

Publications of Wolfgang Lubitz

1. Lubitz, W.; Dinse, K. P.; Möbius, K.; Biehl, R. Fluorine and Proton ENDOR of Aromatic Radicals in Solution. *Chem. Phys.* **1975**, *8* (3), 371–383.
2. Biehl, R.; Lubitz, W.; Möbius, K.; Plato, M. Observation of Deuterium Quadrupole Splittings of Aromatic Free Radicals in Liquid Crystals by ENDOR and TRIPLE Resonance. *J. Chem. Phys.* **1977**, *66* (5), 2074–2078.
3. Biehl, R.; Hinrichs, K.; Kurreck, H.; Lubitz, W.; Mennenga, U.; Roth, K. ESR, NMR and ENDOR Studies of Partially Deuterated Phenyl Substituted Anthracenes. π - σ Delocalization. *J. Am. Chem. Soc.* **1977**, *99* (13), 4278–4286.
4. Lubitz, W.; Biehl, R.; Möbius, K. Sodium and Proton ENDOR and Triple-Resonance Experiments on Biphenyl and Fluorenone Ion-Pairs in Solution. *J. Magn. Reson.* **1977**, *27* (3), 411–417.
5. Biehl, R.; Hass, C.; Kurreck, H.; Lubitz, W.; Oestreich, S. ESR and ENDOR Studies of Partially Deuterated and Chlorinated Phenalenyls - New Synthetic Pathways. *Tetrahedron* **1978**, *34* (4), 419–424.
6. Kirste, B.; Kurreck, H.; Lubitz, W.; Schubert, K. ^{13}C ENDOR Studies of Organic Doublet and Triplet-State Molecules. *J. Am. Chem. Soc.* **1978**, *100* (8), 2292–2299.
7. Fey, H.-J.; Lubitz, W.; Zimmermann, H.; Plato, M.; Möbius, K.; Biehl, R. ^{13}C -ENDOR and Proton-ENDOR Studies of ^{13}C -Labeled Organic Radicals. *Z. Naturforsch.* **1978**, *33a* (5), 514–522.
8. Lubitz, W.; Broser, W.; Kirste, B.; Kurreck, H.; Schubert, K. ^{13}C -ENDOR and ^1H -ENDOR Studies of A Phenoxy Type Radical. *Z. Naturforsch.* **1978**, *33* (9), 1072–1076.
9. Fey, H. J.; Kurreck, H.; Lubitz, W. ENDOR Studies of [6]Helicene Anion Radical. *Tetrahedron* **1979**, *35* (7), 905–907.
10. Lubitz, W.; Plato, M.; Möbius, K.; Biehl, R. Alkali and H ENDOR on Aromatic Ion-Pairs in Solution. An INDO Approach. *J. Phys. Chem.* **1979**, *83* (26), 3402–3413.
11. Kirste, B.; Kurreck, H.; Lubitz, W.; Zimmermann, H. ^1H , ^2H and ^{13}C ENDOR Studies of Labeled Bis-(biphenylenyl)propenyl Type Radicals in Isotropic Solutions and in Liquid-Crystals. *J. Am. Chem. Soc.* **1980**, *102* (2), 817–825.
12. Lubitz, W.; Nyrönen, T. ^{14}N and ^1H ENDOR and TRIPLE Resonance on Azaaromatic Radicals Produced by Sodium Reduction in Liquid Ammonia. *J. Magn. Res.* **1980**, *41* (1), 17–29.
13. Plato, M.; Lubitz, W.; Möbius, K. A Solution ENDOR Sensitivity Study of Various Nuclei in Organic Radicals. *J. Phys. Chem.* **1981**, *85* (9), 1202–1219.
14. Lubitz, W.; Lendzian, F.; Möbius, K. ^{14}N and ^1H Electron Nuclear Multiple Resonance Experiments on Bacteriochlorophyll *a* Anion Radicals in Solution. *Chem. Phys. Lett.* **1981**, *81* (2), 235–241.
15. Lendzian, F.; Lubitz, W.; Scheer, H.; Bubenzer, C.; Möbius, K. *In Vivo* Liquid Solution ENDOR and TRIPLE Resonance of Bacterial Photosynthetic Reaction Centers of *Rhodospseudomonas sphaeroides* R-26. *J. Am. Chem. Soc.* **1981**, *103* (15), 4635–4637.
16. Bock, M.; Lubitz, W.; Kurreck, H.; Fenner, H.; Grauert, R. ^{14}N and ^1H ENDOR and TRIPLE Resonance Experiments of Flavin and Thiaflavin Radical Cations in Liquid Solution. *J. Am. Chem. Soc.* **1981**, *103* (18), 5567–5568.
17. Lubitz, W.; Lendzian, F.; Möbius, K. The Bacteriopheophytin *a* Anion Radical. A Solution ENDOR and TRIPLE Resonance Study. *Chem. Phys. Lett.* **1981**, *84* (1), 33–38.
18. Möhl, W.; Winscom, C. J.; Plato, M.; Möbius, K.; Lubitz, W. Examination of the Conditions for ENDOR-in-Solution Experiments on Transition-Metal Complexes. *J. Phys. Chem.* **1982**, *86* (1), 149–152.
19. Möbius, K.; Plato, M.; Lubitz, W. Radicals in Solution Studied by ENDOR and TRIPLE Resonance Spectroscopy. *Phys. Rep.* **1982**, *87* (4), 171–208.
20. Hoff, A. J.; Lendzian, F.; Möbius, K.; Lubitz, W. Proton and Nitrogen Electron Nuclear Double and Triple Resonance of the Chlorophyll *a* Anion in Liquid Solution. *Chem. Phys. Lett.* **1982**, *85* (1), 3–8.
21. Lendzian, F.; Möbius, K.; Lubitz, W. The Pheophytin *a* Anion Radical. ^{14}N - and ^1H -ENDOR and TRIPLE Resonance in Liquid Solution. *Chem. Phys. Lett.* **1982**, *90* (5), 375–381.
22. Möbius, K.; Fröhling, W.; Lendzian, F.; Lubitz, W.; Plato, M.; Winscom, C. J. Multiple Magnetic-Resonance Studies on Organic Molecules in Their Ground and Excited States. *J. Phys. Chem.* **1982**, *86* (23), 4491–4507.
23. Winscom, C. J.; Lubitz, W.; Diegruber, H.; Mösel, R. In *Metal Microstructures in Zeolites*; Jacobs, P. A., et al., Eds. Elsevier Scientific Publishing Company: Amsterdam, **1982**; pp 15–21.
24. Lubitz, W.; Lendzian, F.; Scheer, H.; Plato, M.; Möbius, K. Electron–Nuclear Multiple Resonance Studies on Primary Product of Bacterial Photosynthesis. In *Photochemistry and Photobiology*; Zewail, A. H., Ed. Harwood Academic Publishers: New York, **1983**; Vol. 2, pp 1057–1069.
25. Kaim, W.; Lubitz, W. Radical Products in Single Electron Transfer Reactions of Lithium Triethylhydridoborate Detected by ESR and Multinuclear (^1H , ^{10}B , ^{11}B , ^{14}N)-ENDOR Spectroscopy. *Angew. Chem., Int. Ed.* **1983**, *22* (11), 892–893.
