, 54, 1141-1156 (1998)
125. E. Navedryk, J. Breton, J.C. Williams, J.P. Allen, M. Kuhn and W. Lubitz
FTIR Characterization of the Primary Electron Donor in Double Mutants Combining the Heterodimer HL (M202) with the LH (L131), HF (L168), FH (M197), or LH (M160) Mutations
Spectrochim. Acta A, 54, 1219-1230 (1998)
126. J. Wachtveitl, H. Huber, R. Feick, J. Rautter, F. Müh and W. Lubitz
Electron Transfer in Bacterial Reaction Centers with an Energetically raised Primary Acceptor: Ultrafast Spectroscopy and ENDOR/TRIPLE Studies
Spectrochim. Acta A, 54, 1231-1245 (1998)
127. F. Lendzian, R. Bittl and W. Lubitz
Pulsed ENDOR of the Photo-Excited Triplet States of Bacteriochlorophyll a and of the Primary Donor P_{865} in Reaction Centers of *Rhodobacter sphaeroides* R-26
Photosyn. Res. 55, 189-197 (1998)

128. O. Nimz, F. Lendzian, C. Boullais and W. Lubitz
Influence of Hydrogen Bonds on the Electronic g-Tensor and ^{13}C -Hyperfine Tensors of ^{13}C -Labeled Ubiquinones. EPR and ENDOR Study
Appl. Magn. Res. 14, 255-274 (1998)
129. F. Müh, C. Schulz, E. Schlodder, M.R. Jones, J. Rautter, M. Kuhn and W. Lubitz
Effects of Zwitterionic Detergents on the Electronic Structure of the Primary Donor and the Charge Recombination Kinetics of $\text{P}^+ \text{Q}_\text{A}^-$ in Native and Mutant Reaction Centers from *Rhodobacter sphaeroides*
Photosyn. Res. 55, 199-205 (1998)
130. M. Rohrer, F. MacMillan, T.F. Prisner, A.T. Gardiner, K. Möbius and W. Lubitz
Pulsed ENDOR at 95 GHz on the Primary Acceptor Ubisemiquinone Q_A^- in Photosynthetic Bacterial Reaction Centers and Related Model Systems
J. Phys. Chem. B 102, 4648-4657 (1998)
131. F. Müh, J.C. Williams, J.P. Allen and W. Lubitz
A Conformational Change of the Photoactive Bacteriopheophytin in Reaction Centers from *Rhodobacter sphaeroides*
Biochemistry 37, 13066-13074 (1998)
132. A. Kamlowski, S.G. Zech, P. Fromme, R. Bittl, W. Lubitz, H.T. Witt and D. Stehlik
The Radical Pair State $\text{P}_{700}^+ \text{A}_1^-$ in Photosystem I Single Crystals: Orientation Dependence of the Transient Spin-Polarized EPR Spectra
J. Phys. Chem. B 102, 8266-8277 (1998)
133. A. Kamlowski, B. Altenberg-Greulich, A. van der Est, S.G. Zech, R. Bittl, P. Fromme, W. Lubitz and D. Stehlik
The Quinone Acceptor A_1 in Photosystem I: Binding Site and Comparison to Q_A in Purple Bacteria Reaction Centers
J. Phys. Chem. B 102, 8278-8287 (1998)
134. F. Lendzian, R. Bittl, A. Telfer, J. Barber and W. Lubitz
Time Resolved ENDOR of the Triplet State of P680 in PS II Reaction Centers
in: Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, Dordrecht, Vol. II, 1057-1060 (1998)

135. A. Telfer, F. Lendzian, E. Schlodder, J. Barber and W. Lubitz
ENDOR and Transient Absorption Studies of P680⁺ and Other Cation Radicals in PS II Reaction Centers before and after Inactivation of Secondary Electron Donors
in: Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, Dordrecht, Vol. II, 1061-1064 (1998)
136. C. Schulz, F. Müh, A. Beyer, R. Jordan, E. Schlodder and W. Lubitz
Investigation of *Rhodobacter sphaeroides* Reaction Center Mutants with Changed Ligands to the Primary Donor
in: Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, Dordrecht, Vol. II, 767-770 (1998)
137. F. Müh, M. Bibikova, F. Lendzian, D. Oesterhelt and W. Lubitz
Pigment-Protein Interactions in Reaction Centers of *Rhodospseudomonas viridis*: ENDOR Study of the Oxidized Primary Donor in Site-Directed Mutants
in: Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, Dordrecht, Vol. II, 763-766 (1998)
138. C. Teutloff, F. MacMillan, R. Bittl, F. Lendzian and W. Lubitz
A Comparative Study of A₁⁻ in PS I from Cyanobacteria, Green Plants and Algae Using EPR and ENDOR Spectroscopy
in: Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, Dordrecht, Vol. I, 607-610 (1998)
139. R. Bittl, S.G. Zech, C. Teutloff, L. Krabben and W. Lubitz
Structural Information on Components of the Electron Transfer Chain in Photosystem I from Time-Resolved EPR Spectroscopy
in: Photosynthesis: Mechanisms and Effects (G. Garab, ed.), Kluwer Academic Publishers, Dordrecht, Vol. I, 509-514 (1998)
140. K.-O. Schäfer, R. Bittl, W. Zweggart, F. Lendzian, G. Haselhorst, T. Weyhermüller, K. Wieghardt and W. Lubitz
Electronic Structure of Antiferromagnetically Coupled Dinuclear Manganese (Mn^{III}Mn^{IV}) Complexes Studied by Magnetic Resonance Techniques
J. Am. Chem. Soc. 120, 13104-13120 (1998)
141. G. Lassmann, L.A. Eriksson, F. Himo, F. Lendzian and W. Lubitz
Electronic Structure of a Transient Histidine Radical in Liquid Aqueous Solution. EPR Continuous-Flow Studies and Density Functional Calculations
J. Phys. Chem. A 103, 1283-1290 (1999)

142. F. Müh, M.R. Jones and W. Lubitz
Reorientation of the Acetyl Group of the Photoactive Bacteriopheophytin in Reaction Centers of *Rhodobacter sphaeroides*. An ENDOR/TRIPLE Resonance Study
Biospectroscopy 5, 35-46 (1999)
143. S.G. Zech, J. Kurreck, G. Renger, W. Lubitz and R. Bittl
Determination of the Distance between $Y_Z^{ox\cdot}$ and $Q_A^{\cdot-}$ in Photosystem II by Pulsed EPR Spectroscopy on Light-Induced Radical Pairs
FEBS Lett. 442, 79-82 (1999)
144. S. Pötsch, F. Lenzian, R. Ingemarson, A. Hörnberg, L. Thelander, W. Lubitz, G. Laßmann and A. Gräslund
The Iron-Oxygen Reconstitution Reaction in Protein R2-Tyr-177 Mutants of Mouse Ribonucleotide Reductase: EPR and ENDOR Studies on a New Transient Tryptophan Radical
J. Biol. Chem. 274, 17696-17704 (1999)
145. M. Fahnenschmidt, H.K. Rau, R. Bittl, W. Haehnel and W. Lubitz
Characterization of a *de novo*-Designed Heme Protein by EPR and ENDOR Spectroscopy
Chem. Eur. J. 5, 2327-2334 (1999)
146. Ch. Geßner, M. Stein, S.P.J. Albracht and W. Lubitz
Orientation-Selected ENDOR of the Active Center in *Chromatium vinosum* [NiFe]-Hydrogenase in the Oxidized, 'Ready' State
J. Biol. Inorg. Chem. 4, 379-389 (1999)
147. W. Lubitz and G. Feher
The Primary and Secondary Acceptors in Bacterial Photosynthesis III. Characterization of the Quinone Radicals $Q_A^{\cdot-}$ and $Q_B^{\cdot-}$ by EPR and ENDOR
Appl. Magn. Res. 17, 1-48 (1999)
148. C. Jegerschöld, F. MacMillan, W. Lubitz and A.W. Rutherford
Effects of Copper and Zinc Ions on Photosystem II Studied by EPR Spectroscopy
Biochemistry 38, 12439-12445 (1999)
149. A.T. Gardiner, S.G. Zech, F. MacMillan, H. Käß, R. Bittl, E. Schlodder, F. Lenzian and W. Lubitz
EPR Studies of Zn-Substituted Reaction Centers from *Rhodospseudomonas viridis*
Biochemistry 38, 11773-11787 (1999)

150. O. Trofanchuk, M. Stein, Ch. Geßner, F. Lenzian, Y. Higuchi and W. Lubitz
Single Crystal EPR Studies of the Oxidized Active Site of [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F
J. Biol. Inorg. Chem. 5, 36-44 (2000)
151. E. Nabedryk, C. Schulz, F. Müh, W. Lubitz and J. Breton
Heterodimeric versus Homodimeric Structure of the Primary Electron Donor in *Rhodobacter sphaeroides* Reaction Centers Genetically Modified at Position M202
Photochem. Photobiol. 71, 582-588 (2000)
152. R. Calvo, E.C. Abresch, R. Bittl, G. Feher, W. Hofbauer, R.A. Isaacson, W. Lubitz, M.Y. Okamura and M.L. Paddock
EPR Study of the Molecular and Electronic Structure of the Semiquinone Biradical $Q_A^- \cdot Q_B^-$ in Photosynthetic Reaction Centers from *Rhodobacter sphaeroides*
J. Am. Chem. Soc. 122, 7327-7341 (2000)
153. F. Müh, M. Bibikova, E. Schlodder, D. Oesterhelt and W. Lubitz
Conformational Relaxation Following Reduction of the Photoactive Bacteriopheophytin in Reaction Centers from *Blastochloris viridis*. Influence of Mutations at Position M208
Biochim. Biophys. Acta 1459, 191-201 (2000)
154. M. Fahnenschmidt, R. Bittl, H.K. Rau, W. Haehnel and W. Lubitz
Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Spectroscopy of a Heme Protein Maquette
Chem. Phys. Lett. 323, 329-339 (2000)
155. R.J. Cogdell, T.D. Howard, R. Bittl, E. Schlodder, I. Geisenheimer and W. Lubitz
How Carotenoids Protect Bacterial Photosynthesis
Phil. Trans. R. Soc. London B 355, (1402), 1345-1349 (2000)
156. S. Sinnecker, W. Koch and W. Lubitz
Bacteriochlorophyll a Radical Cation and Anion – Calculation of Isotropic Hyperfine Coupling Constants by Density Functional Methods
Phys. Chem. Chem. Phys. 2, 4772-4778 (2000)
157. L. Krabben, E. Schlodder, R. Jordan, D. Carbonera, G. Giacometti, H. Lee, A.N. Webber and W. Lubitz
Influence of the Axial Ligands on the Spectral Properties of P700 of Photosystem I: A Study of Site-Directed Mutants
Biochemistry 39, 13012-13025 (2000)

158. S. Zech, W. Hofbauer, A. Kamlowksi, P. Fromme, D. Stehlik, W. Lubitz and R. Bittl
A Structural Model for the Charge Separated State $P_{700}^{+} A_1^{-}$ in Photosystem I from the Orientation of the Magnetic Interaction Tensors
J. Phys. Chem. B 104, 9728-9739 (2000)
159. G. Laßmann, L.A. Eriksson, F. Lenzian and W. Lubitz
Structure of a Transient Neutral Histidine Radical in Solution: EPR Continuous-Flow Studies in a Ti^{3+} /EDTA-Fenton System and Density Functional Calculations
J. Phys. Chem. A 104, 9144-9152 (2000)
160. M. Kolberg, G. Bleifuss, S. Pötsch, A. Gräslund, W. Lubitz, G. Lassmann and F. Lenzian
A New Stable High-Valent Diiron Center in R2 Mutant Y122H of *E. coli* Ribonucleotide Reductase Studied by High-Field EPR and ^{57}Fe -ENDOR
J. Am. Chem. Soc. 122, 9856-9857 (2000)
161. M. Stein, E. van Lenthe, E.J. Baerends and W. Lubitz
g- and A-Tensor Calculations in the Zero-Order Approximation for Relativistic Effects of Ni Complexes $Ni(mnt)_2^{-}$ and $Ni(CO)_3H$ as Model Complexes for the Active Center of [NiFe]-Hydrogenase
J. Phys. Chem. A 105, 416-425 (2001)
162. H. Käß, P. Fromme, H.T. Witt and W. Lubitz
Orientation and Electronic Structure of the Primary Donor Radical Cation P_{700}^{+} in Photosystem I: A Single Crystals EPR and ENDOR Study
J. Phys. Chem. B 105, 1225-1239 (2001)
163. R. Bittl, E. Schlodder, I. Geisenheimer, W. Lubitz and R.J. Cogdell
Transient EPR and Absorption Studies of Carotenoid Triplet Formation in Purple Bacterial Antenna Complexes
J. Phys. Chem. B 105, 5525-5535 (2001)
164. M. Baumgarten, C.J. Winscom and W. Lubitz
Probing the Surrounding of a Cobalt(II)Porphyrin and its Superoxo Complex by EPR Techniques
Appl. Magn. Reson. 20, 35-70 (2001)
165. A.N. Webber and W. Lubitz
P700: The Primary Electron Donor of Photosystem I
Biochim. Biophys. Acta 1507, 61-79, (2001)

166. W. Hofbauer, A. Zouni, R. Bittl, J. Kern, P. Orth, F. Lendzian, P. Fromme, H.T. Witt and W. Lubitz
Photosystem II Single Crystals Studied by EPR Spectroscopy at 94 GHz: the Tyrosine Radical Y_D
Proc. Natl. Acad. Sci. USA 98, 6623-6628 (2001)
167. M. Stein, E. van Lenthe, E.J. Baerends and W. Lubitz
Relativistic DFT Calculations of the Paramagnetic Intermediates of [NiFe]Hydrogenase. Implications for the Enzymatic Mechanism
J. Am. Chem. Soc. 123, 5839-5840 (2001)
168. M. Stein and W. Lubitz
DFT Calculations of the Electronic Structure of the Paramagnetic States Ni-A, Ni-B and Ni-C of [NiFe]-Hydrogenase
Phys. Chem. Chem. Phys. 3, 2668-2675 (2001)
169. M. Fahnenschmidt, R. Bittl, E. Schlodder, W. Haehnel and W. Lubitz
Characterization of *de novo* Synthesized Four-Helix Bundle Proteins with Metalloporphyrin Cofactors
Phys. Chem. Chem. Phys. 3, 4082-4090 (2001)
170. M. Stein and W. Lubitz
The Electronic Structure of the Catalytic Intermediate Ni-C in [NiFe]- and [NiFeSe] Hydrogenases
Phys. Chem. Chem. Phys. 3, 5115-5120 (2001)
171. P. J. S. Albracht, P. Bertrand, B. Bleijlevens, F. Dole, B. Guigliarelli, W. R. Hagen, R. P. Happe, W. Lubitz, M. J. Maroney, Ch. Massanz, J. J. G. Moura, A. S. Pereira, A. J. Pierik, O. Sorgenfrei, M. Stein and P. Tavares
Spectroscopy - the functional puzzle
in: Hydrogen as a Fuel, eds. R. Cammack, M. Frey, R. Robson, Taylor & Francis, London and New York, Chapter 7, 110-158 (2001)
172. C. Teutloff, W. Hofbauer, S.G. Zech, M. Stein, R. Bittl and W. Lubitz
High- Frequency EPR Studies on Cofactor Radicals in Photosystem I
Appl. Magn. Reson. 21, 363-379 (2001)
173. F. Müh, A.T. Gardiner, H. Witt, C. Schulz, J.F. Imhoff, R.J. Cogdell and W. Lubitz
Conserved Electronic Structure of the Primary Donor in Reaction Centers of Sulfur and Non-Sulfur Purple Bacteria
in: Proceedings of the 12th International Congress on Photosynthesis, Brisbane, Australia (2001), CSIRO Publishing, Australia, S7-005