26. Bock, H.; Hierholzer, B.; Kurreck, H.; Lubitz, W. ^{29}Si -E(lectron)N(uclear)DO(uble)R(esonance). *Angew. Chem., Int. Ed.* **1983**, *22* (10), 787–788.
27. Lubitz, W.; Lendzian, F.; Scheer, H.; Gottstein, J.; Plato, M.; Möbius, K. Structural Studies of the Primary Donor Cation Radical $\text{P}_{870}^{+\bullet}$ in Reaction Centers of *Rhodospirillum rubrum* by Electron–Nuclear Double Resonance in

Special Issue: Wolfgang Lubitz Festschrift

Published: October 29, 2015



- Solution. *Proc. Natl. Acad. Sci. U.S.A.* **1984**, 81, 1401–1405.
28. Kurreck, H.; Kirste, B.; Lubitz, W. ENDOR Spectroscopy - A Promising Technique for Investigating the Structure of Organic Radicals. *Angew. Chem., Int. Ed.* **1984**, 23, 173–194.
 29. Kurreck, H.; Bock, M.; Bretz, N.; Elsner, M.; Kraus, H.; Lubitz, W.; Müller, F.; Geissler, J.; Kroneck, P. M. H. Fluid Solution and Solid-State Electron Nuclear Double Resonance Studies of Flavin Model Compounds and Flavoenzymes. *J. Am. Chem. Soc.* **1984**, 106 (3), 737–746.
 30. Smith, I. M.; Sutcliffe, L. H.; Wiesner, S.; Lubitz, W.; Kurreck, H. 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., Faraday Trans. 1* **1984**, 80 (11), 3021–3036.
 31. Lendzian, F.; Möbius, K.; Plato, M.; Smith, U. H.; Thurnauer, M. C.; Lubitz, W. ^{25}Mg ENDOR and TRIPLE Resonance in Liquid Solution of the Bacteriochlorophyll *a* Cation and Anion Radicals. *Chem. Phys. Lett.* **1984**, 111, 583–588.
 32. Lubitz, W.; Isaacson, R. A.; Abresch, E. C.; Feher, G. ^{15}N Electron Nuclear Double-Resonance of the Primary Donor Cation Radical $\text{P}_{865}^{+\bullet}$ in Reaction Centers of *Rhodospseudomonas sphaeroides*: Additional Evidence for the Dimer Model. *Proc. Natl. Acad. Sci. U.S.A.* **1984**, 81 (24), 7792–7796.
 33. Lubitz, W.; Lendzian, F.; Scheer, H. Characterization of 10-Hydroxybacteriochlorophyll *a* by ENDOR and TRIPLE Resonance Spectroscopy. *J. Am. Chem. Soc.* **1985**, 107 (3341), 3343.
 34. Lubitz, W.; Abresch, E. C.; Debus, R. J.; Isaacson, R. A.; Okamura, M. Y.; Feher, G. Electron Nuclear Double Resonance of Semiquinones in Reaction Centers of *Rhodospseudomonas sphaeroides*. *Biochim. Biophys. Acta* **1985**, 808 (3), 464–469.
 35. Lubitz, W.; Lendzian, F.; Plato, M.; Möbius, K.; Tränkle, E. ENDOR Studies of the Primary Donor in Bacterial Reaction Centers. In *Antennas and Reaction Centers of Photosynthetic Bacteria*; Michel-Beyerle, M. E., Ed. Springer-Verlag: Berlin, **1985**; pp 164–173.
 36. Feher, G.; Isaacson, R. A.; Okamura, M. Y.; Lubitz, W. ENDOR of Semiquinones in RC's from *Rhodospseudomonas sphaeroides*. In *Antennas and Reaction Centers of Photosynthetic Bacteria. Structure, Interactions, and Dynamics*; Michel-Beyerle, M. E., Ed. Springer-Verlag: Berlin, **1985**; pp 174–189.
 37. Lendzian, F.; Lubitz, W.; Steiner, R.; Tränkle, E.; Plato, M.; Scheer, H.; Möbius, K. The Radical Cation of Bacteriochlorophyll *b*. A Liquid-Phase ENDOR and TRIPLE Resonance Study. *Chem. Phys. Lett.* **1986**, 126, 290–296.
 38. Plato, M.; Tränkle, E.; Lubitz, W.; Lendzian, F.; Möbius, K. Molecular Orbital Investigation of Dimer Formations of Bacteriochlorophyll *a*. Model Configurations for the Primary Donor of Photosynthesis. *Chem. Phys.* **1986**, 107 (2–3), 185–196.
 39. Huber, M.; Lendzian, F.; Lubitz, W.; Tränkle, E.; Möbius, K.; Wasielewski, M. R. ENDOR and TRIPLE Resonance in Solutions of the Chlorophyll *a* and Bis(chlorophyll)cyclophane Radical Cations. *Chem. Phys. Lett.* **1986**, 132 (4–5), 467–473.
 40. Möbius, K.; Lubitz, W. ENDOR Spectroscopy in Photobiology and Biochemistry. In *Biological Magnetic Resonance*; Berliner, L. J., Reuben, J., Eds. Plenum Press: New York, **1987**; Vol. 7, pp 129–247.
 41. Lubitz, W.; Babcock, G. T. ENDOR Spectroscopy. *Trends Biochem. Sci.* **1987**, 12, 96–100.
 42. Baumgarten, M.; Lubitz, W.; Winscom, C. J. EPR and ENDOR Studies of Cobaloxime (II). *Chem. Phys. Lett.* **1987**, 133 (2), 102–108.
 43. Lubitz, W.; Winscom, C. J.; Diegruber, H.; Mösel, R. EPR Characterization of Bis(dimethylglyoximate) Cobalt(II) Complexes and their Oxygen Adducts Synthesized in an X-Zeolite Matrix. *Z. Naturforsch.* **1987**, 42a, 970–986.
 44. Kurreck, H.; Kirste, B.; Lubitz, W. *Electron Nuclear Double Resonance Spectroscopy of Radicals in Solution - Applications to Organic and Biological Chemistry*. VCH Publishers, Inc.: Deerfield Beach, Florida, **1988**; pp 1–374.
 45. Feher, G.; Isaacson, R.; Okamura, M. Y.; Lubitz, W. 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*; Breton, J., Verméglio, A., Eds. Plenum Press: **1988**; pp 229–235.
 46. Plato, M.; Lendzian, F.; Lubitz, W.; Tränkle, E.; Möbius, K. Molecular Orbital Studies on the Primary Donor P_{960} in Reaction Centers of *Rps. viridis*. In *The Photosynthetic Bacterial Reaction Center, Structure and Dynamics*; Breton, J., Verméglio, A., Eds. Plenum Press: **1988**; pp 379–388.
 47. Lendzian, F.; Lubitz, W.; Scheer, H.; Hoff, A. J.; Plato, M.; Tränkle, E.; Möbius, K. ESR, ENDOR and TRIPLE Resonance Studies of the Primary Donor Radical Cation $\text{P}_{960}^{+\bullet}$ in the Photosynthetic Bacterium *Rhodospseudomonas viridis*. *Chem. Phys. Lett.* **1988**, 148 (5), 377–385.
 48. Plato, M.; Lubitz, W.; Lendzian, F.; Möbius, K. Magnetic Resonance and Molecular Orbital Studies of the Primary Donor Cation Radical $\text{P}_{960}^{+\bullet}$ in the Photosynthetic Bacterium *Rhodospseudomonas viridis*. *Isr. J. Chem.* **1988**, 28 (2–3), 109–119.
 49. Möbius, K.; Plato, M.; Lubitz, W.; Lendzian, F. Electron–nuclear Multiple Resonance on Stable and Transient Radicals. *Isr. J. Chem.* **1988**, 28 (4), 239–248.
 50. Möbius, K.; Plato, M.; Lubitz, W. Bacteriochlorophyll Dimers in Photosynthesis: ENDOR and MO Studies. In 24th Ampere Congress, Magnetic Resonance and Related Phenomena: Posen, **1988**; pp 517–527.
 51. Möbius, K.; Lubitz, W.; Plato, M. Liquid-State ENDOR and TRIPLE Resonance. In *Advanced EPR, Applications in Biology and Biochemistry*; Hoff, A. J., Ed. Elsevier: **1989**; pp 441–499.
 52. Krebber, A. M. L.; Sutcliffe, L. H.; Lubitz, W.; Kurreck, H. Structural Effects on ESR Hyperfine Coupling Constants of Some Dithiazolidinyl Free Radicals. *Magn. Reson. Chem.* **1989**, 27 (3), 288–294.
 53. Lubitz, W.; Isaacson, R. A.; Okamura, M. Y.; Abresch, E. C.; Plato, M.; Feher, G. ENDOR Studies of the Intermediate Electron-Acceptor Radical-Anion $\text{I}^{\bullet-}$ in Photosystem II Reaction Centers. *Biochim. Biophys. Acta* **1989**, 977 (2), 227–232.

54. Lubitz, W.; Bönigk, B.; Plato, M.; Isaacson, R.; Okamura, M. Y.; Feher, G. ENDOR Studies of the Intermediate Electron Acceptor Radical Anion $I^{\bullet-}$ in Reaction Centers of *Rps. viridis*. In *Current Research in Photosynthesis*; Baltscheffsky, M., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1990**; pp 141–144.
55. MacMillan, F.; Gleiter, H.; Renger, G.; Lubitz, W. EPR/ENDOR Studies of Plastoquinone Anion Radical in Photosystem II Q_A^- and in Organic Solvents. In *Current Research in Photosynthesis*; Baltscheffsky, M., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1990**; pp 531–534.
56. Plato, M.; Möbius, K.; Lubitz, W.; Allen, J. P.; Feher, G. Magnetic Resonance and Molecular Orbital Studies of the Primary Donor States in Bacterial Reaction Centers. In *Perspectives in Photosynthesis*; Jortner, J., Pullmann, B., Eds. Kluwer: **1990**; pp 423–434.
57. Lendzian, F.; Endeward, B.; Plato, M.; Bumann, D.; Lubitz, W.; Möbius, K. ENDOR and TRIPLE Resonance Investigation of the Primary Donor Cation Radical $P_{865}^{+\bullet}$ in Single Crystals of *Rhodobacter sphaeroides* R-26 Reaction Centers. In *Springer Series in Biophysics, Vol. 6, Reaction Centers of Photosynthetic Bacteria*; Michel-Beyerle, M. E., Ed. Springer Verlag: **1990**; pp 57–68.
58. Lubitz, W. EPR and ENDOR Studies of Chlorophyll Cation and Anion Radicals. In *Chlorophylls*; Scheer, H., Ed. CRC Press Inc.: Boca Raton, Florida, **1991**; pp 903–944.
59. Plato, M.; Möbius, K.; Lubitz, W. Molecular Orbital Calculations on Chlorophyll Radical Ions. In *Chlorophylls*; Scheer, H., Ed. CRC Press Inc.: Boca Raton, Florida, **1991**; pp 1015–1046.
60. Burghaus, O.; Plato, M.; Bumann, D.; Neumann, B.; Lubitz, W.; Möbius, K. 3 mm EPR Investigation of the Primary Donor Cation Radical $P_{865}^{+\bullet}$ in Single Crystals of *Rb. Sphaeroides* R-26 Reaction Centers. *Chem. Phys. Lett.* **1991**, 185 (3–4), 381–386.
61. Geßner, C.; Lendzian, F.; Bönigk, B.; Plato, M.; Möbius, K.; Lubitz, W. Proton ENDOR and TRIPLE Resonance Investigation of $P_{865}^{+\bullet}$ in Photosynthetic Reaction Center Single Crystals of *Rb. sphaeroides* Wild Type 2.4.1. *Appl. Magn. Reson.* **1992**, 3, 763–777.
62. Rautter, J.; Geßner, C.; Lendzian, F.; Lubitz, W.; Williams, J. C.; Murchison, H. A.; Wang, S.; Woodbury, N. W.; Allen, J. P. EPR and ENDOR Studies of the Primary Donor Cation Radical in Native and Genetically Modified Bacterial Reaction Centers. In *Photosynthetic Bacterial Reaction Center II*; Breton, J., Verméglio, A., Eds. Plenum Press: New York, **1992**; Vol. 237, pp 99–108.
63. Lendzian, F.; Bönigk, B.; Plato, M.; Möbius, K.; Lubitz, W. ^{15}N ENDOR Experiments on the Primary Donor Cation Radical $D^{+\bullet}$ in Bacterial Reaction Center Single Crystals of *Rhodobacter sphaeroides* R-26. In *Photosynthetic Bacterial Reaction Center II*; Breton, J., Verméglio, A., Eds. Plenum Press: New York, **1992**; Vol. 237, pp 89–97.
64. Plato, M.; Lendzian, F.; Lubitz, W.; Möbius, K. Molecular-orbital Study of Electronic Asymmetry in Primary Donors of Bacterial Reaction Centers. In *Photosynthetic Bacterial Reaction Center II*; Breton, J., Verméglio, A., Eds. Plenum Press: New York, **1992**; Vol. 237, pp 109–118.
65. Zweggart, W.; Weyhermüller, T.; Renger, G.; Wieghardt, K.; Lubitz, W. EPR and ENDOR Studies of Manganese Clusters in the Water-oxidizing Complex and Related Model Compounds. In *Research in Photosynthesis, Vol. II*; Murata, N., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1992**; pp 289–292.
66. Lendzian, F.; Geßner, C.; Bönigk, B.; Plato, M.; Möbius, K.; Lubitz, W. ^{15}N - and ^1H -ENDOR/TRIPLE Resonance of the Primary Donor Cation Radical $D^{+\bullet}$ in Isotopically Labeled Reaction Centers of *Rhodobacter sphaeroides*. In *Research in Photosynthesis, Vol. I: IXth International Congress on Photosynthesis*; Murata, N., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1992**; pp 433–436.