174. A.T. Gardiner, A. Kuglstatter, G. Fritzsich, J. Breton, E. Nabedryk and W. Lubitz
The Crystal Structure of the *Rb. sphaeroides* Zn²⁺ Reaction Centre Mutant HC(M266)
in: Proceedings of the 12th International Congress on Photosynthesis, Brisbane, Australia (2001), CSIRO Publishing, Australia, S7-016
175. C. Teutloff, R. Bittl, M. Stein, P. Jordan, P. Fromme, N. Krauß and W. Lubitz
Structure Based Analysis of the Magnetic Resonance Parameters of the Phylloquinone Acceptor A₁ in PS I
in: Proceedings of the 12th International Congress on Photosynthesis, Brisbane, Australia (2001), CSIRO Publishing, Australia, S6-030
176. H. Witt, E. Schlodder, C. Teutloff, E. Bordignon, D. Carbonera, J. Niklas and W. Lubitz
Site-Directed Mutagenesis of Thr A739 of Photosystem I in *Chlamydomonas reinhardtii* Alters Significantly the Excitonic and Electronic Coupling of the Primary Electron Donor P700
in: Proceedings of the 12th International Congress on Photosynthesis, Brisbane, Australia (2001), CSIRO Publishing, Australia, S6-011
177. G. Bleifuss, M. Kolberg, S. Pötsch, W. Hofbauer, R. Bittl, W. Lubitz, A. Gräslund, G. Lassmann and F. Lenzian
Tryptophan and Tyrosine Radicals in Ribonucleotide Reductase: A Comparative High-Field EPR Study at 94 GHz
Biochemistry 40, 15362-15368 (2001)
178. W. Lubitz
Paramagnetic States of Photosynthetic Reaction Centers Studied by Advanced EPR Techniques
in "Advanced EPR Applied to Biosciences", A. Kawamori (ed.), Kwansei Gakuin Univ. Press, Japan, 117-123 (2002)
179. M. Kolberg, G. Bleifuss, B.-M. Sjöberg, A. Gräslund, W. Lubitz, F. Lenzian and G. Laßmann
Generation and EPR Spin Trapping Detection of Thiyl Radicals in Model Proteins and in the R1 Subunit of *E. coli* Ribonucleotide Reductase
Arch. Biochem. Biophys., 397, 57-68 (2002)
180. S. Schenkl, S. Spörlein, F. Müh, H. Witt, W. Lubitz, W. Zinth and J. Wachtveitl
Selective Perturbation of the Second Electron Transfer Step in Mutant Bacterial Reaction Centers
Biochim. Biophys. Acta, 1554, 36-47 (2002)
181. S. Sinnecker, W. Koch and W. Lubitz
Chlorophyll a Radical Ions: A Density Functional Study
J. Phys. Chem. B, 106, 5281-5288 (2002)

182. W. Lubitz, F. Lendzian and R. Bittl
Radicals, Radical Pairs and Triplet States in Photosynthesis
Acc. Chem. Res. 35, 313-320 (2002)
183. F. Müh, F. Lendzian, M. Roy, J.C. Williams, J.P. Allen and W. Lubitz
Pigment-Protein Interactions in Bacterial Reaction Centers and their Influence on Oxidation Potential and Spin Density Distribution of the Primary Donor
J. Phys. Chem. B. 106, 3226-3236 (2002)
184. W. Lubitz, M. Brecht, S. Foerster, M. Stein, Y. Higuchi, T. Buhrke and B. Friedrich
EPR and Theoretical Investigations of [NiFe] Hydrogenase: Insight into the Mechanism of Biological Hydrogen Conversion
in: EPR in the 21th Century: Basics and Applications to Material, Life and Earth Sciences, A. Kawamori, J. Yamauchi and H. Ohta (eds.), Elsevier, p. 437-445, (2002)
185. T. Buhrke, M. Brecht, W. Lubitz and B. Friedrich
The H₂ Sensor of *Ralstonia eutropha*: Biochemical and Spectroscopic Analysis of Mutant Proteins Modified at a Conserved Glutamine Residue Close to the [NiFe] Active Site
J. Biol. Inorg. Chem. 7, 897-908 (2002)
186. M. Stein and W. Lubitz
Quantum Chemical Calculations of [NiFe] Hydrogenase
Curr. Opin. Chem. Biol. 6, 243-249 (2002)
187. M. Kolberg, G. Bleifuss, A. Gräslund, B.-M. Sjöberg, W. Lubitz, F. Lendzian and G. Lassmann
Protein Thiyl Radicals Directly Observed by EPR Spectroscopy
Arch. Biochem. Biophys. 403, 141-144 (2002)
188. A. Schnegg, M. Fuhs, M. Rohrer, W. Lubitz, T. F. Prisner, K. Möbius
Molecular Dynamics of Q_A⁻ and Q_B⁻ in Photosynthetic Bacterial Reaction Centers Studied by Pulsed High-field EPR at 95 GHz
J. Phys. Chem. B. 106, 9454-9462 (2002)
189. H. Witt, E. Schlodder, C. Teutloff, J. Niklas, E. Bordignon, D. Carbonera, S. Kohler, A. Labahn and W. Lubitz
Hydrogen Bonding to P700: Site-Directed Mutagenesis of Threonine A739 of Photosystem I in *Chlamydomonas reinhardtii*
Biochemistry 41, 8557-8569 (2002)
190. E. T. Johnson, F. Müh, E. Nabedryk, J. C. Williams, J. P. Allen, W. Lubitz, J. Breton and W. W. Parson
Electronic and Vibronic Coupling of the Special Pair of Bacteriochlorophylls in Photosynthetic Reaction Centers from Wild-Type and Mutant Strains of *Rhodobacter sphaeroides*
J. Phys. Chem. B 106, 11859-11869 (2002)

191. W. Lubitz
Pulse EPR and ENDOR Studies of Light-Induced Radicals and Triplet States in Photosystem II of Oxygenic Photosynthesis
Phys. Chem. Chem. Phys. 4, 5539-5545 (2002)
192. S. Foerster, M. Stein, M. Brecht H. Ogata, Y. Higuchi and W. Lubitz
Single Crystal EPR Studies of the Reduced Active Site of [NiFe]-Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F
J. Am. Chem. Soc. 125, 83-93 (2003)
193. J. Sarrou, S. Isgandarova, J. Kern, A. Zouni, G. Renger, W. Lubitz, J. Messinger
Nitric Oxid Induced Formation of the S₂ State in the Oxygen Evolving Complex of Photosystem II from *Synechococcus elongatus*
Biochemistry 42, 1016-1023 (2003)
194. K.-O. Schäfer, R. Bittl, F. Lendzian, V. Barynin, T. Weyhermüller, K. Wieghardt and W. Lubitz
Multifrequency EPR Investigation of Dimanganese Catalase and Related Mn(III)Mn(IV) Complexes
J. Phys. Chem. B 107, 1242-1250 (2003)
195. Günter Lassmann, Matthias Kolberg, Günther Bleifuss, Astrid Gräslund, Britt-Marie Sjöberg, Wolfgang Lubitz
Protein thiyl radicals in disordered systems: A comparative EPR study at low temperature
Phys. Chem. Chem. Phys. 5, 2442 - 2453 (2003)
196. W. Lubitz
Photochemical Processes in Photosynthesis Studied by Advanced EPR Techniques
Pure Appl. Chem., 75, 1021-1030 (2003)
197. W. Lubitz, M. Brecht, S. Foerster, M. van Gastel, and M. Stein
EPR and ENDOR Studies of [NiFe] Hydrogenase: Contributions to Understanding the Mechanism of Biological Hydrogen Conversion
ACS Symposium Series: *Paramagnetic Resonance of Metallobio-molecules*, ACS Vol. 858, 128-150 (2003)
198. Friedhelm Lendzian, Robert Bittl, Alison Telfer, and Wolfgang Lubitz
Hyperfine Structure of the Photoexcited Triplet State ³P₆₈₀ in Plant PS II Reaction Centers as Determined by Pulse ENDOR
Biochim. Biophys. Acta, 1605, 35-46 (2003)
199. Michael Kammel, Jan Kern, Wolfgang Lubitz, and Robert Bittl
Photosystem II Single Crystals Studied by Transient EPR: the Light-Induced Triplet State
Biochim. Biophys. Acta, 1605, 47-54 (2003)

200. Martin Plato, Norbert Krauß, Petra Fromme, Wolfgang Lubitz
Molecular Orbital Study of the Primary Electron Donor P700 of Photosystem I Based on a Recent X-Ray Single Crystal Structure Analysis
Chem. Phys. 294, 483-499 (2003)
201. Marc G. Müller, Jens Niklas, Wolfgang Lubitz, Alfred R. Holzwarth
Ultrafast Transient Absorption Studies on Photosystem I Reaction Centers from *Chlamydomonas reinhardtii*. 1. A New Interpretation of the Energy Trapping and Early Electron Transfer Steps in Photosystem I
Biophysical J. 85, 3899-3822 (2003)
202. Martin R. Fuchs, Alexander Schnegg, Martin Plato, Claudia Schulz, Frank Müh, Wolfgang Lubitz, Klaus Möbius
The primary donor cation P⁺ in photosynthetic reaction centers of site-directed mutants of *Rhodobacter sphaeroides*: g-tensor shifts revealed by high-field EPR at 360 GHz / 12.8 T
Chem. Phys. 294, 371-384 (2003)
203. M. Flores, R. A. Isaacson, R. Calvo, G. Feher, W. Lubitz
Probing hydrogen bonding to quinone anion radicals by ¹H and ²H ENDOR Spectroscopy at 35 GHz
Chem. Phys. 294, 401-413 (2003)
204. M. Brecht, M. van Gastel, T. Buhrke, B. Friedrich, W. Lubitz
Direct Detection of a Hydrogen Ligand in the [NiFe] Center of the Regulatory H₂-Sensing Hydrogenase from *Ralstonia eutropha* in its Reduced State by HYSCORE and ENDOR Spectroscopy
J. Am. Chem. Soc. 125, 13075-13083 (2003)
205. C. Fichtner, M. van Gastel and W. Lubitz
Wavelength Dependence of the Photo-induced Conversion of the Ni-C to the Ni-L Redox State in the [NiFe] Hydrogenase of *D. vulgaris* Miyazaki F
Phys. Chem. Chem. Phys. 5, 5507-5513 (2003)
206. H. Witt, E. Bordignon, D. Carbonera, J. P. Dekker, N. Karapetyan, Ch. Teutloff, A. Webber, W. Lubitz, E. Schlodder
Species Specific Differences of the Spectroscopic Properties of P700 - Analysis of the Influence of Non-conserved Amino Acid Residues Investigated by Site-directed Mutagenesis of Photosystem I from *Chlamydomonas reinhardtii*
J. Biol. Chem. 278 (47), 46760-46771 (2003)
207. M. van Gastel, W. Lubitz, G. Lassmann, F. Neese
The Electronic Structure of the Cysteine Thiyl Radical: a DFT and Correlated Ab Initio Study
J. Am. Chem. Soc. 126, 2237-2246 (2004)

208. S. Sinnecker, F. Neese, L. Noodleman and W. Lubitz
Calculating the Electron Paramagnetic Resonance Parameters of Exchange Coupled Transition Metal Complexes Using Broken Symmetry Density Functional Theory. Application to a Mn^{III}/Mn^{IV} Model Compound
J. Am. Chem. Soc. 126, 2613-2622 (2004)
209. Sebastian Sinnecker, Eduard Reijerse, Frank Neese, Wolfgang Lubitz
Hydrogen Bond Geometries from EPR and ENDOR Parameters. A Density Functional Study of Quinone Radical Anion - Solvent Interactions
J. Am. Chem. Soc. 126, 3280-3290 (2004)
210. C. Teutloff, R. Bittl, W. Lubitz
Pulse ENDOR Studies on the Radical Pair P₇₀₀^{•+} A₁^{•-} and the Photoaccumulated Quinone Acceptor A₁^{•-} of Photosystem I
Appl. Magn. Res. 26, 5-21 (2004)
211. M. Stein, W. Lubitz
Relativistic DFT Calculation of the Reaction Cycle Intermediates of [NiFe] Hydrogenase: A Contribution to Understanding the Enzymatic Mechanism
J. Inorg. Biochem. 98, 862-877 (2004)
212. N. D'Amelio, E. Gaggelli, P. Mlynarz, E. Molteni, G. Valensin, W. Lubitz
NMR Structural Model of the Interaction of Herbicides with the Photosynthetic Reaction Center from *Rhodobacter sphaeroides*
ChemBioChem, 5, 1237-1244 (2004)
213. Y.N. Pushkar, D. Stehlik, M. van Gastel, W. Lubitz
An EPR/ENDOR Study of the Asymmetric Hydrogen Bond between the Quinone Electron Acceptor and the Protein Backbone in Photosystem I
J. Mol. Structure, 700, 233-241 (2004)
214. D. Koulougliotis, Ch. Teutloff, Y. Sanakis, W. Lubitz, V. Petrouleas
The S₁Y_z[•] Metalloradical Intermediate in Photosystem II: an X- and W-Band EPR Study
Phys. Chem. Chem. Phys., 6, 4859-4863 (2004)
215. W. Lubitz
EPR in Photosynthesis
in: Electron Paramagnetic Resonance. A Specialist Periodical Report, Royal Society of Chemistry (B. Gilbert, M. Davies, D. Murphy) Vol. 19, 5, 174-242 (2004)
216. G. Lassmann, P. Schmidt, W. Lubitz
An Advanced EPR Stopped-flow Apparatus Based on a Dielectric Ring Resonator
J. Magn. Reson. 172, 312-323 (2005)

217. S. Foerster, M. van Gastel, M. Brecht, W. Lubitz
An Orientation-Selected ENDOR and HYSCORE Study of the Ni-C Active State of *Desulfovibrio vulgaris* Miyazaki F Hydrogenase.
J. Biol. Inorg. Chem. 10, 51-62 (2005)
218. A. Goenka, J. K. Voordouw, W. Lubitz, W. Gärtner, G. Voordouw
Construction of a [NiFe]-hydrogenase Deletionmutant of *Desulfovibrio vulgaris* Hildenborough
Biochem. Soc. Trans., 33, 59-60 (2005)
219. M. van Gastel, C. Fichtner, F. Neese, W. Lubitz
EPR Experiments to Elucidate the Structure of the Ready and Unready States of the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F
Biochem. Soc. Trans., 33, 7-11 (2005)
220. M. Kolberg, D. T. Logan, G. Bleifuss, S. Pötsch, B.-M. Sjöberg, A. Gräslund, W. Lubitz, G. Lassmann, F. Lendzian
A New Tyrosyl Radical on F208 as Ligand to the Diiron Center in *E. coli* Ribonucleotide Reductase, Mutant R2-Y122H: Combined X-ray Diffraction, and EPR/ENDOR Studies
J. Biol. Chem. 280, 11233-11246 (2005)
221. A. R. Holzwarth, M. G. Müller, J. Niklas, W. Lubitz
Charge Recombination Fluorescence in Photosystem I Reaction Centers from *Chlamydomonas reinhardtii*
J. Phys. Chem. B. 109, 5903-5911 (2005)
222. L. Kulik, B. Epel, J. Messinger, W. Lubitz
Pulse EPR, ⁵⁵Mn-ENDOR and ELDOR-detected NMR of the S₂-state of the Oxygen Evolving Complex in Photosystem II
Photosyn. Research, 84, 347-353 (2005)
223. L.V. Kulik, B. Epel, W. Lubitz, J. Messinger
⁵⁵Mn Pulse ENDOR at 34 GHz of the S₀- and S₂-States of the Oxygen Evolving Complex of Photosystem II
J. Am. Chem. Soc. 127, 2392-2393 (2005)
224. R. Pogni, M. C. Baratto, St. Giansanti, Ch. Teutloff, J. Verdin, B. Valderrama, F. Lendzian, W. Lubitz, R. Vazquez-Duhalt, R. Basosi
A Tryptophan Based Radical in the Catalytic Mechanism of Versatile Peroxidase from *Bjerkandere adusta*
Biochemistry 44, 4267-4274 (2005)
225. B. Epel, K.-O. Schäfer, A. Quentmeier, C. Friedrich, W. Lubitz
Multifrequency EPR Analysis of the Dimanganese Cluster of the Putative Sulfate Thiohydrolase SoxB of *Paracoccus pantotrophus*
J. Biol. Inorg. Chem. 10, 636-642 (2005)