67. Bittl, R.; van der Est, A.; Fücksle, G.; Lubitz, W.; Stehlik, D. Transient EPR of Photosynthetic Reaction Centers: Structural Information on the Radical Pair $P^+ Q^-$ in Zn-substituted *Rhodobacter sphaeroides* and Photosystem I. In *Research in photosynthesis, Vol. 1; IXth International Congress on Photosynthesis*; Murata, N., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1992**; pp 461–464.
68. Klette, R.; Törring, J. T.; Plato, M.; Möbius, K.; Bönigk, B.; Lubitz, W. 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.* **1993**, 97 (9), 2015–2020.
69. Fücksle, G.; Bittl, R.; van der Est, A.; Lubitz, W.; Stehlik, D. Transient EPR Spectroscopy of the Charge Separated State $P^+ Q^-$ in Photosynthetic Reaction Centers: Comparison of Zinc-substituted *Rhodobacter sphaeroides* R-26 and Photosystem I. *Biochim. Biophys. Acta* **1993**, 1142 (1), 23–35.
70. Burghaus, O.; Plato, M.; Rohrer, M.; Möbius, K.; MacMillan, F.; Lubitz, W. Three mm High-field EPR on Semiquinone Radical Anions $Q^{\bullet-}$ Related to Photosynthesis and on the Primary Donor $P^{+\bullet}$ and Acceptor $Q_A^{\bullet-}$ in Reaction Centers of *Rhodobacter sphaeroides* R-26. *J. Phys. Chem.* **1993**, 97 (29), 7639–7647.
71. Van der Est, A.; Bittl, R.; Abresch, E. C.; Lubitz, W.; Stehlik, D. Transient EPR Spectroscopy of Perdeuterated Zn-substituted Reaction Centers of *Rhodobacter sphaeroides* R-26. *Chem. Phys. Lett.* **1993**, 212 (6), 561–568.
72. Lendzian, F.; Huber, M.; Isaacson, R. A.; Endeward, B.; Plato, M.; Bönigk, B.; Möbius, K.; Lubitz, W.; Feher, G. 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* **1993**, 1183 (1), 139–160.
73. Käss, H.; Rautter, J.; Zweggart, W.; Struck, A.; Scheer, H.; Lubitz, W. EPR, ENDOR, and TRIPLE Resonance Studies of Modified Bacteriochlorophyll Cation Radicals. *J. Phys. Chem.* **1994**, 98 (1), 354–363.
74. Zweggart, W.; Thanner, R.; Lubitz, W. An Improved TM_{110} ENDOR Cavity for the Investigation of Transition Metal Complexes. *J. Magn. Reson., Ser. A* **1994**, 109 (2), 172–176.
75. Bittl, R.; van der Est, A.; Kamrowski, A.; Lubitz, W.; Stehlik, D. Time-Resolved EPR of the Radical Pair $P_{865}^{+\bullet} Q_A^{\bullet-}$ in Bacterial Reaction Centers. Observation of Transient Nutations, Quantum Beats and Envelope

- Modulation Effects. *Chem. Phys. Lett.* **1994**, 226 (3–4), 349–358.
76. Rautter, J.; Lendzian, F.; Lubitz, W.; Wang, S.; Allen, J. P. Comparative Study of Reaction Centers from Photosynthetic Purple Bacteria: Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Spectroscopy. *Biochemistry* **1994**, 33 (40), 12077–12084.
77. Käss, H.; Rautter, J.; Bönigk, B.; Höfer, P.; Lubitz, W. 2D ESEEM of the ^{15}N -labeled Radical Cations of Bacteriochlorophyll *a* and of the Primary Donor in Reaction Centers of *Rhodobacter sphaeroides*. *J. Phys. Chem.* **1995**, 99 (1), 436–448.
78. Lubitz, W.; Rautter, J.; Käss, H.; Lendzian, F. Light-induced Charge Separation in Photosynthetic Reaction Centers - Magnetic Resonance Studies. *Sol. Energy Mater. Sol. Cells* **1995**, 38 (1–4), 77–89.
79. Shuvalov, V. A.; Fiege, R.; Schreiber, U.; Lendzian, F.; Lubitz, W. EPR Study of Cytochrome in the D1D2 Cyt b-559 Complex. *Biochim. Biophys. Acta, Bioenerg.* **1995**, 1228 (2–3), 175–180.
80. Cui, L. Y.; Bingham, S. E.; Kuhn, M.; Käss, H.; Lubitz, W.; Webber, A. N. 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 P_{700} . *Biochemistry* **1995**, 34 (5), 1549–1558.
81. Van der Est, A.; Sieckmann, I.; Lubitz, W.; Stehlik, D. Differences in the Binding of the Primary Quinone Acceptor in Photosystem I and Reaction Centers of *Rhodobacter sphaeroides* R26 Studied with Transient EPR Spectroscopy. *Chem. Phys.* **1995**, 194 (2–3), 349–359.
82. Prisner, T. F.; van der Est, A.; Bittl, R.; Lubitz, W.; Stehlik, D.; Möbius, K. Time-Resolved W-Band (95 GHz) EPR Spectroscopy of Zn-Substituted Reaction Centers of *Rhodobacter sphaeroides* R-26. *Chem. Phys.* **1995**, 194 (2–3), 361–370.
83. Käss, H.; Bittersmann-Weidlich, E.; Andréasson, L. E.; Bönigk, B.; Lubitz, W. ENDOR and ESEEM of the ^{15}N Labeled Radical Cations of Chlorophyll *a* and the Primary Donor P_{700} in Photosystem I. *Chem. Phys.* **1995**, 194 (2–3), 419–432.
84. MacMillan, F.; Lendzian, F.; Renger, G.; Lubitz, W. EPR and ENDOR Investigation of the Primary Electron Acceptor Radical Anion $\text{Q}_\text{A}^{\bullet-}$ in Iron-Depleted Photosystem II Membrane Fragments. *Biochemistry* **1995**, 34 (25), 8144–8156.
85. Rautter, J.; Lendzian, F.; Schulz, C.; Fetsch, A.; Kuhn, M.; Lin, X.; Williams, J. C.; Allen, J. P.; Lubitz, W. ENDOR Studies of the Primary Donor Cation Radical in Mutant Reaction Centers of *Rhodobacter sphaeroides* with Altered Hydrogen-Bond Interactions. *Biochemistry* **1995**, 34 (25), 8130–8143.
86. Isaacson, R. A.; Lendzian, F.; Abresch, E. C.; Lubitz, W.; Feher, G. Electronic Structure of $\text{Q}_\text{A}^{\bullet-}$ in Reaction Centers from *Rb. Sphaeroides*. I. Electron Paramagnetic Resonance in Single Crystals. *Biophys. J.* **1995**, 69 (2), 311–322.
87. Rohrer, M.; Plato, M.; MacMillan, F.; Grishin, Y.; Lubitz, W.; Möbius, K. Orientation-selected 95 GHz High-field Endor Spectroscopy of Randomly Oriented Plastoquinone Anion-Radicals. *J. Magn. Reson.* **1995**, 116 (1), 59–66.
88. MacMillan, F.; Lendzian, F.; Lubitz, W. EPR and ENDOR Characterization of Semiquinone Anion Radicals Related to Photosynthesis. *Magn. Reson. Chem.* **1995**, 33, S81–S93.