226. A. R. Holzwarth, M. G. Müller, J. Niklas, H. Witt, W. Lubitz
A New Model for the Energy Transfer and Early Electron Transfer Processes in Photosystem I
in: Photosynthesis: Fundamental Aspects to Global Perspectives, A. van der Est and D. Bruce (Eds), Vol. 1, pp. 52-54, Int. Soc. Photosynth. (2005)
227. L. Kulik, B. Epel, W. Lubitz, J. Messinger
Q-band Pulse EPR and ^{55}Mn -ENDOR Studied of the S_0 -state of the Oxygen Evolving Complex in Photosystem II
in: Photosynthesis: Fundamental Aspects to Global Perspectives, A. van der Est and D. Bruce (Eds), Vol. 1, pp. 380-382, Int. Soc. Photosynth. (2005)
228. S. Sinnecker, F. Neese, W. Lubitz
Dimanganese Catalase – Spectroscopic Parameters from Broken Symmetry Density Functional Theory of the Superoxidized $\text{Mn}^{\text{III}}/\text{Mn}^{\text{IV}}$ State
J. Biol. Inorg. Chem. 10, 231-238 (2005)
229. L. V. Kulik, W. Lubitz, J. Messinger
Electron Spin-Lattice Relaxation of the S_0 state of the Oxygen-Evolving Complex in Photosystem II and of Dinuclear Manganese Model Complexes
Biochemistry 44, 9368-9374 (2005)
230. J. Petersen, Ch. Gessner, K. Fisher, C. J. Mitchell, D. J. Lowe, W. Lubitz
 $\text{Mn}(\text{II})$ -Adenosine Nucleotide Complexes in the Presence of the Nitrogenase Iron-Protein from *Klebsiella pneumoniae*; Detection of Conformational Rearrangements Directly at the Nucleotide Binding Site by EPR and 2D-ESEEM Spectroscopy
Biochem. J. 391, 527-539 (2005)
231. Ch. Teutloff, K.-O. Schäfer, S. Sinnecker, V. Barynin, R. Bittl, K. Wieghardt, F. Lendzian, W. Lubitz
High-Field EPR Investigations of $\text{Mn}^{\text{III}}\text{Mn}^{\text{IV}}$ and $\text{Mn}^{\text{II}}\text{Mn}^{\text{III}}$ States of Dimanganese Catalase and Related Model Systems
Magn. Reson. Chem. 43, S51-S64 (2005)
232. W. Lubitz
EPR Studies of the Primary Electron Donor P700 in Photosystem I
in: Advances in Photosynthesis AND Respiration (Series editor Govindjee). Photosystem I. The Plastocyanin: Ferredoxin Oxidoreductase in Photosynthesis, J.H. Golbeck (ed), Springer, Dordrecht, The Netherlands, (2006) Vol. 24, pp. 245-269

233. A. R. Holzwarth, M. G. Müller, J. Niklas, W. Lubitz
Ultrafast Transient Absorption Studies on Photosystem I Reaction Centers from *Chlamydomonas reinhardtii*. 2. Mutations around the P700 reaction center chlorophylls provide a new view on the nature of the primary electron donor
Biophysical Journal 90, 552-565 (2006)
234. M. van Gastel, M. Stein, M. Brecht, O. Schroeder, F. Lendzian, R. Bittl, H. Ogata, Y. Higuchi, W. Lubitz
A Single Crystal ENDOR and Density Functional Theory Study of the Oxidized States of the [NiFe] Hydrogenase from *D. vulgaris* Miyazaki F
J. Biol. Inorg. Chem. 11, 41-51 (2006)
235. D. Biglino, P. P. Schmidt, E. J. Reijerse, W. Lubitz
PELDOR Study on the Tyrosyl Radicals in the R2 Protein of Mouse Ribonucleotide Reductase
Phys. Chem. Chem. Phys. 8, 58-62 (2006)
236. M. Flores, R. Isaacson, E. Abresch, R. Calvo, W. Lubitz, G. Feher
Protein-cofactor Intercations in Bacterial Reaction Centers from *Rb. Sphaeroides* R-26. I. Identification of the ENDOR Lines Associated with the Hydrogen Bonds to the Primary Quinone Q_A^{*-}
Biophys. J. 90, 3356-3362 (2006)
237. A. Goenka Agrawal, M. van Gastel, W. Gärtner, W. Lubitz
Hydrogen-Bonding Affects the [NiFe] Active Site of *Desulfovibrio vulgaris* Miyazaki F Hydrogenase. A Hyperfine Sublevel Correlation Spectroscopy and Density Functional Theory Study.
J. Phys. Chem. B 110, 8142-8150 (2006)
238. B. Epel, J. Niklas, S. Sinnecker, H. Zimmermann, W. Lubitz
Phylloquinone and Related Radical Anions Studied by Pulse ENDOR Spectroscopy at 34 GHz and Density Functional Theory.
J. Phys. Chem. B. 110, 11549-11560 (2006)
239. C. Fichtner, Ch. Laurich, E. Bothe, W. Lubitz
Spectroelectrochemical Characterization of the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F
Biochemistry 45, 9706-9716 (2006)
240. K. A. Vincent, N. A. Belsey, W. Lubitz, F. A. Armstrong
Rapid and Reversible Reactions of [NiFe]-hydrogenases with Sulfide
J. Am. Chem. Soc., 128, 7448-7449 (2006)
241. A. Mennenga, W. Gärtner, W. Lubitz, H. Görner
Effects of noncovalently bound quinones on the ground and triplet states of zinc chlorins in solution and bound to *de novo* peptides
Phys. Chem. Chem. Phys., 8, 5444-5453 (2006)

242. S. Sinnecker, M. Flores, W. Lubitz
Protein-cofactor interactions in bacterial reaction centers from *Rhodobacter sphaeroides* R-26: Effect of hydrogen bonding on the electronic and geometric structure of the primary quinone. A density functional theory study
Phys. Chem. Chem. Phys. 8, 5659-5670 (2006)
243. B. Epel, J. Niklas, M. L. Antonkine, W. Lubitz
Absolute Signs of Hyperfine Coupling Constants as Determined by Pulse ENDOR of Polarized Radical Pairs
Appl. Magn. Res., 30, 311-327 (2006)
244. E.J. Reijerse, P. P. Schmidt, G. Klichm, W. Lubitz
A CW and Pulse EPR Spectrometer Operating at 122/244 GHz Using a Quasi-optical Bridge and a Cryogen-free 12 T Superconducting Magnet
Appl. Magn. Res. 31, 611-626 (2007)
245. A. Schnegg, A. A. Dubinskii, M. R. Fuchs, Yu. A. Grishin, E. P. Kirilina, W. Lubitz, M. Plato, A. Savitsky, K. Möbius
High-field EPR, ENDOR and ELDOR on Bacterial Photosynthetic Reaction Centers
Appl. Magn. Res. 31, 59-98 (2007)
246. W. Lubitz, M. v. Gastel, W. Gärtner
Nickel Iron Hydrogenases
Met. Ions Life Sci. 2, 279-322 (2007)
247. M. Flores, R. Isaacson, E. Abresch, R. Calvo, W. Lubitz, G. Feher
Protein-cofactor Interactions in Bacterial Reaction Centers from *Rhodobacter Sphaeroides* R-26: II. Geometry of the Hydrogen Bonds to the Primary Quinone Q_A^- by ^1H and ^2H ENDOR Spectroscopy
Biophys. J., 92, 671-682 (2007)
248. O. Schröder, B. Bleijlevens, T. E. de Jongh, Z. Chen, T. Li, J. Fischer, J. Förster, C. G. Friedrich, K. A. Bagley, S. P. J. Albracht, W. Lubitz
Characterization of a Cyanobacterial-like Uptake [NiFe]-hydrogenase: EPR and FTIR Spectroscopic Studies of the Enzyme from *Acidithiobacillus ferrooxidans*
J. Biol. Inorg. Chem. 12, 212-233 (2007)
249. A. Savitsky, A. A. Dubinskii, M. Flores, W. Lubitz, K. Möbius
Orientation-resolving Pulsed Electron Dipolar High-field EPR Spectroscopy on Disordered Solids: I. Structure of Spin-correlated Radical Pairs in Bacterial Photosynthetic Reaction Centers
J. Phys. Chem. B 111, 6245-6262 (2007)

250. E. J. Reijerse, M. Sommerhalter, P. Hellwig, A. Quentmeier, D. Rother, Ch. Laurich, E. Bothe, W. Lubitz, C. G. Friedrich
The Unusual Redox Centers of SoxXA, a Novel c-Type Heme-enzyme Essential for Chemotrophic Sulfur-oxidation of *Paracoccus pantotrophus*
Biochemistry 46, 7804-7810 (2007)
251. L. V. Kulik, B. Epel, W. Lubitz, J. Messinger
Electronic Structure of the Mn₄O_xCa Cluster in the S₀ and S₂ States of the Oxygen-evolving Complex of Photosystem II Based on Pulse ⁵⁵Mn-ENDOR and EPR Spectroscopy
J. Am. Chem. Soc. 129, 13421 -13435 (2007)
252. A. Silakov, E. J. Reijerse, S. P. J. Albracht, E. C. Hatchikian, W. Lubitz
The Electronic Structure of the H-cluster in the [FeFe]-hydrogenase from *Desulfovibrio desulfuricans*: A Q-band ⁵⁷Fe-ENDOR and HYSCORE Study
J. Am. Chem. Soc. 129, 11447-11458 (2007)
253. W. Lubitz, E.J. Reijerse, M. van Gastel
[NiFe] and [FeFe] Hydrogenases Studied by Advanced Magnetic Resonance Techniques
Chem. Rev. 107, 4331-4365 (2007)
254. W. Lubitz, W. Tumas
Hydrogen: An Overview
Chem. Rev. 107, 3900-3903 (2007)
255. B. H. Monien, F. Drepper, M. Sommerhalter, W. Lubitz, W. Haehnel
Detection of Heme Oxygenase Activity in a Library of Four-helix Bundle Proteins: Towards the *de Novo* Synthesis of Functional Heme Proteins
J. Mol. Biol. 371, 739-753 (2007)
256. A. Marchanka, M. Paddock, W. Lubitz, M. van Gastel
Low-temperature Pulsed EPR Study at 34 GHz of the Triplet States of the Primary Electron Donor P₈₆₅ and the Carotenoid in Native and Mutant Bacterial Reaction Centers of *Rhodobacter Sphaeroides*
Biochemistry 46, 14782-14794 (2007)
257. J. Niklas, T. Schulte, S. Prakash, M. van Gastel, E. Hofmann, W. Lubitz
Spin-Density Distribution of the Carotenoid Triplet State in the Peridinin-chlorophyll-protein Antenna. A Q-Band Pulse Electron-Nuclear Double Resonance and Density Functional Theory Study
J. Am. Chem. Soc. 129, 15442-15443 (2007)

258. A. Mennenga, W. Gärtner, W. Lubitz
Interaction of Heme- and Chlorophyll-based Cofactors with *de Novo* Synthesized Peptides
Peptides 2006. Proceedings of the Twenty-Ninth European Peptide Symposium; K. Rolka, P. Rekowski, J. Silberring, eds.; Kenes International, 388-389 (2007)
259. S. Zein, C. Duboc, W. Lubitz, F. Neese
A Systematic Density Functional Study of the Zero-field Splitting in Mn(II) Coordination Compounds
Inorg. Chem. 47, 134-142 (2008)
260. V.P. Denysenkov, D. Biglino, W. Lubitz, T.F. Prisner, M. Bennati
Structure of the Tyrosyl Biradical in Mouse R2 Ribonucleotide Reductase from High-field PELDOR
Angew. Chem. 120, 1244-1247 (2008), Angew. Chem. Int. Ed. 47, 1224-1227 (2008)
261. J.-H. Su, W. Lubitz, J. Messinger
Probing Mode and Site of Substrate Water Binding to the Oxygen-evolving Complex in the S₂ State of Photosystem II by ¹⁷O-HYSCORE Spectroscopy
J. Am. Chem. Soc. 130, 786-787 (2008)
Correction published: J. Am. Chem. Soc. 133, 12317 (2011)
262. S. Zein, L. V. Kulik, J. Yano, J. Kern, Y. Pushkar, A. Zouni, V. K. Yachandra, W. Lubitz, F. Neese, J. Messinger
Focusing the View on Nature's Water-Splitting Catalyst
Phil. Trans. R. Soc. London, Ser. B 363, 1167-1177 (2008)
263. J. Niklas, S. Prakash, T. Schulte, M. van Gestel, E. Hofmann, W. Lubitz
Electron Spin Density Distribution of the Carotenoid Triplet State in the Peridinin-chlorophyll-protein Antenna of Dinoflagellates Determined by Pulse ENDOR Spectroscopy and Density Functional Theory
Photosynthesis: Energy from the Sun, J.F. Allen, E. Gantt, J.H. Golbeck, B. Osmond (eds.), Springer Dordrecht, 291-294 (2008)
264. A. Marchanka, W. Lubitz, M. Paddock, M. van Gestel
Triplet States in Photosynthetic Reaction Centers of *Rb. sphaeroides*
Photosynthesis: Energy from the Sun, J.F. Allen, E. Gantt, J.H. Golbeck, B. Osmond (eds.), Springer Dordrecht, 133-136 (2008)

265. M. L. Antonkine, C. Breitenstein; B. Epel, E. Bill, W. Gärtner, W. Lubitz
De novo Peptides Modeling the Binding Sites of [4Fe-4S] Clusters in Photosystem I
Photosynthesis: Energy from the Sun, J.F. Allen, E. Gantt, J.H. Golbeck, B. Osmond (eds.), Springer Dordrecht, 1257-1260 (2008)
266. J.-H. Su, W. Lubitz, J. Messinger
Substrate Water Bound to the S₂-state of the Mn₄O_xCa Cluster in Photosystem II Studied by Advanced Pulse EPR Spectroscopy
Photosynthesis: Energy from the Sun, J.F. Allen, E. Gantt, J.H. Golbeck, B. Osmond (eds.), Springer Dordrecht, 503-507 (2008)
267. M. Flores, A. Savitsky, E.C. Abresch, W. Lubitz, K. Möbius
Structure of Radical Pairs D⁺ Q_A⁻ in Bacterial Photosynthetic Reaction Centers Cooled to Cryogenic Temperatures in the Dark and Under Illumination: A High-Field EPR/PELDOR Study
Photosynthesis: Energy from the Sun, J.F. Allen, E. Gantt, J.H. Golbeck, B. Osmond (eds.), Springer Dordrecht, 59-63 (2008)
268. M. Flores, A. Goenka Agrawal, M. van Gestel, W. Gärtner, W. Lubitz
Electron–Electron Double Resonance-Detected NMR to Measure Metal Hyperfine Interactions: ⁶¹Ni in the Ni–B state of the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F
J. Am. Chem. Soc. 130, 2402-2403 (2008)
269. Ch. Kamp, A. Silakov, M. Winkler, E.J. Reijerse, W. Lubitz, Th. Happe
Isolation and First EPR Characterization of the [FeFe]-hydrogenases from Green Algae
Biochim. Biophys. Acta 1777, 410-416 (2008)
270. M. Fedin, V. Ovcharenko, R. Sagdeev, E.J. Reijerse, W. Lubitz, E. Bagryanskaya
Light-induced Excited Spin State Trapping in an Exchange-Coupled Nitroxide-copper(II)-nitroxide Cluster
Angew. Chem. 120, 7003-7005 (2008)
Angew. Chem. Int. Ed. 47, 6897-6899 (2008)
271. M. S. Koay, M. L. Antonkine, W. Gärtner, W. Lubitz
Modelling Low-potential [Fe₄S₄] Clusters in Proteins
Chem. Biodivers. 5, 1571-1587 (2008)
272. P. Kellers, H. Ogata, W. Lubitz
Purification, Crystallization and Preliminary X-ray Analysis of the Membrane-bound [NiFe] Hydrogenase from *Allochromatium vinosum*
Acta Crystallogr. F64, 719-722 (2008)

273. W. Lubitz, E. J. Reijerse, J. Messinger
Solar Water-splitting into H₂ and O₂: Design Principles of Photosystem II and Hydrogenases
Energy Environ. Sci. 1, 15-31 (2008)
274. B. Brogioni, D. Biglino, D. Sinicropi, E.J. Reijerse, P. Giardina, G. Sannia, W. Lubitz, R. Basosi, R. Pogni
Characterization of Radical Intermediates in the Laccase-mediator Systems. A multifrequency EPR, ENDOR and DFT/PCM Investigation
Phys. Chem. Chem. Phys. 10, 7284-7292 (2008)
275. H. Ogata, A. Goenka Agrawal, A. Kaur, R. Goddard, W. Gärtner and W. Lubitz
Purification, Crystallization and Preliminary X-ray Analysis of Adenylylsulfate Reductase from *Desulfovibrio vulgaris* Miyazaki F
Acta Crystallogr. F64, 1010-1012 (2008)
276. M. van Gastel, J. L. Shaw, A. J. Blake, M. Flores, M. Schröder, J. McMaster, W. Lubitz
Electronic Structure of a Binuclear Nickel Complex of Relevance to [NiFe] Hydrogenase
Inorg. Chem. 47, 11688-11697 (2008)
277. M. v. Gastel, W. Lubitz
EPR Investigation of [NiFe] Hydrogenases
in: High Resolution EPR: Applications to Metalloenzymes and Metals in Medicine, G.R. Hanson and L.J. Berliner (Eds.), Biol. Magn. Res. 28, Springer, Dordrecht 441-470 (2009)
278. J. P. Allen, J.M. Cordova, C.C. Jolley, T.A. Murray, J.W. Schneider, N. W. Woodbury, J. C. Williams, J. Niklas, G. Kllhm, M. Reus, W. Lubitz
EPR, ENDOR, and Special TRIPLE Measurements of P^{•+} in Wild Type and Modified Reaction Centers from *Rb. Sphaeroides*
Photosyn. Res. 99, 1-10 (2009)
279. A.Silakov, B.Wenk, E.Reijerse, S.P.J. Albracht, W.Lubitz
Spin Distribution of the H-cluster in the H_{ox}-CO State of the [FeFe] Hydrogenase from *Desulfovibrio desulfuricans*: HYSCORE and ENDOR Study of ¹⁴N and ¹³C Nuclear Interactions
J. Biol. Inorg. Chem. 14, 301-313 (2009)
280. M. van Gastel, C.C. Lu, K. Wieghardt, W. Lubitz
Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Investigation of the Diradical Bis(α-iminopyridinato)zinc Complex
Inorg. Chem. 48, 2626-2632 (2009)

281. Kulik, L., Lubitz, W.
Electron-nuclear Double Resonance
Photosyn. Res. 102 (2), 391-401, (2009)
282. E.J. Reijerse, A. Silakov, W. Lubitz
In Search of Non-fossil Fuels. Understanding the Active Site of [FeFe] Hydrogenase: Basis for a Biohydrogen Technology
The Treasures of EUREKA. Volume 1. Electron Paramagnetic Resonance. From Fundamental Research to Pioneering Applications & Zavoisky Award. Part III, ed. by K.M. Salikhov, 166-167, 2009
283. J. Messinger, L. Kulik, W. Lubitz
Mastering Sustainable Energy. Light-induced Water-splitting in Nature: Electronic Structure of the Manganese Cluster in Photosystem II
The Treasures of EUREKA. Volume 1. Electron Paramagnetic Resonance. From Fundamental Research to Pioneering Applications & Zavoisky Award. Part III, ed. by K.M. Salikhov, 164-165, 2009
284. G. Feher, W. Lubitz, K. Möbius
The Most Important Biochemical Process on Earth. EPR and ENDOR of Primary Reactants in Bacterial Photosynthesis
The Treasures of EUREKA. Volume 1. Electron Paramagnetic Resonance. From Fundamental Research to Pioneering Applications & Zavoisky Award. Part III, ed. by K.M. Salikhov, 158-159, 2009
285. M. L. Antonkine, M. S. Koay, B. Epel, C. Breitenstein, O. Gopta, W. Gärtner, E. Bill, W. Lubitz
Synthesis and Characterization of *De Novo* Designed Peptides Modelling the Binding Sites of [4Fe-4S] Clusters in Photosystem I
Biochim. Biophys. Acta 1787, 995-1008 (2009)
286. B. Conlan, N. Cox, J.-H. Su, W. Hillier, J. Messinger, W. Lubitz, P.L. Dutton, T. Wydrzynski
Photo-catalytic Oxidation of a Di-nuclear Manganese Centre in an Engineered Bacterioferritin 'Reaction Centre'
Biochim. Biophys. Acta 1787, 1112-1121 (2009)
287. D. A. Pantazis, M. Orio, T. Petrenko, S. Zein, E. Bill, W. Lubitz, J. Messinger, F. Neese
A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transition-metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystem II
Chem. Eur.J. 15, 5108-5123 (2009)
288. A. Marchanka, W. Lubitz, M. van Gastel
Spin Density Distribution of the Excited Triplet State of Bacteriochlorophylls. Pulsed ENDOR and DFT Studies
J. Phys. Chem. B 113, 6917-6927 (2009)

289. A. Silakov, B. Wenk, E.J. Reijerse, W. Lubitz
¹⁴N HYSORE Investigation of the H-cluster of [FeFe] Hydrogenase: Evidence for a Nitrogen in the Dithiol Bridge
Phys. Chem. Chem. Phys. 11, 6592 – 6599 (2009)
290. J. Niklas, B. Epel, M. L. Antonkine, S. Sinnecker, M.E. Pandelia, W. Lubitz
Electronic Structure of the Quinone Radical Anion A₁⁻ of Photosystem I Investigated by Advanced Pulse EPR and ENDOR Techniques
J. Phys. Chem. B 113, 10367-10379 (2009)
291. H. Ogata, W. Lubitz, Y. Higuchi
[NiFe] Hydrogenases: Structural and Spectroscopic Studies of the Reaction Mechanism
Dalton Trans. 37, 7577-7587 (2009)
292. M.V. Fedin, S.L. Veber, G.V. Romanenko, V.I. Ovcharenko, R.Z. Sagdeev, G. Klihm, E.J. Reijerse, W. Lubitz, E.G. Bagryanskaya
Dynamic Mixing Processes in Spin Triads of “Breathing Crystals” Cu(hfac)₂L^R: A Multifrequency EPR Study at 34, 122 and 244 GHz
Phys. Chem. Chem. Phys. 11, 6654-6663 (2009)
293. M. E. Pandelia, H. Ogata, L.J. Currell, M. Flores, W. Lubitz
Probing Intermediates in the Activation Cycle of [NiFe] Hydrogenase by Infrared Spectroscopy: The Ni-SI_r State and its Light Sensitivity
J. Biol. Inorg. Chem. 14, 1227-1241 (2009)
294. D. A. Pantazis, M. Orio, T. Petrenko, S. Zein, W. Lubitz, J. Messinger, F. Neese
Structure of the Oxygen-evolving Complex of Photosystem II: Information on the S₂ State through Quantum Chemical Calculation of its Magnetic Properties
Phys. Chem. Chem. Phys. 11, 6788-6798 (2009)
295. A.Silakov, C.Kamp, E.Reijerse, T.Happe , W. Lubitz
Spectroelectrochemical Characterization of the Active Site of the [FeFe] Hydrogenase HydA1 from *Chlamydomonas reinhardtii*
Biochemistry 48, 7780–7786 (2009)
296. H. Ogata, P. Stolle, M. Stehr, G. Auling, W. Lubitz
Crystallization and Preliminary X-ray Analysis of the Small Subunit (R2F) of Native Ribonucleotide Reductase from *Corynebacterium ammoniagenes*
Acta Crystallogr. F 65, 878-880 (2009)

297. P. Kellers, M.E. Pandelia, L.J. Currell, H. Görner, W. Lubitz
FTIR Study on the Light Sensitivity of the [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F: Ni-C to Ni-L Photoconversion, Kinetics of Proton Rebinding and H/D Isotope Effect
Phys. Chem. Chem. Phys. 11, 8680-8683 (2009)
298. D. Millo, M.E. Pandelia, T. Utesch, N. Wisitruangsakul, M. A. Mroginski, W. Lubitz, P. Hildebrandt, I. Zebger
Spectroelectrochemical Study of the [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F in Solution and Immobilized on Biocompatible Gold Surfaces
J. Phys. Chem. B 113, 15344–15351 (2009)
299. A. van der Est, Y. Puskar, I. Karyagina, B. Fonovic, T. Dudding, J. Niklas, W. Lubitz, J. Golbeck
Incorporation of 2,3-Disubstituted-1,4-naphthoquinones into the A₁ Binding Site of Photosystem I Studied by EPR and ENDOR Spectroscopy
Appl. Magn. Res. 37, 65–83 (2010)
300. M.E. Pandelia, H. Ogata, L. J. Currell, M. Flores, W. Lubitz
Inhibition of the [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F by Carbon Monoxide: An FTIR and EPR Spectroscopy Study
Biochim. Biophys. Acta 1797, 304-313 (2010)
301. J. Niklas, O. Gupta, B. Epel, W. Lubitz, M. L. Antonkine
Investigation of the Stationary and Transient A₁⁻ Radical in Trp → Phe Mutants of Photosystem I
Appl. Magn. Res. 38, 187-203 (2010)
302. I. Czech, A. Silakov, W. Lubitz, Th. Happe
The [FeFe]-hydrogenase Maturase HydF from *Clostridium acetobutylicum* Contains a CO and CN⁻ Ligated Iron Cofactor
FEBS Lett. 584, 638-642 (2010)
303. M. Saggiu, C. Teutloff, M. Ludwig, M. Brecht, M.E. Pandelia, O. Lenz, B. Friedrich, W. Lubitz, P. Hildebrandt, F. Lenzian, R. Bittl
Comparison of the Membrane-bound [NiFe] Hydrogenases from *R. eutropha* H16 and *D. vulgaris* Miyazaki F in the Oxidized Ready State by Pulsed EPR
Phys. Chem. Chem. Phys. 12, 2139-2148 (2010)
304. M.E. Pandelia, H. Ogata, W. Lubitz
Intermediates in the Catalytic Cycle of [NiFe] Hydrogenase: Functional Spectroscopy of the Active Site
Chem. Phys. Chem. 11, 1127-1140 (2010)

305. J. Grzyb, F. Xu, L. Weiner, E.J. Reijerse, W. Lubitz, V. Nanda, D. Noy
De Novo Design of a Non-natural Fold for an Iron-sulfur Protein: Alpha-helical Coiled-coil with a Four-iron Four-sulfur Cluster Binding Site in its Central Core
Biochim. Biophys Acta 1797, 406-413 (2010)
306. M.E. Pandelia, V. Fourmond, P. Tron-Infossi, E. Lojou, P. Bertrand, C. Léger, M.-Th. Giudici-Ortoni, W. Lubitz
The Membrane-Bound Hydrogenase I from the Hyperthermophilic Bacterium *Aquifex aeolicus*: Enzyme Activation, Redox Intermediates and Oxygen Tolerance
J. Am. Chem. Soc. 132, 6991-7004 (2010)
307. A. Marchanka, A. Savitsky, W. Lubitz, K. Möbius, M. van Gastel
B-branch Electron Transfer in the Photosynthetic Reaction Center of a *Rhodobacter sphaeroides* Quadruple Mutant. Q- and W-band Electron Paramagnetic Resonance Studies of Triplet and Radical-pair Cofactor States
J. Phys. Chem. B 114, 14364–14372 (2010)
308. P. Stolle, O. Barckhausen, W. Oehlmann, N. Knobbe, C. Vogt, A. J. Pierik, N. Cox, P. P. Schmidt, E.J. Reijerse, W. Lubitz, G. Auling
Homologous Expression of the *nrdF* Gene of *Corynebacterium ammoniagenes* Strain ATCC 6872 generates a Manganese-Metallo-Cofactor (R2F) and a Stable Tyrosyl Radical (Y^{*}) involved in Ribonucleotide Reduction
FEBS Journal 277; 4849–4862 (2010)
309. N. Cox, H. Ogata, P. Stolle, E.J. Reijerse, G. Auling, W. Lubitz
A Tyrosyl-Dimanganese Coupled Spin System is the Native Metalloradical Cofactor of the R2F Subunit of the Ribonucleotide Reductase of *Corynebacterium ammoniagenes*
J. Am Chem. Soc. 132, 11197–11213 (2010)
310. M.E. Pandelia, P. Infossi, M-Th. Giudici-Ortoni, W. Lubitz
The Oxygen-tolerant Hydrogenase I from *Aquifex aeolicus* Weakly Interacts with Carbon Monoxide: An Electrochemical and Time-Resolved FTIR Study
Biochemistry 49, 8873–8881 (2010)
311. H. Ogata, P. Kellers, W. Lubitz
The Crystal Structure of the [NiFe] Hydrogenase from the Photosynthetic Bacterium *Allochromatium vinosum*: Characterization of the Oxidized Enzyme (Ni-A state)
J. Mol. Biol. 402, 428-444 (2010)

312. H. Ogata, Y. Shomura, A. Goenka Agrawal, A. Pal Kaur, W. Gärtner, Y. Higuchi, W. Lubitz
Purification, Crystallization and Preliminary X-ray Analysis of the Dissimilatory Sulfite Reductase from *Desulfovibrio vulgaris*
Miyazaki F
Acta Crystallogr. F66, 1470-1472 (2010)
313. A. Silakov, J.L. Shaw, E.J. Reijerse, W. Lubitz
Advanced Electron Paramagnetic Resonance and Density Functional Theory Study of a {2Fe3S} Cluster Mimicking the Active Site of [FeFe] Hydrogenase
J. Am. Chem. Soc. 132, 17578 – 17587 (2010)
314. M. Flores, A. Savitsky, M. Paddock, E. Abresch, A. Dubinskii, M.Y. Okamura, W. Lubitz, K. Möbius
Electron-Nuclear and Electron-Electron Double Resonance Spectroscopies Show that the Primary Quinone Acceptor Q_A in Reaction Centers from Photosynthetic Bacteria *Rhodobacter sphaeroides* Remains in the Same Orientation Upon Light-Induced Reduction
J. Phys.Chem B 114, 16894–16901 (2010)
315. K. Kulon, W. Lubitz, M.L. Antonkine
Modelling the Binding Site of a Linear [3Fe-4S] Cluster
in: 10th European Biological Inorganic Chemistry Conference EUROBIIC 10 (D. Kessissoglou, T. Salifoglou (Eds.) Medimond, Pianoro 39 – 42, 2010
316. A.W.U. Busch , E.J. Reijerse, W. Lubitz, E. Hofmann, N. Frankenberg-Dinkel
Radical Mechanism of Cyanophage Phycoerythrobilin Synthase (PebS)
Biochem. J. 433, 469 – 476 (2011)
317. S.C. Drew, E.J. Reijerse, A. Quentmeier, D. Rother, C.G. Friedrich, W. Lubitz
Spectroscopic Characterization of the Molybdenum Cofactor of the Sulfane Dehydrogenase SoxCD from *Paracoccus pantotrophus*
Inorg. Chem. 50, 409-411 (2011)
318. Ö. Erdem, L. Schwartz, M. Stein, A. Silakov, S. Kaur-Ghumaan, P. Huang, S. Ott, E.J. Reijerse, W. Lubitz
A Model of the [FeFe] Hydrogenase Active Site with a Biologically Relevant Azadithiolate Bridge: A Spectroscopic and Theoretical Investigation
Angew. Chem. Int. Ed. 50, 1439-1443 (2011)
Angew. Chem. 123, 1475 –1479 (2011)

319. D. Millo, P. Hildebrandt, M.E. Pandelia, W. Lubitz, I. Zebger
SEIRA Spectroscopy of the Electrochemical Activation of an Immobilized [NiFe] Hydrogenase under Turnover and Non-Turnover Conditions
Angew. Chemie Int. Ed., 50, 2632-2632 (2011)
Angew. Chem. Dt. Ed., 123, 2680 – 2683 (2011)
320. A. Silakov, E.J. Reijerse, W. Lubitz
Unraveling the Electronic Properties of the Photo-Induced States of the H-cluster in the [FeFe] Hydrogenase from *D. desulfuricans*
Eur. J. Inorg. Chem., 1056-1066 (2011)
321. C. Greco, A. Silakov, M. Bruschi, U. Ryde, L. De Gioia, W. Lubitz
Magnetic Properties of [FeFe]-hydrogenases: A Theoretical Investigation Based on Extended QM and QM/MM Models of the H-Cluster and its Surroundings
Eur. J. Inorg. Chem., 1043-1049 (2011)
322. N. Cox, L. Rapatskiy, J.-H. Su, D.A. Pantazis, M. Sugiura, L. Kulik, P. Dorlet, A.W. Rutherford, F. Neese, A. Boussac, W. Lubitz, J. Messinger
Effect of Ca²⁺/Sr²⁺ Substitution on the Electronic Structure of the Oxygen-evolving Complex of Photosystem II: A Combined Pulse ⁵⁵Mn-ENDOR, Multi-frequency EPR and DFT Study of the S₂ State
J. Am. Chem. Soc., 133, 3635 - 3648 (2011). Addition published: J. Am. Chem. Soc. 133, 14149 (2011)
323. M.E. Pandelia, W. Nitschke, P. Infossi, M.-T. Giudici-Ortoni, E. Bill, W. Lubitz
Characterization of a Unique [FeS] Cluster in the Electron Transfer Chain of the Oxygen Tolerant [NiFe] Hydrogenase from *Aquifex aeolicus*
P. Natl. Acad. Sci. USA, 108, 6097-6102 (2011)
324. J.-H. Su, N. Cox, W. Ames, D.A. Pantazis, L. Rapatskiy, T. Lohmiller, L. Kulik, P. Dorlet, A.W. Rutherford, F. Neese, A. Boussac, W. Lubitz, J. Messinger
The Electronic Structures of the S₂ States of the Oxygen-evolving Complexes of Photosystem II in Plants and Cyanobacteria in the Presence and Absence of Methanol
Biochim. Biophys. Acta – Bioenergetics, 1807, 829-840 (2011)
325. I. Cohen-Ofri, M. van Gastel, J. Grzyb, A. Brandis, I. Pinkas, W. Lubitz, D. Noy
Zinc–bacteriochlorophyllide Dimers in *De Novo* Designed Four-Helix Bundle Proteins. A Model System for Natural Light Energy Harvesting and Dissipation
J. Am. Chem. Soc., 133, 9526–9535 (2011)