89. Gardiner, A. T.; Lendzian, F.; MacMillan, F.; Zech, S. G.; Bittl, R.; Kuhn, M.; Lubitz, W. EPR Characterization of $\text{Q}_\text{A}^{\bullet-}$ from Biosynthetically and Chemically Substituted Zn(II) Reaction Centres from *Rhodobacter sphaeroides* and *Rhodospseudomonas viridis*. In *Photosynthesis: from Light to Biosphere, Vol. I*; Mathis, P., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1995**; pp 655–658.
90. MacMillan, F.; Kurreck, J.; Adir, N.; Lendzian, F.; Käss, H.; Reifarth, F.; Renger, G.; Lubitz, W. EPR, ENDOR and ESEEM Investigation of the Electron Acceptor Radical Anion $\text{Q}_\text{A}^{\bullet-}$ in Photosystem II (PS II) Reaction Centres. In *Photosynthesis: from Light to Biosphere, Vol. I*; Mathis, P., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1995**; pp 659–662.
91. Krabben, L.; Käss, H.; Schlodder, E.; Kuhn, M.; Lubitz, W.; Xu, H.; Bingham, S.; Webber, A. Site-directed Mutations of PsaB for the Study of Cofactor-protein and Protein–protein Interactions of Photosystem I. In *Photosynthesis: From Light to Biosphere, Vol. II*; Mathis, P., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1995**; pp 123–126.
92. Lubitz, W.; Müh, F.; Rautter, J.; Lendzian, F.; Allen, J. P.; Williams, J. C. Magnetic Resonance Studies of Bacterial Reaction Centers: Effects of Hydrogen Bonds on the Electronic Structure of $\text{P}^{\bullet+}$ and $\text{I}^{\bullet+}$. In *Photosynthesis: from Light to Biosphere, Vol. I*; Mathis, P., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1995**; pp 413–418.
93. Fiege, R.; Zweggart, W.; Irrgang, K. D.; Adir, N.; Geiken, B.; Renger, G.; Lubitz, W. EPR/ENDOR Studies of the Water Oxidizing Complex in Photosystem II. In *Photosynthesis: From Light to Biosphere, Vol. II*; Mathis, P., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1995**; pp 369–372.
94. Huber, M.; Törring, J. T.; Plato, M.; Fink, U.; Lubitz, W.; Feick, R.; Schenck, C. C.; Möbius, K. 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. Energy Mater. Sol. Cells* **1995**, 38 (1–4), 119–126.
95. Van der Est, A.; Sieckmann, I.; Lubitz, W.; Stehlik, D. Quinone Binding in *Rhodobacter sphaeroides* and Photosystem I Studied by Transient EPR. In *Photosynthesis: From Light to Biosphere, Vol. II*; Mathis, P., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1995**; pp 143–146.
96. Fiege, R.; Schreiber, U.; Renger, G.; Lubitz, W.; Shuvalov, V. A. Study of Heme Fe(III) Ligated by OH^- in Cytochrome *b*-559 and Its Low Temperature Photochemistry in Intact Chloroplasts. *FEBS Lett.* **1995**, 377 (3), 325–329.
97. Lubitz, W.; Lendzian, F. ENDOR Spectroscopy. In *Advances in Photosynthesis. Biophysical Techniques in Photosynthesis*; Ames, J., Hoff, A. J., Eds. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1996**; pp 255–275.

98. Rautter, J.; Lendzian, F.; Lin, X.; Williams, J. C.; Allen, J. P.; Lubitz, W. 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*; Michel-Beyerle, M. E., Ed. Springer-Verlag Publishers: Berlin, **1996**; pp 37–50.
99. Isaacson, R. A.; Abresch, E. C.; Lendzian, F.; Boullais, C.; Paddock, M.; Mioskowski, C.; Lubitz, W.; Feher, G. 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*; Michel-Beyerle, M. E., Ed. Springer Verlag Publishers: Berlin, **1996**; pp 353–367.
100. Käss, H.; Lubitz, W. Evaluation of 2D-ESEEM Data of ^{15}N -labeled Radical Cations of the Primary Donor P_{700} in Photosystem I and Chlorophyll *a*. *Chem. Phys. Lett.* **1996**, 251 (3–4), 193–203.
101. Bittl, R.; Zech, S. G.; Lubitz, W. Light-induced Changes in Transient EPR Spectra of $P_{865}^{+\bullet}Q_A^{-\bullet}$. In *The Reaction Center of Photosynthetic Bacteria, Structure and Dynamics*; Michel-Beyerle, M. E., Ed. Springer Verlag Publishers: Berlin, **1996**; pp 333–339.
102. Muegge, I.; Apostolakis, J.; Ermiler, U.; Fritzsche, G.; Lubitz, W.; Knapp, E. W. Shift of the Special Pair Redox Potential: Electrostatic Energy Computations of Mutants of the Reaction Center from *Rhodobacter sphaeroides*. *Biochemistry* **1996**, 35 (25), 8359–8370.
103. Allen, J. P.; Artz, K.; Lin, X.; Williams, J. C.; Ivancich, A.; Albouy, D.; Mattioli, T. A.; Fetsch, A.; Kuhn, M.; Lubitz, W. Effects of Hydrogen Bonding to a Bacteriochlorophyll–Bacteriopheophytin Dimer in Reaction Centers from *Rhodobacter sphaeroides*. *Biochemistry* **1996**, 35 (21), 6612–6619.
104. Zweggart, W.; Bittl, R.; Wieghardt, K.; Lubitz, W. 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.* **1996**, 261 (3), 272–276.
105. Fiege, R.; Zweggart, W.; Bittl, R.; Adir, N.; Renger, G.; Lubitz, W. EPR and ENDOR Studies of the Water Oxidizing Complex of Photosystem II. *Photosynth. Res.* **1996**, 48 (1–2), 227–237.
106. Webber, A. N.; Su, H.; Bingham, S. E.; Käss, H.; Krabben, L.; Kuhn, M.; Jordan, R.; Schlodder, E.; Lubitz, W. Site-directed Mutations Affecting the Spectroscopic Characteristics and Mid-Point Potential of the Primary Donor in Photosystem I. *Biochemistry* **1996**, 35 (39), 12857–12863.
107. Geßner, C.; Trofanchuk, O.; Kawagoe, K.; Higuchi, Y.; Yasuoka, N.; Lubitz, W. Single Crystal EPR Study of the Ni Center of $[\text{NiFe}]$ Hydrogenase. *Chem. Phys. Lett.* **1996**, 256 (4–5), 518–524.
108. Käss, H.; Fromme, P.; Lubitz, W. Quadrupole Parameters of Nitrogen Nuclei in the Cation Radical $P_{700}^{+\bullet}$ Determined by ESEEM of Single Crystals of Photosystem I. *Chem. Phys. Lett.* **1996**, 257 (1–2), 197–206.
109. Lendzian, F.; Sahlin, M.; MacMillan, F.; Bittl, R.; Fiege, R.; Pötsch, S.; Sjöberg, B. M.; Gräslund, A.; Lubitz, W.; Lassmann, G. Electronic Structure of Neutral Tryptophan Radicals in Ribonucleotide Reductase Studied by EPR and ENDOR Spectroscopy. *J. Am. Chem. Soc.* **1996**, 118 (34), 8111–8120.