326. A. Sedoud, N. Cox, M. Sugiura, W. Lubitz, A. Boussac, A.W. Rutherford
The Semiquinone-Iron Complex of Photosystem II: EPR Signals Assigned to the Low-Field Edge of the Ground State Doublet of $Q_A^{\bullet-} Fe^{2+}$ and $Q_B^{\bullet-} Fe^{2+}$
Biochemistry, 50, 6012-6021 (2011)
327. A. Hoppe, M.E. Pandelia, W. Gärtner, W. Lubitz
[Fe₄S₄]- and [Fe₃S₄]-Cluster Formation in Synthetic Peptides
Biochim. Biophys. Acta – Bioenergetics, 1807, 1414-1422 (2011)
328. A.W.U. Busch, E.J. Reijerse, W. Lubitz, N. Frankenberg-Dinkel, E. Hofmann
Structural and Mechanistic Insight into the Ferredoxin-Mediated two Electron Reduction of Bilins
Biochem. J., 439, 257-264 (2011)
329. N. Cox, W. Ames, B. Epel, L.V. Kulik, L. Rapatskiy, F. Neese, J. Messinger, K. Wieghardt, W. Lubitz
The Electronic Structure of a Weakly Antiferromagnetically Coupled Mn^{II}Mn^{III} Model Relevant to Manganese Proteins: A Combined EPR, ⁵⁵Mn-ENDOR and DFT Study
Inorg. Chem., 50, 8238-8251 (2011)
330. W. Ames, D.A. Pantazis, V. Krewald, N. Cox, J. Messinger, W. Lubitz, F. Neese
A Theoretical Evaluation of Structural Models of the S₂ State in the Oxygen Evolving Complex: Protonation States and Magnetic Interactions
J. Am. Chem. Soc. 133, 19743-19757 (2011)
331. S.L. Veber, M.V. Fedin, K.Y. Maryunina, A. Potapov, D. Goldfarb, E.J. Reijerse, W. Lubitz, R.Z. Sagdeev, V.I. Ovcharenko, E. G. Bagryanskaya
Temperature-Dependent Exchange Interaction in Molecular Magnets Cu(hfac)₂L^R Studied by EPR: Methodology and Interpretations
Inorg. Chem. 50, 10204 – 10212 (2011)
332. A. Savitsky, A. Dubinskii, H. Zimmermann, W. Lubitz, K. Möbius
High-Field Dipolar Electron Paramagnetic Resonance (EPR) Spectroscopy of Nitroxide Biradicals for Determining Three-Dimensional Structures of Biomacromolecules in Disordered Solids
J. Phys Chem B, 115, 11950–11963 (2011)
333. K. Möbius, W. Lubitz, A. Savitsky
Photo-Induced Electron Spin Polarization in Chemical and Biological reactions: Probing Structure and Dynamics of Transient

Intermediates by Multifrequency EPR Spectroscopy

Appl. Magn. Res. 41, 113-143 (2011)

334. E.J. Reijerse, F. Lendzian, R. Isaacson, W. Lubitz
A Tunable General Purpose Q-Band Resonator for CW and Pulse EPR/ENDOR Experiments with Large Sample Access and Optical Excitation
J. Magn. Reson. 214, 237-243 (2012)
335. M.E. Pandelia, P. Infossi, M. Stein, M.-T. Giudici-Ortoni, W. Lubitz
Spectroscopic Characterization of the Key Catalytic Intermediate Ni-C in the O₂-Tolerant [NiFe] Hydrogenase I from *Aquifex aeolicus*: Evidence of a Weakly Bound Hydride
Chem. Commun. 48, 823-825 (2012)
336. W. Lubitz, H. Ogata, E.J. Reijerse, Y. Higuchi
Structure and Function of Hydrogenase Enzymes
in: RSC Energy and Environment Series No. 5. Molecular Solar Fuels, Edited by T.J. Wydrzynski and W. Hillier, Royal Society of Chemistry, 288 – 325 (2012)
337. P. Knörzer, A. Silakov, C.E. Foster, F.A. Armstrong, W. Lubitz, T. Happe
The Importance of the Protein Framework for the Catalytic Activity of [FeFe]-Hydrogenases
J. Biol. Chem. 287, 1489-1499 (2012)
338. S. Mula, A. Savitsky, K. Möbius, W. Lubitz, J.H. Golbeck, M.D. Mamedov, A.Y. Semenov, A. van der Est
Incorporation of a High Potential Quinone Reveals that Electron Transfer in Photosystem I Becomes Highly Asymmetric at Low Temperature
Photochem. Photobiol. Sci. 11, 946-956 (2012)
339. J. Grzyb; F. Xu; V. Nanda; R. Łuczowska; E.J. Reijerse; W. Lubitz; D. Noy
Empirical and Computational Design of Iron-Sulfur Cluster Proteins
Biochim. Biophys. Acta 1817, 1256-1262 (2012)
340. T. Lohmiller, N. Cox, J.-H. Su, J. Messinger, W. Lubitz
An EPR and ENDOR Spectroscopic Investigation of the Ca²⁺-Depleted Oxygen-Evolving Complex of Photosystem II
In: Photosynthesis: Research for Food, Fuel and Future-15th International Conference on Photosynthesis, Congming Lu, Tingyun Kuang, Lixin Zhang, 239 – 243 (2012)

341. A. Adamska, A. Silakov, C. Lambertz, O. Rüdiger, T. Happe, E.J. Reijerse, W. Lubitz
Identification and Characterization of the “super-reduced” state of the H-cluster in [FeFe] Hydrogenase: A New Building Block for the Catalytic Cycle?
Angew. Chem. Int. Ed. 51, 11458-11462 (2012)
Angew. Chem. 124, 11624-11629 (2012)
342. H.S. Shafaat, K. Weber, T. Petrenko, F. Neese, W. Lubitz
Key Hydride Vibrational Modes in [NiFe] Hydrogenase Model Compounds Studied by Resonance Raman Spectroscopy and Density Functional Calculations
Inorg. Chem. 51, 11787-11797 (2012)
343. D.A. Pantazis, W. Ames, N. Cox, W. Lubitz, F. Neese
Two Interconvertible Structures Explain the Spectroscopy of the Oxygen Evolving Complex in the S₂ State
Angew. Chem. Int. Ed. 51, 9935 –9940 (2012)
Angew.Chem. 124, 10074 –10079 (2012)
344. M.E. Pandelia, W. Lubitz, W. Nitschke
Evolution and Diversification of Group 1 [NiFe] Hydrogenases. Is there a Phylogenetic Marker for O₂ Tolerance?
Biochim. Biophys. Acta 1817, 1565-1575 (2012)
345. T. Lohmiller, N. Cox, J.-H. Su, J. Messinger, W. Lubitz
The Basic Properties of the Electronic Structure of the Oxygen-evolving Complex of Photosystem II are not Perturbed by Ca²⁺ Removal
J. Biol. Chem. 287, 24721-24733 (2012)
346. L. Rapatskiy, N. Cox, A. Savitsky, W. Ames, J. Sander, M. Nowaczyk, M. Rögner, A. Boussac, F. Neese, J. Messinger, W. Lubitz
Detection of the Water Binding Sites of the Oxygen-evolving Complex of Photosystem II Using W-band ¹⁷O Electron-Electron Double Resonance Detected NMR Spectroscopy
J. Am. Chem. Soc. 134, 16619-16634 (2012)
347. M. Flores, M.Y. Okamura, J. Niklas, M.E. Pandelia, W. Lubitz
Pulse Q-Band EPR and ENDOR Spectroscopies of the Photochemically Generated Monoprotonated Benzosemiquinone Radical in Frozen Alcoholic Solution
J. Phys.Chem.B 116, 8890-8900 (2012)

348. C.-H. Hsieh, Ö. Erdem, S.D. Harman, M. Singleton, E.J. Reijerse, W. Lubitz, C. Popescu, J.H. Reibenspies, S.M. Brothers, M.B. Hall, M.Y. Darensbourg,
Structural and Spectroscopic Features of Mixed Valent Fe^{II}Fe^I Complexes and Factors Related to the Rotated Configuration of Diiron Hydrogenase
J. Am. Chem. Soc. 134, 13089-13102 (2012)
349. A. Silakov, M. Olsen, S. Sproules, E.Reijerse, T. Rauchfuss, W. Lubitz
EPR/ENDOR, Mössbauer, and Quantum Chemical Investigation of Di-iron Complexes Mimicking the Active Oxidized State of [FeFe] Hydrogenase
Inorg. Chem 51, 8617-8628 (2012)
350. E.V. Tretyakov, S. Tolstikov, A.O. Suvorova, A.V. Polushkin, G.V. Romanenko, A.S. Bogomyakov, S.L. Veber, M.V. Fedin, D.V. Stass, E.J. Reijerse, W. Lubitz, E.M. Zueva, V.I. Ovcharenko.
Crucial Role of Paramagnetic Ligand for Magnetostructural Anomalies in “Breathing Crystals”
Inorg. Chem 51, 9385-9394 (2012)
351. M. Karnahl, S. Tschierlei, Ö. Erdem, S. Pullen, M.P. Santoni, E.J. Reijerse, W. Lubitz, S. Ott
Mixed-Valence [Fe^IFe^{II}] Hydrogenase Active Site Model Complexes Stabilized by a Bidentate Carborane bis-Phosphine Ligand
Dalton Trans. 41, 12468 – 12477 (2012)
352. M. Kampa, W. Lubitz, M. van Gastel, F. Neese
Computational Study of the Electronic Structure and Magnetic Properties of the Ni-C State in [NiFe] Hydrogenases Including the Second Coordination Sphere
J. Biol. Inorg. Chem. 7, 1269–1281 (2012)
353. K. Weber, T. Krämer, H.S. Shafaat, T. Weyhermüller, E. Bill, M. van Gastel, F. Neese, W. Lubitz
A Functional [NiFe]-Hydrogenase Model Compound that Undergoes Biologically Relevant Reversible Thiolate Protonation
J. Am. Chem. Soc. 134, 20745–20755 (2012)
354. N. Cox, W. Lubitz
Molecular Concepts of Water Splitting: Nature’s Approach
in: R. Schlögl (ed.) Chemical Energy Storage, Chapter 3.4, 185-224 (2013) Berlin/Boston: Walter de Gruyter GmbH
355. N. Cox, W. Lubitz
Molecular Concepts of Water Splitting: Nature's Approach
De Gruyter Bookshelf
Green 3, 235-263 (2013)

356. M.E. Pandelia, D. Bykov, R. Izsak, P. Infossi, M.-T. Giudici-Ortoni, E. Bill, F. Neese, W. Lubitz
Electronic Structure of the Unique [4Fe-3S] Cluster in O₂-tolerant Hydrogenases Characterized by ⁵⁷Fe Mössbauer and EPR spectroscopy
Proc. Natl. Acad. Sci. USA 110, 483-488 (2013)
357. H. Ogata, W. Lubitz
Hydrogenase Structure and Function
In: Lennarz, W.J. and Lane, M.D. (eds.) The Encyclopedia of Biological Chemistry, Vol. 2, pp. 562-567 (2013) Waltham, MA: Academic Press
358. S. Kamali, H. Wang, D. Mitra, H. Ogata, W. Lubitz, B.C. Manor, T.B. Rauchfuss, D. Byrne, V. Bonnefoy, F.E. Jenney Jr, M.W.W. Adams, Y. Yoda, E. Alp, J. Zhao, S.P. Cramer
Observation of the Fe-CN and Fe-CO Vibrations in the Active Site of [NiFe] Hydrogenase by Nuclear Resonance Vibrational Spectroscopy
Angew. Chem. Int. Ed. 52, 724-728 (2013)
Angew. Chem. 125, 752-756 (2013)
359. A. Savitsky, Y. Grishin, R. Rakhmatullin, E.J. Reijerse, W. Lubitz
An Improved Coupling Design for High-frequency TE₀₁₁ EPR Cavities
Rev. Sci. Instrum. 84, 014704 (2013), DOI 10.1063/1.4788735
360. H.S. Shafaat, O. Rüdiger, H. Ogata, W. Lubitz
[NiFe] Hydrogenases: A Common Active Site for Function under Diverse Environments
Biochim. Biophys. Acta. 1827, 986-1002 (2013)
361. T.A. Faunce, W. Lubitz, A.W. Rutherford, D. MacFarlane, G.F. Moore, P. Yang, D.G. Nocera, T.A. Moore, D.H. Gregory, S. Fukuzumi, K.B. Yoon, F.A. Armstrong, M.R. Wasielewski
Energy and Environment Policy Case for a Global Project on Artificial Photosynthesis
Energy Environ. Sci. 6, 695-698 (2013)
362. W. Lubitz, N. Cox
Wie Pflanzen Wasser spalten
Spektrum der Wissenschaften 9, 34-43 (2013)
363. T. Lohmiller, W. Ames, W. Lubitz, N. Cox, S. Misra
EPR Spectroscopy and the Electronic Structure of the Oxygen-evolving Complex of Photosystem II
Appl. Magn. Res. 44, 691-720 (2013)

364. C. He, K. Nishikawa, Ö.F. Erdem, E.J. Reijerse, H. Ogata, W. Lubitz, M. Knipp
Complexes of Ferriheme Nitrophorin 4 with Low-Molecular Weight Thiol(ate)s Occurring in Blood Plasma
J. Inorg. Biochem. 122, 38-48 (2013)
365. M. Kampa, M.E. Pandelia, W. Lubitz, M. van Gestel, F. Neese
A Metal-metal Bond in the Light-induced State of [NiFe] Hydrogenases with Relevance to Hydrogen Evolution
J. Am. Chem. Soc. 135, 3915–3925 (2013)
366. N. Cox, D.A. Pantazis, F. Neese, W. Lubitz
Biological Water Oxidation
Acc. Chem. Res. 46, 1588-1596 (2013)
367. G. Berggren, A. Adamska, C. Lambertz, T. Simmons, J. Esselborn, M. Atta, S. Gambarelli, J.M. Mousesca, E.J. Reijerse, W. Lubitz, T. Happe, V. Artero, M. Fontecave
Biomimetic Assembly and Activation of [FeFe]-Hydrogenases
Nature 499, 66–69 (2013)
368. A. Thapper, S. Styring, G. Saracco, A.W. Rutherford, B. Robert, A. Magnuson, W. Lubitz, A. Llobet, P. Kurz, A. Holzwarth, S. Fiechter, H. de Groot, S. Campagna, A. Braun, H. Bercegol, V. Artero
Artificial Photosynthesis for Solar Fuels – an Evolving Research Field within AMPEA, a Joint Programme of the European Energy Research Alliance
Green 3, 43-57 (2013)
369. A. Savitsky, J. Niklas, J.H. Golbeck, K. Möbius, W. Lubitz
Orientation Resolving Dipolar High-field EPR Spectroscopy on Disordered Solids: II. Structure of Spin-correlated Radical Pairs in Photosystem I
J. Phys. Chem B. 117, 11184-11199 (2013)
370. T. Krämer, M. Kampa, W. Lubitz, M. van Gestel, F. Neese
Theoretical Spectroscopy of the Ni^{II} Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenases
Chem. Bio. Chem. 14, 1898-1905 (2013)
371. J. Riethausen, O. Rüdiger, W. Gärtner, W. Lubitz, H.S. Shafaat
Spectroscopic and Electrochemical Characterization of the [NiFeSe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F: Reversible Redox Behavior and Interactions Between Electron Transfer Centers
Chem. Bio. Chem. 14, 1714-1719 (2013)

372. J.J. Griese, K. Roos, N. Cox, H.S. Shafaat, R.M.M. Branca, J. Lehtiö, A. Gräslund, W. Lubitz, P.E.M. Siegbahn, M. Högbom
Direct Observation of Structurally Encoded Metal Discrimination and Ether Bond Formation in a Heterodinuclear Metalloprotein
Proc. Natl. Acad. Sci. USA 110, 17189-17194 (2013)
373. M. Pérez Navarro, W.M. Ames, H. Nilsson, T. Lohmiller, D.A. Pantazis, L. Rapatskiy, M.M. Nowaczyk, F. Neese, A. Boussac, J. Messinger, W. Lubitz, N. Cox
Ammonia Binding to the Oxygen-evolving Complex of Photosystem II Identifies the Solvent-exchangeable μ -oxo of the Manganese Tetramer
Proc. Natl. Acad. Sci. USA 110, 15561-15566 (2013)
374. B. Molitor, M. Staßen, A. Modi, S. El-Mashtoly, C. Laurich, W. Lubitz, J.H. Dawson, M. Rother, N. Frankenberg-Dinkel
A Heme-based Redox Sensor in the Methanogenic Archaeon *Methanosarcina acetivorans*
J. Biol. Chem. 288, 18458-18472 (2013)
375. J. Esselborn, C. Lambertz, A. Adamska-Venkatesh, T. Simmons, G. Berggren, J. Noth, J. Siebel, A. Hemschemeier, V. Artero, E.J. Reijerse, M. Fontecave, W. Lubitz, T. Happe
Spontaneous Activation of [FeFe]-hydrogenases by an inorganic [2Fe] Active Site Mimic
Nat. Chem. Biol. 9, 607-609 (2013)
376. N. Cox, W. Lubitz, A. Savitsky
W-band ELDOR-detected NMR (EDNMR) Spectroscopy as a Versatile Technique for the Characterization of Transition Metal-Ligand Interactions
Mol. Phys. 111, 2788-2808 (2013)
377. K. Möbius, W. Lubitz, A. Savitsky
High-Field EPR on Membrane Proteins – Crossing the GAP to NMR
Prog. Nucl. Magn. Reson. Spectrosc. 75, 1-49 (2013)
378. Ö.F. Erdem, M. Stein, S. Kaur-Ghumaan, E.J. Reijerse, S. Ott, W. Lubitz
Effect of Cyanide Ligands on the Electronic Structure of [FeFe] Hydrogenase Active Site Model Complexes with an Azadithiolate Ligand
Chem. Eur. J. 19, 14566-14572 (2013)

379. O. Gutiérrez-Sanz, M. Marques, I.A.C. Pereira, A.L. de Lacey, W. Lubitz, O. Rüdiger
Orientation and Function of a Membrane Bound Enzyme Monitored by Electrochemical Surface Enhanced Infrared Absorption Spectroscopy
J. Phys. Chem. Lett. 4, 2794-2798 (2013)
380. H. Wang, H. Ogata, W. Lubitz, S.P. Cramer
A Dynamic View of [NiFe] Hydrogenase by Means of Nuclear Resonance Vibrational Spectroscopy
Spring-8 Res. Front. 2012, 80-81 (2013)
381. K. Weber, I. Heise, T. Weyhermüller, W. Lubitz
Synthesis and Characterization of Nickel Compounds with Tetradentate Thiolate-Thioether Ligands as Precursors for [NiFe]-Hydrogenase Models
Eur. J. Inorg. Chem., 148-155 (2014)
382. H. Ogata, E. Decaneto, M. Grossman, M. Havenith, I. Sagi, W. Lubitz, M. Knipp
Crystallization and Preliminary X-ray Crystallographic Analysis of the Catalytic Domain of Membrane Type 1 Matrix Metalloproteinase
Acta Crystallogr. F70, 232-235 (2014)
383. M. Malferrari, A. Nalepa, G. Venturoli, F. Francia, W. Lubitz, K. Möbius, A. Savitsky
Structural and Dynamical Characteristics of Trehalose and Sucrose Matrices at Different Hydration Levels as Probed by FTIR and High-Field EPR
Phys. Chem. Chem. Phys. 16, 9831-9848 (2014)
384. A. Marchanka, W. Lubitz, M. van Gastel, M. Plato
Comparative ENDOR Study at 34 GHz and the Triplet State of the Primary Donor in Bacterial Reaction Centers of *Rb. sphaeroides* and *Bl. Viridis*
Photosynth. Res. 120, 99-111 (2014)
385. W. Lubitz, H. Ogata, O. Rüdiger, E.J. Reijerse
Hydrogenases
Chem. Rev. 114, 4081-4148 (2014)
386. A. Nalepa, K. Möbius, W. Lubitz, A. Savitsky
High-Field ELDOR-Detected NMR Study of a Nitroxide Radical in Disordered Solids: Towards Characterization of Heterogeneity of Microenvironments in Spin-Labeled Systems
J. Magn. Reson. 242, 203-213 (2014)

387. T. Lohmiller, V. Krewald, M. Pérez Navarro, M. Retegan, L. Rapatskiy, M.M. Nowaczyk, A. Boussac, F. Neese, W. Lubitz, D.A. Pantazis, N. Cox
Structure, Ligands and Substrate Coordination of the Oxygen-Evolving Complex of Photosystem II in the S₂ State: A Combined EPR and DFT Study
Phys. Chem. Chem. Phys. 16, 11877-11892 (2014)
388. M. Retegan, N. Cox, W. Lubitz, F. Neese, D.A. Pantazis
The First Tyrosyl Radical Intermediate Formed in the S₂-S₃ Transition of Photosystem II
Phys. Chem. Chem. Phys. 16, 11901-11910 (2014)
389. C.-H. Hsieh, Ö. F. Erdem, S. Ding, D. J. Crouthers, T. Liu, C.C.L. McCrory, W. Lubitz, C. V. Popescu, J. H. Reibenspies, M. B. Hall, M.Y. Darensbourg
In Search of an Iron-Nitrosyl Paradigm for Base Metal Proton Reduction Electrocatalysis
Nat. Commun. 5, 3684 (2014), doi 10.1038/ncomms4684
390. K. Weber, Ö.F. Erdem, E. Bill, T. Weyhermüller, W. Lubitz
Modeling the Active Site of [NiFe]-Hydrogenases and the [NiFe_u] Subside of the H-Cluster of Carbon Monoxide Dehydrogenases: Iron(II) Low Spin vs. Iron(II) High Spin
Inorg. Chem. 53, 6329-6337 (2014)
391. N. Plumeré, O. Rüdiger, A. A. Oughli, R. Williams, J. Vivekananthan, S. Pöller, W. Schuhmann, W. Lubitz
A Redox Hydrogel Protects Hydrogenase from High Potential Deactivation and Oxygen Damage
Nat. Chem. 6, 822-827 (2014)
392. A. Adamska-Venkatesh, D. Krawietz, J. Siebel, K. Weber, T. Happe, E. Reijerse, W. Lubitz
New Redox States Observed in [FeFe] Hydrogenases Reveal Redox Coupling within the H-Cluster
J. Am. Chem. Soc. 136, 11339-11346 (2014)
393. S. Rumpel, J. F. Siebel, C. Farès, J. Duan, E. Reijerse, T. Happe, W. Lubitz and M. Winkler
Enhancing Hydrogen Production of Microalgae by Redirecting Electrons from Photosystem I to Hydrogenase
Energy Environ. Sci. 7, 3296-3301 (2014)
394. N. Cox, M. Retegan, F. Neese, D.A. Pantazis, A. Boussac, W. Lubitz
Electronic Structure of the Oxygen-evolving Complex in Photosystem II Prior to O-O Bond Formation
Science 345, 804-808 (2014)

395. H. S. Shafaat, J. J. Griese, D. A. Pantazis, K. Roos, C. S. Andersson, A. Popović-Bijelić, A. Gräslund, P. E. M. Siegbahn, F. Neese, W. Lubitz, M. Högbom, N. Cox
Electronic Structural Flexibility of Heterobimetallic Mn/Fe Cofactors: R2lox and R2c Proteins
J. Am. Chem. Soc. 136, 13399-13409 (2014)
396. D.A. Pantazis, N. Cox, W. Lubitz, F. Neese
Oxygen-Evolving Photosystem II
In: Encyclopedia of Inorganic and Bioinorganic Chemistry, John Wiley & Sons, Ltd. 1-13 (2014), doi 10.1002/9781119951438.eibc2166
397. Ogata, H. Lubitz, W.
Protein Crystallography Using Free-Electron Lasers: Water Oxidation in Photosynthesis
Angew. Chem., Int. Ed. 53, 13007-13008 (2014)
Angew. Chem. 126, 13221-13222 (2014)
398. H. Vondracek, J. Dielmann-Gessner, W. Lubitz, M. Knipp, M. Havenith
THz Absorption Spectroscopy of Solvated β -Lactoglobulin
J. Chem. Phys. 141, 22D534 (2014)
399. H. Ogata, K. Nishikawa, W. Lubitz
Hydrogens Detected by Subatomic Resolution Protein Crystallography in a [NiFe] Hydrogenase
Nature 520, 571-574 (2015)
400. K. Möbius, A. Savitsky, A. Nalepa, M. Malferrari, F. Francia, W. Lubitz, G. Venturoli
The Magic of Disaccharide Glass Matrices for Protein Function as Decoded by High-Field EPR and FTIR Spectroscopy
Appl. Magn. Res. 46, 435-464 (2015)
401. S. Kiesel, D. Wätzlich, C. Lange, E. Reijerse, M.J. Bröcker, W. Rüdiger, W. Lubitz, H. Scheer, J. Moser, D. Jahn
Iron-Sulfur Cluster-Dependent Catalysis of Chlorophyllide Oxidoreductase from *Roseobacter denitrificans*
J. Biol. Chem. 290, 1141-1154 (2015)
402. E. Decaneto, S. Abbruzzetti, I. Heise, W. Lubitz, C. Viappiani, M. Knipp
A Caged Substrate Peptide for Matrix Metalloproteinases
Photochem. Photobiol. Sci. 14, 300-307 (2015)
403. V. Krewald, M. Retegan, N. Cox, J. Messinger, W. Lubitz, S. DeBeer, F. Neese, D.A. Pantazis
Metal Oxidation States in Biological Water Splitting
Chem. Sci. 6, 1676-1695 (2015)

404. A. Adamska-Venkatesh, T.R. Simmons, J. Siebel, V. Artero, M. Fontecave, E. Reijerse, W. Lubitz
Artificially Maturated [FeFe] Hydrogenase from *Chlamydomonas reinhardtii*: A HYSCORE and ENDOR Study of a Non-Natural H-cluster
Phys. Chem. Chem. Phys. 17, 5421—5430 (2015)
405. J.F. Siebel, A. Adamska-Venkatesh, K. Weber, S. Rumpel, E. Reijerse, W. Lubitz
Hybrid [FeFe]-hydrogenases with Modified Active Sites Show Remarkable Residual Enzymatic Activity
Biochemistry 54, 1474-1483 (2015)
406. K. Möbius, M. Pato, G. Kllhm, C. Laurich, A. Savitsky, W. Lubitz, B. Szyszko, M. Stepien, L. Latos-Grazynski
Möbius-Hückel Topology Switching in an Expanded Porphyrin Cation Radical as Studied by EPR and ENDOR Spectroscopy
Phys. Chem. Chem. Phys. 17, 6644-6652 (2015)
407. N. Cox, D. Pantazis, F. Neese, W. Lubitz
Artificial Photosynthesis: Understanding Water Splitting in Nature
Interface Focus 5, 20150009, doi 10.1098/rsfs.2015.0009 (2015)
408. C. He, B. D. Howes, G. Smulevich, S. Rumpel, E.J. Reijerse, W. Lubitz, N. Cox, M. Knipp
Nitrite Dismutase Reaction Mechanism: Kinetic and Spectroscopic Investigation of the Interaction between Nitrophorin and Nitrite
J. Am. Chem. Soc. 137, 4141-4150 (2015)
409. V. Fourmond, S. Stapf, H. Li, D. Buesen, J. Birrell, O. Rüdiger, W. Lubitz, W. Schuhmann, N. Plumeré, C. Léger
Mechanism of Protection of Catalysts Supported in Redox Hydrogel Films
J. Am. Chem. Soc. 137, 5494-5505 (2015)
410. P. Rodriguez-Macià, A. Dutta, W. Lubitz, W. Shaw, O. Rüdiger
Direct Comparison of the Performance of a Bio-inspired Synthetic Ni-Catalyst and a [NiFe]-Hydrogenase Covalently Attached to Electrodes
Angew. Chem., Int. Ed., 54, 12303-12307 (2015)
Angew. Chem., 127, 12478-12482 (2015)
411. A. A. Oughli, F. Conzuelo, M. Winkler, T. Happe, W. Lubitz, W. Schuhmann, O. Rüdiger, N. Plumeré
A Redox Hydrogel Protects the O₂-Sensitive [FeFe]-Hydrogenase from *Chlamydomonas reinhardtii* from Oxidative Damage
Angew. Chem., Int. Ed. (2015), 54, 12329-12333
Angew. Chem., 127, 12506–12510 (2015)

412. S. Rumpel, J.F. Siebel, M. Diallo, C. Farès, E. Reijerse, W. Lubitz
Structural Insight into the Complex of Ferredoxin and [FeFe] Hydrogenase from *Chlamydomonas reinhardtii*
ChemBioChem 16, 1663-1669 (2015)
413. F. Roncaroli, E. Bill, B. Friedrich, O. Lenz, W. Lubitz, M.E. Pandelia
Cofactor Composition and Function of a H₂-sensing Regulatory Hydrogenase as Revealed by Mössbauer and EPR spectroscopy
Chem. Sci. 6, 4495-4507 (2015)
414. J. L. Barilone, H. Ogata, W. Lubitz, M. van Gastel
Structural Differences between the Active Sites of the Ni-A and Ni-B States of the [NiFe] Hydrogenase: An Approach by Quantum Chemistry and Single Crystal ENDOR Spectroscopy
Phys. Chem. Chem. Phys. 17, 16204-16212 (2015)
415. K. Weber, T. Weyhermüller, E. Bill, Ö.F. Erdem, W. Lubitz
Design and Characterization of Phosphine Iron Hydrides: Toward Hydrogen-Producing Catalysts
Inorg Chem. 54, 6928-6937 (2015)
416. R. Gilbert-Wilson, J.F. Siebel, A. Adamksa-Venkatesh, C.C. Pham, E. Reijerse, H. Wang, Hongxin, S.P. Cramer, W. Lubitz, T.B. Rauchfuss
Spectroscopic Investigations of [FeFe] Hydrogenase Matured with [Fe(adt)(CN)(CO)]
J. Am. Chem. Soc. 137, 8998-9005 (2015)
417. H. Ogata, T. Krämer, H. Wang, D. Schilter, V. Pelmeshnikov, M. van Gastel, F. Neese, T. B. Rauchfuss, L.B. Gee, A.D. Scott, Y. Yoda, Y. Tanaka, W. Lubitz, S. P. Cramer
Hydride Bridge in [NiFe]-hydrogenase Observed by Nuclear Resonance Vibrational Spectroscopy
Nat. Commun. 6:7890 doi: 10.1038/ncomms8890 (2015)
418. N. Cox, A. Nalepa, M.-E. Pandelia, W. Lubitz, A. Savitsky
Double-Resonance EPR Techniques for the Study of Metallobiomolecules
in: *Methods in Enzymology*, Qin, P.Z., Warncke, K., Eds. Elsevier, Oxford, 563, 211-249 (2015)
419. A. Adamska-Venkatesh, S. Roy, J. F. Siebel, T. R. Simmons, M. Fontecave, V. Artero, E. Reijerse, W. Lubitz
Spectroscopic Identification of the Bridging Amine in the Active Site of [FeFe] Hydrogenase Using Isotopologues of the H-Cluster
J. Am. Chem. Soc. 137, 12744-12747 (2015)

420. T. Lohmiller, N. Cox, W. Lubitz
Ein Enzym, das die Welt veränderte: Die Wasserspaltungsmaschine der Photosynthese
labor & more 08.15, 10-15 (2015)
421. E. Decaneto, S. Suladze, C. Rosin, M. Havenith, W. Lubitz, R. Winter
Pressure and Temperature Effects on the Activity and Structure of the Catalytic Domain of Human MT1-MMP
Biophys. J. 109, 2371-2381 (2015)
422. H. Wang, Y. Yoda, H. Ogata, Y. Tanaka, W. Lubitz
A Strenuous Experimental Journey Searching for Spectroscopic Evidence of a Bridging Nickel-iron-hydride in [NiFe] Hydrogenase
J. Synchrotron Rad. 22, 1334-1344 (2016)
423. M. Retegan, V. Krewald, F. Mamedov, F. Neese, W. Lubitz, N. Cox, D. A. Pantazis
A Five-coordinate Mn(IV) Intermediate in Biological Water Oxidation: Spectroscopic Signature and a Pivot Mechanism for Water Binding
Chem. Sci. 7, 72-84 (2016)
424. V. Krewald, M. Retegan, F. Neese, W. Lubitz, D. A. Pantazis, N. Cox
Spin State as a Marker for the Structural Evolution of Nature's Water Splitting Catalyst
Inorg. Chem. 55, 488-501 (2016)
425. G. M. Chambers, M.T. Huynh, S. Hammes-Schiffer, T.B. Rauchfuss, E. Reijerse, W. Lubitz
Models of the Ni-L and Ni-SI_a States of the [NiFe]-Hydrogenase Active Site
Inorg. Chem. 55, 419-431 (2016)
426. P. Costa, T. Lohmiller, I. Trosien, A. Savitsky, W. Lubitz, M. Fernandez-Oliva, E. Sanchez-Garcia, W. Sander
Light and Temperature Control of the Spin State of Bis(*p*-methoxyphenyl)carbene: a Bistable Carbene
J. Am. Chem. Soc. 138, 1622-1629 (2016)
427. S. Hugenbruch, H.S. Shafaat, T. Kraemer, M.U. Delgado-Jaime, K. Weber, F. Neese, E. Lubitz, S. DeBeer
In Search of Metal Hydrides: An X-ray Absorption and Emission Study of [NiFe] Hydrogenase Model Complexes
Phys. Chem. Chem. Phys. 18, 10688-10699 (2016)
428. M. Pérez-Navarro, F. Neese, W. Lubitz, D.A. Pantazis, N. Cox
Recent Developments in Biological Water Oxidation
Curr. Opin. Chem. Biol. 31, 113-119 (2016)