110. Zech, S. G.; Lubitz, W.; Bittl, R. Pulsed EPR Experiments on Radical Pairs in Photosynthesis: Comparison of the Donor–acceptor Distances in Photosystem I and Bacterial Reaction Centers. *Ber. Bunsen-Ges.* **1996**, 100 (12), 2041–2044.
111. Müh, F.; Rautter, J.; Lubitz, W. Effects of Zwitterionic Detergents on the Primary Donor of Bacterial Reaction Centers. *Ber. Bunsen-Ges.* **1996**, 100 (12), 1974–1977.
112. Lendzian, F.; Rautter, J.; Käss, H.; Gardiner, A.; Lubitz, W. ENDOR and Pulsed EPR Studies of Photosynthetic Reaction Centers: Protein–Cofactor Interactions. *Ber. Bunsen-Ges.* **1996**, 100 (12), 2036–2040.
113. Lubitz, W.; Fiege, R.; Bittl, R.; Irrgang, K. D.; Renger, G. EPR and ENDOR Investigations of the Manganese Cluster in Photosystem II. In *Bioinorganic Chemistry: Transition Metals in Biology and their Coordination Chemistry*; Trautwein, A. X., Ed. VCH Publishers: Weinheim, **1996**; pp 673–680.
114. Lubitz, W.; Zweggart, W.; Bittl, R.; Wieghardt, K.; Haselhorst, G.; Weyhermüller, T. 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*; Trautwein, A. X., Ed. VCH Publishers: Weinheim, **1996**; pp 665–672.
115. Renger, G.; Kurreck, H.; Haag, E.; Reifarth, F.; Bergmann, A.; Parak, F.; Garbers, A.; MacMillan, F.; Lendzian, F.; Lubitz, W. The Nonheme Iron Center of Photosystem II and Modulatory Effects of Exogenous Copper(II). In *Bioinorganic Chemistry: Transition Metals in Biology and their Coordination Chemistry*; Trautwein, A. X., Ed. VCH Publishers: Weinheim, **1996**; pp 260–276.
116. Van der Est, A.; Prisner, T.; Bittl, R.; Fromme, P.; Lubitz, W.; Möbius, K.; Stehlik, D. Time-Resolved X -, K -, and W -Band EPR of the Radical Pair State $P_{700}^{+\bullet}A_1^{-\bullet}$ of Photosystem I in Comparison with $P_{865}^{+\bullet}Q_A^{-\bullet}$ in Bacterial Reaction Centers. *J. Phys. Chem. B* **1997**, 101 (8), 1437–1443.
117. Müh, F.; Rautter, J.; Lubitz, W. Two Distinct Conformations of the Primary Electron Donor in Reaction Centers from *Rhodobacter sphaeroides* Revealed by ENDOR/TRIPLE-spectroscopy. *Biochemistry* **1997**, 36 (14), 4155–4162.
118. Albouy, D.; Kuhn, M.; Williams, J. C.; Allen, J. P.; Lubitz, W.; Mattioli, T. A. Fourier Transform Raman Investigation of the Electronic Structure and Charge Localization in a Bacteriochlorophyll–Bacteriopheophytin Dimer of Reaction Centers from *Rhodobacter sphaeroides*. *Biochim. Biophys. Acta* **1997**, 1321 (2), 137–148.
119. Bittl, R.; Zech, S. G.; Fromme, P.; Witt, H. T.; Lubitz, W. Pulsed EPR Structure Analysis of Photosystem I Single Crystals: Localization of the Phylloquinone Acceptor. *Biochemistry* **1997**, 36 (40), 12001–12004.
120. Zech, S. G.; Kurreck, J.; Eckert, H. J.; Renger, G.; Lubitz, W.; Bittl, R. Pulsed EPR Measurement of the Distance between $P_{680}^{+\bullet}$ and $Q_A^{-\bullet}$ in Photosystem II. *FEBS Lett.* **1997**, 414 (2), 454–456.
121. Lubitz, W.; Lendzian, F.; Plato, M.; Scheer, H.; Möbius, K. The Bacteriochlorophyll *a* Cation Radical Revisited. An ENDOR and TRIPLE Resonance Study. *Appl. Magn. Reson.* **1997**, 13 (3–4), 531–551.
122. Zech, S. G.; Bittl, R.; Gardiner, A. T.; Lubitz, W. Transient and Pulsed EPR Spectroscopy on the Radical

- Pair State $P_{865}^{+\bullet} Q_A^{-\bullet}$ to Study Light-induced Changes in Bacterial Reaction Centers. *Appl. Magn. Reson.* **1997**, *13* (3–4), 517–529.
123. Artz, K.; Williams, J. C.; Allen, J. P.; Lendzian, F.; Rautter, J.; Lubitz, W. Relationship Between the Oxidation Potential and Electron Spin Density of the Primary Electron Donor in Reaction Centers from *Rhodobacter sphaeroides*. *Proc. Natl. Acad. Sci. U.S.A.* **1997**, *94* (25), 13582–13587.
 124. Käss, H.; Lubitz, W.; Hartwig, G.; Scheer, H.; Noy, D.; Scherz, A. ENDOR Studies of Substituted Chlorophyll Cation Radicals. *Spectrochim. Acta, Part A* **1998**, *54* (9), 1141–1156.
 125. Nabedryk, E.; Breton, J.; Williams, J. C.; Allen, J. P.; Kuhn, M.; Lubitz, W. 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, Part A* **1998**, *54* (9), 1219–1230.
 126. Wachtveitl, J.; Huber, H.; Feick, R.; Rautter, J.; Müh, F.; Lubitz, W. Electron Transfer in Bacterial Reaction Centers with an Energetically Raised Primary Acceptor: Ultrafast Spectroscopy and ENDOR/TRIPLE Studies. *Spectrochim. Acta, Part A* **1998**, *54* (9), 1231–1245.
 127. Lendzian, F.; Bittl, R.; Lubitz, W. Pulsed ENDOR of the Photoexcited Triplet States of Bacteriochlorophyll *a* and of the Primary Donor P_{865} in Reaction Centers of *Rhodobacter sphaeroides* R-26. *Photosynth. Res.* **1998**, *55* (2–3), 189–197.
 128. Nimz, O.; Lendzian, F.; Boullais, C.; Lubitz, W. 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. Reson.* **1998**, *14* (2–3), 255–274.
 129. Müh, F.; Schulz, C.; Schlodder, E.; Jones, M. R.; Rautter, J.; Kuhn, M.; Lubitz, W. Effects of Zwitterionic Detergents on the Electronic Structure of the Primary Donor and the Charge Recombination Kinetics of $P^+Q_A^-$ in Native and Mutant Reaction Centers from *Rhodobacter sphaeroides*. *Photosynth. Res.* **1998**, *55* (2–3), 199–205.
 130. Rohrer, M.; MacMillan, F.; Prisner, T. F.; Gardiner, A. T.; Möbius, K.; Lubitz, W. Pulsed ENDOR at 95 GHz on the Primary Acceptor Ubisemiquinone $Q_A^{-\bullet}$ in Photosynthetic Bacterial Reaction Centers and Related Model Systems. *J. Phys. Chem. B* **1998**, *102* (23), 4648–4657.
 131. Müh, F.; Williams, J. C.; Allen, J. P.; Lubitz, W. A Conformational Change of the Photoactive Bacteriopheophytin in Reaction Centers from *Rhodobacter sphaeroides*. *Biochemistry* **1998**, *37* (38), 13066–13074.
 132. Kamlowski, A.; Zech, S. G.; Fromme, P.; Bittl, R.; Lubitz, W.; Witt, H. T.; Stehlik, D. The Radical Pair State $P_{700}^{+\bullet} A_1^{-\bullet}$ in Photosystem I Single Crystals: Orientation Dependence of the Transient Spin-Polarized EPR Spectra. *J. Phys. Chem. B* **1998**, *102* (42), 8266–8277.
 133. Kamlowski, A.; Altenberg-Greulich, B.; van der Est, A.; Zech, S. G.; Bittl, R.; Fromme, P.; Lubitz, W.; Stehlik, D. The Quinone Acceptor A_1 in Photosystem I: Binding Site and Comparison to Q_A in Purple Bacteria Reaction Centers. *J. Phys. Chem. B* **1998**, *102* (42), 8278–8287.
 134. Lendzian, F.; Bittl, R.; Telfer, A.; Barber, J.; Lubitz, W. Time Resolved ENDOR of the Triplet State of P_{680} in PS II Reaction Centers. In *Photosynthesis: mechanisms and effects: Proceedings of the XIth International Congress on Photosynthesis, Budapest, Hungary, August 17–22, 1998*; Garab, G., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1998**; Vol. 2, pp 1057–1060.
 135. Telfer, A.; Lendzian, F.; Schlodder, E.; Barber, J.; Lubitz, W. ENDOR and Transient Absorption Studies of $P_{680}^{+\bullet}$ and other Cation Radicals in PS II Reaction Centres before and after Inactivation of Secondary Electron Donors. In *Photosynthesis: Mechanisms and Effects: Proceedings of the XIth International Congress on Photosynthesis, Budapest, Hungary, August 17–22, 1998*; Garab, G., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1998**; Vol. 2, pp 1061–1064.
 136. Schulz, C.; Müh, F.; Beyer, A.; Jordan, R.; Schlodder, E.; Lubitz, W. Investigation of *Rhodobacter sphaeroides* Reaction Center Mutants with Changed Ligands to the Primary Donor. In *Photosynthesis: Mechanisms and Effects: Proceedings of the XIth International Congress on Photosynthesis, Budapest, Hungary, August 17–22, 1998*; Garab, G., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1998**; Vol. 2, pp 767–770.
 137. Müh, F.; Bibikova, M.; Lendzian, F.; Oesterheld, D.; Lubitz, W. Pigment–protein Interactions in Reaction Centers of *Rhodospseudomonas viridis*: ENDOR-study of Oxidized Primary Donor in Site-directed Mutants. In *Photosynthesis: Mechanisms and Effects: Proceedings of the XIth International Congress on Photosynthesis, Budapest, Hungary, August 17–22, 1998*; Garab, G., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1998**; Vol. 2, pp 763–766.
 138. Teutloff, C.; MacMillan, F.; Bittl, R.; Lendzian, F.; Lubitz, W. A Comparative Study of $A_1^{-\bullet}$ in PS I from Cyanobacteria, Green Plants and Algae using EPR and ENDOR Spectroscopy. In *Photosynthesis: Mechanisms and Effects: Proceedings of the XIth International Congress on Photosynthesis, Budapest, Hungary, August 17–22, 1998*; Garab, G., Ed. Kluwer Academic Publishers: Dordrecht, The Netherlands, **1998**; Vol. 1, pp 607–610.
 139. Bittl, R.; Zech, S. G.; Teutloff, C.; Krabben, L.; Lubitz, W. Structural Information on Components of the Electron Transfer Chain in Photosystem I from Time-resolved EPR Spectroscopy. In *Photosynthesis: Mechanisms and Effects: Proceedings of the XIth International Congress on Photosynthesis, Budapest, Hungary, August 17–22, 1998*; Garab, G., Ed. Kluwer Academic Press: Dordrecht, The Netherlands, **1998**; Vol. 1, pp 509–514.
 140. Schäfer, K. O.; Bittl, R.; Zweggart, W.; Lendzian, F.; Haselhorst, G.; Weyhermüller, T.; Wieghardt, K.; Lubitz, W. Electronic Structure of Antiferromagnetically Coupled Dinuclear Manganese ($\text{Mn}^{\text{III}} \text{Mn}^{\text{IV}}$) Complexes Studied by Magnetic Resonance Techniques. *J. Am. Chem. Soc.* **1998**, *120* (50), 13104–13120.
 141. Lassmann, G.; Eriksson, L. A.; Himo, F.; Lendzian, F.; Lubitz, W. Electronic Structure of a Transient Histidine Radical in Liquid Aqueous Solution: EPR Continuous-flow Studies and Density Functional Calculations. *J. Phys. Chem. A* **1999**, *103* (9), 1283–1290.
 142. Müh, F.; Jones, M. R.; Lubitz, W. Reorientation of the Acetyl Group of the Photoactive Bacteriopheophytin in Reaction Centers of *Rhodobacter sphaeroides*: An ENDOR/TRIPLE Resonance Study. *Biospectroscopy* **1999**, *5* (1), 35–46.

143. Zech, S. G.; Kurreck, J.; Renger, G.; Lubitz, W.; Bittl, R. Determination of the Distance between $Y_Z^{ox\bullet}$ and $Q_A^{-\bullet}$ in Photosystem II by Pulsed EPR Spectroscopy on Light-induced Radical Pairs. *FEBS Lett.* **1999**, 442 (1), 79–82.
144. Pötsch, S.; Lendzian, F.; Ingemarsson, R.; Hörnberg, A.; Thelander, L.; Lubitz, W.; Lassmann, G.; Gräslund, A. 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.* **1999**, 274 (25), 17696–17704.
145. Fahnenschmidt, M.; Rau, H. K.; Bittl, R.; Haehnel, W.; Lubitz, W. Characterization of a *de novo* Designed Heme Protein by EPR and ENDOR Spectroscopy. *Chem. Eur. J.* **1999**, 5 (8), 2327–2334.
146. Geßner, C.; Stein, M.; Albracht, S. P. J.; Lubitz, W. Orientation-selected ENDOR of the Active Center in *Chromatium vinosum* [NiFe] Hydrogenase in the Oxidized “Ready” State. *J. Biol. Inorg. Chem.* **1999**, 4 (4), 379–389.
147. Lubitz, W.; Feher, G. The Primary and Secondary Acceptors in Bacterial Photosynthesis III. Characterization of the Quinone Radicals $Q_A^{-\bullet}$ and $Q_B^{-\bullet}$ by EPR and ENDOR. *Appl. Magn. Reson.* **1999**, 17 (1), 1–48.