429. M. Kühner, P. Schweyen, M. Hoffmann, J. Vazquez Ramos, E. J. Reijerse, W. Lubitz, M. Bröring, G. Layer
The Auxiliary [4Fe-4S] Cluster of the Radical SAM Heme Synthase from *Methanosarcina barkeri* is Involved in Electron Transfer
Chem. Sci. 7, 4633-4643 (2016)
430. Y. Kutin, V. Srinivas, M. Fritz, R. Kositzki, H. S. Shafaat, J. Birrell, E. Bill, M. Haumann, W. Lubitz, M. Högbom, J. J. Griese, N. Cox
Divergent Assembly Mechanisms of the Manganese/Iron Cofactors in R2lox and R2c Proteins
J. Inorg. Biochem. 162, 164-177 (2016)
431. C. He, H. Ogata, W. Lubitz
Elucidation of the Heme Active Site Electronic Structure Affecting the Unprecedented Nitrite Dismutase Activity of the Ferriheme *b* Proteins, the Nitrophorins
Chem. Sci. 7, 5332-5340 (2016)
432. F. Wang, R. Büchel, A. Savitsky, M. Zalibera, D. Widmann, S. E. Pratsinis, W. Lubitz, F. Schüth
***In situ* EPR Study of the Redox Properties of CuO-CeO₂ Catalysts for the Preferential CO Oxidation (PROX)**
ACS Catal. 6, 3520-3530 (2016)
433. M. Malferrari, A. Savitsky, M. D. Mamedov, G. E. Milanovsky, W. Lubitz, K. Möbius, A. Y. Semenov, G. Venturoli
Trehalose Matrix Effects on Charge-recombination Kinetics in Photosystem I of Oxygenic Photosynthesis at Different Dehydration levels
Biochim. Biophys. Acta Bioenerg. 1857, 1440-1454 (2016)
434. J. Milić, M. Zalibera, I. Pochorovski, N. Trapp, J. Nomrowski, D. Neshchadin, L. Ruhlmann, C. Boudon, O. S. Wenger, A. Savitsky, W. Lubitz, G. Gescheidt, F. Diederich
Paramagnetic Molecular Grippers: The Elements of Six-State Redox Switches
J. Phys. Chem. Lett. 7, 2470–2477 (2016)
435. K. Möbius, A. Savitsky, W. Lubitz, M. Plato
Möbius-Hückel Topology Switching in Expanded Porphyrins: EPR, ENDOR, and DFT Studies of Doublet and Triplet Open-Shell Systems
Appl. Magn. Res. 47, 757–780 (2016)
436. J.A. Birrell, C. Laurich, E. Reijerse, H. Ogata, W. Lubitz
Importance of Hydrogen Bonding in Fine Tuning the [2Fe-2S] Cluster Redox Potential of HydC from *Thermotoga maritima*
Biochemistry 55, 4344-4355 (2016)

437. J. A. Birrell, K. Wrede, K. Pawlak, P. Rodriguez-Marciá, O. Rüdiger, E., W. Lubitz
Artificial Maturation of the Highly Active Heterodimeric [FeFe] Hydrogenase from *Desulfovibrio desulfuricans* ATCC 7757
Isr. J. Chem. 56, 852-863 (2016)
438. P. Rodriguez-Maciá, N. Priyadarshani, A. Dutta, C. Weidenthaler, W. Lubitz, W.J. Shaw, O. Rüdiger
Covalent Attachment of the Water-insoluble Ni(PCy₂N^{Phe}₂)₂ Electrocatalyst to Electrodes Showing Reversible Catalysis in Aqueous Solution
Electroanalysis 28, 2452-2458 (2016)
439. H. Ogata, W. Lubitz, Y. Higuchi
Structure and Function of [NiFe] Hydrogenase
J. Biochem. 160, 251-258 (2016)
440. M. Mirmohades, A. Adamska-Venkatesh, C. Sommer, E. Reijerse, R. Lomoth, W. Lubitz, L. Hammarström
Following [FeFe] Hydrogenase Active Site Intermediates by Time-Resolved Mid-IR Spectroscopy
J. Phys. Chem. Lett. 7, 3290-3293 (2016)
441. W. Lubitz, T. Lohmiller, N. Cox
Water Oxidation and Oxygen Evolution in Photosynthesis. An Enzyme that Changed the World
Bunsen-Magazin 6, 216-223 (2016)
442. G. Caserta, A. Adamska-Venkatesh, L. Pecqueur, M. Atta, V. Artero, S. Roy, E. Reijerse, W. Lubitz, M. Fontecave
Chemical Assembly of Multiple Metal Cofactors: The Heterologously Expressed Multidomain [FeFe]-hydrogenase from *Megasphaera elsdenii*
Biochim. Biophys. Acta 1857, 1734-1740 (2016)
443. M. Malferrari, A. Savitsky, W. Lubitz, K. Möbius, G. Venturoli, G.
Protein Immobilization Capabilities of Sucrose and Trehalose Glasses: The Effect of Protein/Sugar Concentration Unraveled by High-field EPR
J. Phys. Chem. Lett. 7, 4871-4877 (2016)
444. C. Sommer, A. Adamska-Venkatesh, K. Pawlak, J. Birrell, E. Reijerse, W. Lubitz
Proton Coupled Electron Transfer within the H-Cluster as an Essential Step in the Catalytic Cycle of [FeFe] Hydrogenases
J. Am. Chem. Soc. 139, 1440-1443 (2017)

445. S. Sinnecker, W. Lubitz
Probing the Electronic Structure of Bacteriochlorophyll Radical Ions – A Theoretical Study of the Effect of Substituents on Hyperfine Parameters
Photochem. Photobiol. 93, 755-761 (2017)
446. T. Lohmiller, M.A. Vibhute, W. Lubitz, A. Savitsky
Multifrequency Multiresonance EPR Investigation of Halogen-bonded Complexes Involving Neutral Nitroxide Radicals
Z. Phys. Chem. 231, 867-886 (2017)
447. P. Rodriguez-Maciá, J. A. Birrell, W. Lubitz, O. Rüdiger
Electrochemical Investigations on the Inactivation of the [FeFe]-Hydrogenase from *Desulfovibrio desulfuricans* by O₂ or Light Under Hydrogen Producing Conditions
ChemPlusChem 82, 540-545 (2017)
448. E. Decaneto, W. Lubitz, H. Ogata
Structural Studies of Matrix Metalloproteinase by X-ray Diffraction
Methods Mol. Biol. 1579, 49-60 (2017)
449. E. Reijerse, C. Pham, V. Pelmeshnikov, R. Gilbert-Wilson, A. Adamska-Venkatesh, J. Siebel, L. Gee, Y. Yoda, K. Tamasaku, W. Lubitz, T. Rauchfuss, S. Cramer
Direct Observation of an Iron-bound Terminal Hydride in [FeFe]-hydrogenase by Nuclear Resonance Vibrational Spectroscopy
J. Am. Chem. Soc. 139, 4306-4309 (2017)
450. F. Zhao, F. Conzuelo, V. Hartmann, H. Li, S. Stapf, M.M. Nowaczyk, M. Rögner, N. Plumeré, W. Lubitz, W. Schuhmann
A Novel Versatile Microbiosensor for Local Hydrogen Detection by Means of Scanning Photoelectrochemical Microscopy
Biosensors & Bioelectronics 94, 433–437 (2017)
451. S. Kacprzak, I. Nijmona, A. Renz, J. Feng, E. Reijerse, W. Lubitz, N. Krauß, P. Scheerer, S. Nagano, T. Lamparter, S. Weber
Spatial Arrangement of Dimer Subunits in the Full-Length Bacterial Phytochrome Agp1 as Determined by PELDOR Spectroscopy
J. Biol. Chem. 292, 7598-7606 (2017)
452. G. Caserta, L. Pecqueur, A. Adamska-Venkatesh, C. Papini, S. Roy, V. Artero, M. Atta, E. Reijerse, W. Lubitz, M. Fontecave
Structural and Functional Characterization of the Hydrogenase Maturation HydF Protein
Nat. Chem. Biol. 13, 779-784 (2017)

453. N. Cox, A. Nalepa, W. Lubitz, A. Savitsky
ELDOR-detected NMR (EDNMR): A General, Robust Method for Electron-nuclear Hyperfine Spectroscopy
J. Magn. Reson. 280, 63-78 (2017)
454. V. Engelbrecht, P. Rodríguez-Maciá, J. Esselborn, A. Sawyer, A. Hemschemeier, O. Rüdiger, W. Lubitz, M. Winkler, T. Happe
The Structurally Unique Photosynthetic *Chlorella variabilis* NC64A Hydrogenase Does Not Interact Directly With Plant-type Ferredoxins
Biochim. Biophys. Acta Bioenerg. 1858, 771-778 (2017)
455. J. Birrell, E. Reijerse, O. Rüdiger, W. Lubitz
Semisynthetic Hydrogenases Propel Biological Energy Research into a New Era
Joule 1, 61-76 (2017)
456. E. A. Lukina, E. Suturina, E. Reijerse, W. Lubitz, L. V. Kulik
Spin Dynamics of Light-induced Charge Separation in Composites of Semiconducting Polymers and PCBM Revealed by Q-band Pulse EPR
Phys. Chem. Chem. Phys. 33, 22141-22152 (2017)
457. P. Rodriguez-Maciá, K. Pawlak, O. Rüdiger, E. Reijerse, W. Lubitz, J. Birrell
Inter-cluster Redox Coupling Influences Protonation at the H-cluster in [FeFe] Hydrogenases
J. Am. Chem. Soc. 139, 15122-15134 (2017)
458. P. Rodriguez-Maciá, E. Reijerse, W. Lubitz, J.A. Birrell, O. Rüdiger
Spectroscopic Evidence of Reversible Disassembly of the [FeFe] Hydrogenase Active Site
J. Phys. Chem. Lett. 8, 3834-3839, (2017)
459. T. Lohmiller, V. Krewald, A. Sedoud, A. W. Rutherford, F. Neese, W. Lubitz, D. A. Pantazis, N. Cox
The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived μ -Hydroxo Bridge
J. Am. Chem. Soc. 139, 14412-14424 (2017)
460. A. Nalepa, M. Malferrari, W. Lubitz, G. Venturoli, K. Möbius, A. Savitsky
Local Water Sensing: Water Exchange in Bacterial Photosynthetic Reaction Centers Embedded in a Trehalose Glass Studied by Multiresonance EPR
Phys. Chem. Chem. Phys. 460, 28388-28400 (2017)

461. V. Pelmeshnikov, J. Birrell, C. Pham, N. Mishra, H. Wang, C. Sommer, E. Reijerse, C.P. Richers, K. Tamasaku, Y. Yoda, T. Rauchfuss, W. Lubitz, S. Cramer
Reaction Coordinate Leading to H₂ Production in [FeFe]-Hydrogenase Identified by NRVs and DFT
J. Am Chem. Soc. 139, 16894-16902 (2017)
462. K. Möbius, W. Lubitz, A. Savitsky
Jim Hyde and the ENDOR Connection: A Personal Account
Appl. Magn. Reson. 48, 1149-1183 (2017)
463. J. W. Sidabras, E. J. Reijerse, W. Lubitz
Uniform Field Re-Entrant Cylindrical TE_{01U} Cavity for Pulse Electron Paramagnetic Resonance Spectroscopy at Q-band
Appl. Magn. Reson. 48, 1301-1314 (2017)
464. L. Kertess, W. Lubitz, O. Rüdiger, A. Adamska, P. Rodriguez, T. Happe
Influence of the [4Fe-4S] Cluster Coordinating Cysteines on Active Site Maturation and Catalytic Properties of *C. reinhardtii* [FeFe]-Hydrogenase
Chem. Sci. 8, 8127-8137, (2017)
465. O. Lampret, A. Adamska-Venkatesh, H. Konegger, F. Wittkamp, U.-P. Apfel, E. J. Reijerse, W. Lubitz, O. Rüdiger, T. Happe, M. Winkler
Interplay Between the CN⁻ Ligands and the Secondary Coordination Sphere of the H-cluster in [FeFe]-hydrogenases
J. Am. Chem. Soc. 139, 18222-18230 (2017)
466. L. Kertess, F. Wittkamp, C. Sommer, J. Esselborn, O. Ruediger, E. Reijerse, E. Hofmann, W. Lubitz, M. Winkler, T. Happe, U.-P. Apfel
Chalcogenide substitution in the [2Fe]-cluster of [FeFe]-hydrogenases conserves high enzymatic activity
Dalton Trans. 46, 16958-16958 (2017)
467. E. Decaneto, T. Vasilevskaya, Y. Kutin, H. Ogata, M. Grossman, I. Sagi, M. Havenith, W. Lubitz, W. Thiel, N. Cox
Solvent Water Interactions Within The Active Site of the Membrane Type I Matrix Metalloproteinase
Phys. Chem. Chem. Phys. 19, 30316-30331 (2017)
468. M. Zalibera, D.S. Krylov, D. Karagiannis, P.-A. Will, F. Ziegls, S. Schiemenz, W. Lubitz, S. Reineke, A. Savitsky, A.A. Popov
Thermally-activated Delayed Fluorescence in Y₃N@C₈₀ Endohedral Fullerene: Time Resolved Luminescence and Electron Paramagnetic Resonance Studies
Angew. Chem. Int. Ed. 57, 277-281 (2018)
Angew. Chem. 130, 283-287 (2018)

469. J. Morton, M. Chrysinia, V.S. Craig, F. Akita, Y. Nakajima, W. Lubitz, N. Cox, J.-R. Shen, E. Krausz
Structured Near-infrared Magnetic Circular Dichroism spectra of the Mn₄CaO₅ Cluster of PS II in *T. vulcanus* are Dominated by Mn(IV) d-d 'spin-flip' Transitions
Biochim. Biophys. Acta Bioenerg. 1859, 88-98 (2018)
470. S. Rumpel, E. Ravera, C. Sommer, E. Reijerse, C. Farés, C. Luchinat, W. Lubitz
¹H NMR Spectroscopy of [FeFe] Hydrogenase: Insight into the Electronic Structure of the Active Site
J. Am. Chem. Soc. 140, 131-134 (2018)
471. N. Chongdar, J. A. Birrell, K. Pawlak, C. Sommer, E. J. Reijerse, W. Lubitz, H. Ogata
Unique Spectroscopic Properties of the H-cluster in a Putative Sensory [FeFe] Hydrogenase
J. Am. Chem. Soc. 140, 1057-1068 (2018)
472. J. Milić, M. Zalibera, D. Talaat, J. Nomrowski, N. Trapp, L. Ruhlmann, C. Boudon, O. S. Wenger, A. Savitsky, W. Lubitz, F. Diederich
Photoredox-Switchable Resorcin[4]arene Cavitands: Radical Control of Molecular Gripping Machinery via Hydrogen Bonding
Chem. Eur. J. 24, 1431-1440 (2018)
473. K. Wiegand, M. Winkler, S. Rumpel, D. Kannchen, S. Rexroth, T. Hase, C. Farès, T. Happe, W. Lubitz, M. Rögner
Rational Redesign of the Ferredoxin-NADP⁺-Oxidoreductase / Ferredoxin-interaction for Photosynthesis-dependent H₂-production
Biochem. Biophys. Acta Bioenergetics 1859, 253-262 (2018)
474. A. A. Oughli, A. Ruff, N. Priyadarshani Boralugodage, P. Rodríguez-Maciá, N. Plumeré, W. Lubitz, W. J. Shaw, W. Schuhmann, O. Rüdiger
Dual Properties of a Hydrogen Oxidation Ni-catalyst within a Polymer Promote Self-defense Against Oxygen
Nat. Commun. 9, 864 (2018)
475. S. Rumpel, C. Sommer, E. Reijerse, C. Farès, W. Lubitz
Direct Detection of the Terminal Hydride Intermediate in [FeFe] Hydrogenase by NMR Spectroscopy
J. Am. Chem. Soc. 140, 3863-3866 (2018)
476. V. Haskamp, S. Karrie, T. Mingers, F. Alberge, A. Magalon, K. Müller, E. Bill, W. Lubitz, K. Kleeberg, P. Schweyen, M. Bröring, W. Sassen, R. Köster, M. Jahn, D. Jahn
The Radical SAM Protein HemW is a Heme Chaperone
J. Biol. Chem. 293, 2558-2572 (2018)

477. G. Caserta, C. Papini, A. Adamska-Venkatesh, L. Pecqueur, C. Sommer, E. Reijerse, W. Lubitz, Wolfgang; C. Gauquelin, I. Meynial-Salles, D. Pramanik, V. Artero, M. Atta, M. del Barrio, B. Faivre, V. Fourmond, C. Léger, M. Fontecave
Engineering an [FeFe]-hydrogenase: Do Accessory Clusters Influence O₂ Resistance and Catalytic Bias?
J. Am. Chem. Soc. 140, 5516-5526 (2018)
478. C. Sommer, C. P. Richers, W. Lubitz, T. B. Rauchfuss; E. J. Reijerse
[RuRu] Analogue of [FeFe]-Hydrogenase Traps the Key Hydride Intermediate in the Enzyme's Catalytic Cycle
Angew. Chem. Int. Ed. 57, 5429-5432 (2018)
479. C. Sommer, S. Rumpel, S. Roy, C. Farès, V. Artero, M. Fontecave, E. Reijerse, W. Lubitz
Spectroscopic Investigations of a Semi-synthetic [FeFe] Hydrogenase with Propane Di-selenol as Bridging Ligand in the Binuclear Subsite
J. Biol. Inorg. Chem. 23, 481-491 (2018)
480. M.Y. Okamura, W. Lubitz, J.P. Allen
Remembering George Feher (1924-2017)
Photosyn. Res. 137, 361-375 (2018)
481. P. Rodriguez-Macià, E.J. Reijerse, M. van Gaste, S. DeBeer, W. Lubitz, O. Rüdiger, J.A. Birrell
Sulfide Protects [FeFe] Hydrogenase From O₂
J. Am. Chem. Soc. 140, 9346-9350 (2018). Correction published: J. Am. Chem. Soc., 140, 17806 (2018)
482. A. Agostini, J. Niklas, T. Schulte, M. Di Valentin, M. Bortolus, E. Hofmann, W. Lubitz, D. Carbonera
Changing the Site Energy of Per614 in Peridinin-Chlorophyll a-Protein Does Not Alter Its Capability of Chl Triplet Quenching
Biochem. Biophys. Acta Bioenerg. 1859, 612-618 (2018)
483. A. A. Oughli, M. Vélez, J. Birrell, W. Schuhmann, W. Lubitz, N. Plumeré, O. Rüdiger
Viologen-modified Electrodes for Protection of Hydrogenases from High Potential Inactivation while Performing H₂ Oxidation at Low Overpotential
Dalton Trans. 47, 10685-10691 (2018)
484. Li, H., Buesen, D., Williams, R., Henig, J., Stapf, S., Mukherjee, K., Freier, E., Lubitz, W., Winkler, M.; Happe, T.; Plumere, N., **Preventing the Coffee-Ring Effect and Aggregate Sedimentation by *in situ* Gelation of Monodisperse Materials**
Chem. Sci. 9, 7596-7605 (2018)

485. A. Ruff, J. Szczesny, N. Marković, F. Conzuelo, S. Zacarias, I. A. C. Pereira, W. Lubitz, W. Schuhmann
A Fully Protected Hydrogenase/Polymer Based Bioanode for High-performance Hydrogen/Glucose Biofuel Cells
Nat. Commun. 9, 3675, doi: 10.1038/s41467-018-06106-3 (2018)
486. J. Szczesny, N. Marković, F. Conzuelo, S. Zacarias, I.A.C. Pereira, W. Lubitz, N. Plumeré, W. Schuhmann, A. Ruff
A Gas Breathing Hydrogen/Air Biofuel Cell Comprising a Redox Polymer/Hydrogenase-based Bioanode
Nat. Commun. 9, 4715, doi: 10.1038/s41467-018-07137-6 (2018)
487. N. Siemer, A. Lüken, M. Zalibera, J. Frenzel, D. Muñoz-Santiburcio, A. Savitsky, W. Lubitz, M. Muhler, D. Marx, J. Strunk
Atomic Scale Explanation of O₂ Activation at the Au-TiO₂ Interface
J. Am. Chem. Soc. 140, 18082-18092 (2018)
488. K. Möbius, W. Lubitz, N. Cox, A. Savitsky
Biomolecular EPR Meets NMR at High Magnetic Fields
Magnetochemistry, 4, 50, doi: 10.3390/magnetochemistry4040050 (2018)
489. E. A. Lukina, E. Reijerse, W. Lubitz, L. V. Kulik
Spin-dependent Recombination of the Charge-transfer State in Photovoltaic Polymer/Fullerene Blends
Mol. Phys. 117, 2654-2663 (2019)
490. J. M. Schuller, J. A. Birrell, H. Tanaka, T. Konuma, H. Wulfhorst, N. Cox, S. K. Schuller, J. Thiemann, W. Lubitz, P. Sétif, T. Ikegami, B. D. Engel, G. Kurisu, M. M. Nowaczyk
Structural Adaptations of Photosynthetic Complex I Enable Ferredoxin-Dependent Electron Transfer
Science 363, 257-260 (2019)
491. P. Rodríguez-Maciá, L. Kertess, J. Burni, J. A. Birrell, E. Hofman, W. Lubitz, T. Happe, O. Rüdiger
His-Ligation to the [4Fe-4Fe] Sub-Cluster Tunes the Catalytic Bias of the [FeFe] Hydrogenase
J. Am. Chem. Soc. 141, 472-481(2019)
492. A. Nalepa, K. Möbius, M. Plato, W. Lubitz, A. Savitsky
Nitroxide Spin Labels – Magnetic Parameters and Hydrogen-Bond Formation: A High-field EPR and EDNMR Study
Appl. Magn. Reson. 50, 1-16 (2019)

493. M. S. Sim, H. Ogata, W. Lubitz, J. F. Adkins, A. L. Sessions, V.J Orphan, S. E. McGlynn
Role of APS Reductase in Biogeochemical Sulfur Isotope Fractionation
Nat. Commun. 10:44, doi: /10.1038/s41467-018-07878-4 (2019)
494. A. Ruff, S. Janke, J. Szczesny, S. Alsaoub, I. Ruff, W. Lubitz, W. Schuhmann,
Polymer-bound DuBois-type Molecular H₂ Oxidation Ni Catalysts are Protected by Redox Polymer Matrices.
ACS Appl. Energy Mater. 2, 2921-2929 (2019)
495. C. Papini, C. Sommer, L. Pecqueur, D. Pramanik, S. Roy, E. J. Reijerse, F. Wittkamp, V. Artero, W. Lubitz, M. Fontecave
A Bioinspired Artificial [FeFe]-hydrogenase with a Synthetic H-Cluster
ACS Catal. 9, 4495–4501 (2019)
496. W. Lubitz, M. Chrysina, N. Cox
Water Oxidation in Photosystem II
Photosyn. Res. 142, 105-125 (2019)
497. M. Chrysina, E. Heyno, Y. Kutin, M. Reus, H. Nilsson, M. M. Nowaczyk, S. DeBeer, F. Neese, J. Messinger W. Lubitz, N. Cox
Five-coordinate Mn(IV) intermediate in the activation of nature's water splitting cofactor
Proc. Natl. Acad. Sci. USA 116, 16841–16846 (2019)
498. M. L. K. Sanchez, C. Sommer, E. Reijerse, J.A. Birrell, W. Lubitz, R. B. Dyer
Investigating the Kinetic Competency of CrHydA1 [FeFe] Hydrogenase Intermediate States via Time-resolved Infrared Spectroscopy
J. Am. Chem. Soc. 141, 16064-16070 (2019)
499. J. W. Sidabras, J. Duan, M. Winkler, T. Happe, R. Hussein, A. Zouni, D. Suter, A. Schnegg, W. Lubitz, E. Reijerse
Extending Electron Paramagnetic Resonance to nano-Liter Volume Protein Single-Crystals Using a Self-Resonant micro-Helix
Sci. Adv. 5: eaay1394 (2019)
500. E. Reijerse, V. Pelmeshnikov, J. A. Birrell, C. P. Richers, T. B. Rauchfuss, S. P. Cramer, W. Lubitz
Asymmetry in the Ligand Coordination Sphere of the [FeFe] Hydrogenase Active site is Reflected in the Magnetic Spin Interactions of the Aza-Propane-Dithiolate Ligand
J. Phys. Chem. Lett. 10, 6794-6799 (2019)

501. Y. Kutin, N. Cox, W. Lubitz, A. Schnegg, O. Rüdiger
In Situ EPR Characterization of a Cobalt Oxide Water Oxidation Catalyst at Neutral pH
Catalysts 9, 926; doi:10.3390/catal9110926 (2019)
502. N. Cox, D. Pantazis, W. Lubitz
Current Understanding of the Mechanism of Water Oxidation in Photosystem II and Its Relation to XFEL Data
Annual Reviews of Biochemistry 89, 795-820 (2020)
503. J. A. Birrell, V. Pelmeshnikov, N. Mishra, H. Wang, Y. Yoda, K. Tamasaku, T. B. Rauchfuss, S. P. Cramer, W. Lubitz, S. DeBeer
Spectroscopic and Computational Evidence that [FeFe] Hydrogenases Operate Exclusively with CO-Bridged Intermediates
J. Am. Chem. Soc. 142, 222-232 (2020)
504. N. Chongdar, K. Pawlak, O. Rüdiger, E. J. Reijerse, P. Rodríguez-Maciá, W. Lubitz, J. A. Birrell, H. Ogata
Spectroscopic and biochemical insight into an electron-bifurcating [FeFe] hydrogenase
JBIC Journal of Biological Inorganic Chemistry 25, 135–149 (2020)
505. H. Li, U. Münchberg, A.A. Oughli, D. Buesen, W. Lubitz, E. Freier, N. Plumeré
Suppressing hydrogen peroxide generation to achieve oxygen-insensitivity of a [NiFe] hydrogenase in redox active films
Nat Commun 11:920; doi: 10.1038/s41467-020-14673-7 (2020)
506. E. Reijerse, J. A. Birrell, W. Lubitz
Spin Polarization Reveals the Coordination Geometry of the [FeFe] Hydrogenase Active Site in Its CO-Inhibited State
J. Phys. Chem. Lett. 11, 4597-4602 (2020)
507. L. Kang, B. Wang, Q. Bing, M. Zalibera, R. Büchel, R. Xu, Q. Wang, Y. Liu, D. Gianolio, C. C. Tang, E. K. Gibson, M. Danaie, C. Allen, K. Wu, S. Marlow, L. Sun, Q. He, S. Guan, A. Savitsky, J.J. Velasco-Vélez, J. Callison, C. W. M. Kay, S. E. Pratsinis, W. Lubitz, J. Liu, F. R. Wang
Adsorption and activation of molecular oxygen over atomic copper (I/II) site on ceria
Nat Commun 11:4008; doi: 10.1038/s41467-020-17852-8 (2020)
508. K. Möbius, A. Savitsky, M. Malferrari, F. Francia, M.D. Mamedov, A.Y. Semenov, W. Lubitz, G. Venturoli
Soft Dynamic Confinement of Membrane Proteins by Dehydrated Trehalose Matrices: High-Field EPR and Fast-Laser Studies
Appl. Magn. Reson. 51, 773-850 (2020)

509. M. Massmig, E. Reijerse, J. Krausze, C. Laurich, W. Lubitz, D. Jahn, J. Moser
Carnitine metabolism in the human gut: characterization of the two-component carnitine monooxygenase CntAB from *Acinetobacter baumannii*
J. Biol. Chem. 295, 13065-13078 (2020)
510. J. Szczesny, J. A. Birrell, F. Conzuelo, W. Lubitz, A. Ruff, W. Schuhmann
Redox-Polymer-Based High-Current-Density Gas-Diffusion H₂-Oxidation Bioanode Using [FeFe] Hydrogenase from *Desulfovibrio desulfuricans* in a Membrane-free Biofuel Cell
Angew. Chem. Int. Ed. 59, 16506–16510 (2020)
511. M. L. K. Sanchez, S. E. Konecny, S. M. Narehood, E. J. Reijerse, W. Lubitz, J. A. Birrell, R. B. Dyer
The Laser-Induced Potential Jump: A Method for Rapid Electron Injection into Oxidoreductase Enzymes
J. Phys. Chem. B 124, 8750-8760 (2020)
512. B. P. Jagilinki, S. Ilic, C. Trncik, A. M. Tyryshkin, D. H. Pike, W. Lubitz, E. Bill, O. Einsle, J. A. Birrell, B. Akabayov, D. Noy, V. Nanda
In vivo biogenesis of a de novo designed iron-sulfur protein
ACS Synth. Biol. 9, 3400-3407 (2020)
513. M. Zalibera, F. Ziegls, S. Schiemenz, V. Dubrovin, W. Lubitz, A. Savitsky, S. H. M. Deng, X.-B. Wang, S. M. Avdoshenko, A. A. Popov
Metallofullerene photoswitches driven by photoinduced fullerene-to-metal electron transfer
Chem. Sci. 12, 7818-7838 (2021)
514. V. Pelmeshnikov, J. A. Birrell, L. B. Gee, C. P. Richers, E. J. Reijerse, H. Wang, S. Arragain, N. Mishra, Y. Yoda, H. Matsuura, L. Li, K. Tamasaku, T. B. Rauchfuss, W. Lubitz, S. P. Cramer
Vibrational Perturbation of the [FeFe] Hydrogenase H-Cluster Revealed by ¹³C²H-ADT Labeling
J. Am. Chem. Soc. 143, 8237-8243 (2021)
515. H. Ogata, W. Lubitz
Hydrogenases Structure and Function
in Jez Joseph (eds.) Encyclopedia of Biological Chemistry, 3rd edition, Vol. 2, pp. 66 - 73 (2021), Oxford: Elsevier.
516. I. Caspy, E. Neumann, M. Fadeeva, V. Liveanu, A. Savitsky, A. Frank, Y. L. Kalisman, Y. Shkolnisky, O. Murik, H. Treves, V. Hartmann, M. M. Nowaczyk, W. Schuhmann, M. Rögner, I. Willner, A. Kaplan, G. Schuster, N. Nelson, W. Lubitz, R. Nechushtai
Cryo-EM photosystem I structure reveals adaptation mechanisms

to extreme high light in *Chlorella ohadii*

Nature Plants 7, 1314–1322 (2021)

517. J. Birrell, P. Rodriguez-Maciá, E. Reijerse, M.A. Martini, W. Lubitz
The catalytic cycle of [FeFe] hydrogenase: A tale of two sites
Coord. Chem. Rev. 449, 214191 (2021)
518. K Möbius, W Lubitz, A Savitsky
CIDEP-Enhanced ENDOR of short-lived radicals. Recollections of first joint experiments with Renad Sagdeev
Russian Chemical Bulletin 70, 2445-2456 (2021)
519. N. Cox, J. A. Birrell, W. Lubitz
Molecular Concepts of Water Splitting and Hydrogen Production: Nature's Approach
in Chemical Energy Storage, 2nd Edition; R. Schlögl Ed., de Gruyter, Chpt 8, pp. 183 – 241 (2022)
520. A. Lielpetere, J. M. Becker, J. Szczesny, F. Conzuelo, A. Ruff, J. A. Birrell, W. Lubitz, W. Schuhmann **Enhancing the catalytic current response of H₂ oxidation gas diffusion bioelectrodes using an optimized viologen-based redox polymer and [NiFe] hydrogenase**
Electrochemical Science Advances 2, e2100100 (2022)
521. M. L. K. Sanchez, S. Wiley, E. Reijerse, W. Lubitz, J. A. Birrell, R. B. Dyer
Time-Resolved Infrared Spectroscopy Reveals the pH-Independence of the First Electron Transfer Step in the [FeFe] Hydrogenase Catalytic Cycle
J. Phy. Chem. Lett. 13, 5986-5990 (2022)
522. C. Furlan, N. Chongdar, P. Gupta, W. Lubitz, H. Ogata, J. N. Blaza, J. A. Birrell
Structural insight on the mechanism of an electron-bifurcating [FeFe] hydrogenase
Elife 11, e79361 (2022)
523. A. Savitsky, A. Nalepa, T. Petrenko, M. Plato, K. Möbius, W. Lubitz
Hydrogen-bonded complexes of neutral nitroxide radicals with 2-propanol studied by multifrequency EPR/ENDOR
Applied Magnetic Resonance 53, 1239-1263 (2022)

524. J. Niklas, A. Agostini, D. Carbonera, M. Di Valentin, W. Lubitz
Primary donor triplet states of Photosystem I and II studied by Q-band pulse ENDOR spectroscopy
Photosyn. Res. 152, 213 – 234 (2022)
525. F. Piskol, K. Neubauer, M. Eggers, L. M. Bode, J. Jasper, A. Slusarenko, E. Reijerse, W. Lubitz, D. Jahn, J. Moser
Two-component carnitine monooxygenase from Escherichia coli: functional characterization, inhibition and mutagenesis of the molecular interface
Bioscience Reports 42, BSR20221102 (2022)
526. W. Lubitz, D. A. Pantazis, N. Cox
Water oxidation in oxygenic photosynthesis studied by magnetic resonance techniques
FEBS Lett. 597, 6 - 29 (2023)