148. Jegerschöld, C.; MacMillan, F.; Lubitz, W.; Rutherford, A. W. Effects of Copper and Zinc Ions on Photosystem II Studied by EPR Spectroscopy. *Biochemistry* **1999**, 38 (38), 12439–12445.
149. Gardiner, A. T.; Zech, S. G.; MacMillan, F.; Käss, H.; Bittl, R.; Schlodder, E.; Lendzian, F.; Lubitz, W. Electron Paramagnetic Resonance Studies of Zn-substituted Reaction Centers from *Rhodospseudomonas viridis*. *Biochemistry* **1999**, 38 (36), 11773–11787.
150. Trofanchuk, O.; Stein, M.; Geßner, C.; Lendzian, F.; Higuchi, Y.; Lubitz, W. Single Crystal EPR Studies of the Oxidized Active Site of [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F. *J. Biol. Inorg. Chem.* **2000**, 5 (1), 36–44.
151. Nabedryk, E.; Schulz, C.; Müh, F.; Lubitz, W.; Breton, J. Heterodimeric versus Homodimeric Structure of the Primary Electron Donor in *Rhodobacter sphaeroides* Reaction Centers Genetically Modified at Position M202. *Photochem. Photobiol.* **2000**, 71 (5), 582–588.
152. Calvo, R.; Abresch, E. C.; Bittl, R.; Feher, G.; Hofbauer, W.; Isaacson, R. A.; Lubitz, W.; Okamura, M. Y.; Paddock, M. L. EPR Study of the Molecular and Electronic Structure of the Semiquinone Biradical $Q_A^{-\bullet}$ $Q_B^{-\bullet}$ in Photosynthetic Reaction Centers from *Rhodobacter sphaeroides*. *J. Am. Chem. Soc.* **2000**, 122 (30), 7327–7341.
153. Müh, F.; Bibikova, M.; Schlodder, E.; Oesterhelt, D.; Lubitz, W. Conformational Relaxation Following Reduction of the Photoactive Bacteriopheophytin in Reaction Centers from *Blastochloris viridis*. Influence of Mutations at Position M208. *Biochim. Biophys. Acta, Bioenerg.* **2000**, 1459 (1), 191–201.
154. Fahnenschmidt, M.; Bittl, R.; Rau, H. K.; Haehnel, W.; Lubitz, W. Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Spectroscopy of a Heme Protein Maquette. *Chem. Phys. Lett.* **2000**, 323 (3–4), 329–339.
155. Cogdell, R. J.; Howard, T. D.; Bittl, R.; Schlodder, E.; Geisenheimer, I.; Lubitz, W. How Carotenoids Protect Bacterial Photosynthesis. *Philos. Trans. R. Soc., B* **2000**, 355 (1402), 1345–1349.
156. Sinnecker, S.; Koch, W.; Lubitz, W. Bacteriochlorophyll *a* Radical Cation and Anion—calculation of Isotropic Hyperfine Coupling Constants by Density Functional Methods. *Phys. Chem. Chem. Phys.* **2000**, 2 (20), 4772–4778.
157. Krabben, L.; Schlodder, E.; Jordan, R.; Carbonera, D.; Giacometti, G.; Lee, H.; Webber, A. N.; Lubitz, W. Influence of the Axial Ligands on the Spectral Properties of P700 of Photosystem I: A Study of Site-directed Mutants. *Biochemistry* **2000**, 39 (42), 13012–13025.
158. Zech, S. G.; Hofbauer, W.; Kamrowski, A.; Fromme, P.; Stehlik, D.; Lubitz, W.; Bittl, R. A Structural Model for the Charge Separated State $P_{700}^{+\bullet}A_1^{-\bullet}$ in Photosystem I from the Orientation of the Magnetic Interaction Tensors. *J. Phys. Chem. B* **2000**, 104 (41), 9728–9739.
159. Lassmann, G.; Eriksson, L. A.; Lendzian, F.; Lubitz, W. 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* **2000**, 104 (40), 9144–9152.
160. Kolberg, M.; Bleifuss, G.; Pötsch, S.; Gräslund, A.; Lubitz, W.; Lassmann, G.; Lendzian, F. A New Stable High-valent Diiron Center in R2Mutant Y122H of *E. coli* Ribonucleotide Reductase Studied by High-field EPR and ^{57}Fe -ENDOR. *J. Am. Chem. Soc.* **2000**, 122 (40), 9856–9857.
161. Stein, M.; van Lenthe, E.; Baerends, E. J.; Lubitz, W. 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* **2001**, 105 (2), 416–425.
162. Käss, H.; Fromme, P.; Witt, H. T.; Lubitz, W. Orientation and Electronic Structure of the Primary Donor Radical Cation $P_{700}^{+\bullet}$ in Photosystem I: A Single Crystals EPR and ENDOR Study. *J. Phys. Chem. B* **2001**, 105 (6), 1225–1239.
163. Bittl, R.; Schlodder, E.; Geisenheimer, I.; Lubitz, W.; Cogdell, R. J. Transient EPR and Absorption Studies of Carotenoid Triplet Formation in Purple Bacterial Antenna Complexes. *J. Phys. Chem. B* **2001**, 105 (23), 5525–5535.
164. Baumgarten, M.; Winscom, C. J.; Lubitz, W. Probing the Surrounding of a Cobalt(II) Porphyrin and its Superoxo Complex by EPR Techniques. *Appl. Magn. Reson.* **2001**, 20 (1–2), 35–70.
165. Webber, A. N.; Lubitz, W. P700: The Primary Electron Donor of Photosystem I. *Biochim. Biophys. Acta, Bioenerg.* **2001**, 1507 (1–3), 61–79.
166. Hofbauer, W.; Zouni, A.; Bittl, R.; Kern, J.; Orth, P.; Lendzian, F.; Fromme, P.; Witt, H. T.; Lubitz, W. Photosystem II Single Crystals Studied by EPR Spectroscopy at 94 GHz: The Tyrosine Radical Y_D^{\bullet} . *Proc. Natl. Acad. Sci. U.S.A.* **2001**, 98 (12), 6623–6628.
167. Stein, M.; van Lenthe, E.; Baerends, E. J.; Lubitz, W. Relativistic DFT Calculations of the Paramagnetic Intermediates of [NiFe] Hydrogenase. Implications for the Enzymatic Mechanism. *J. Am. Chem. Soc.* **2001**, 123 (24), 5839–5840.
168. Stein, M.; Lubitz, W. DFT Calculations of the Electronic Structure of the Paramagnetic States Ni-A, Ni-B and

- Ni–C of [NiFe]-hydrogenase. *Phys. Chem. Chem. Phys.* **2001**, 3 (13), 2668–2675.
169. Fahnenschmidt, M.; Bittl, R.; Schlodder, E.; Haehnel, W.; Lubitz, W. Characterization of *de novo* Synthesized Four-helix Bundle Proteins with Metalloporphyrin Cofactors. *Phys. Chem. Chem. Phys.* **2001**, 3 (18), 4082–4090.
170. Stein, M.; Lubitz, W. The Electronic Structure of the Catalytic Intermediate Ni–C in [NiFe] and [NiFeSe] Hydrogenases. *Phys. Chem. Chem. Phys.* **2001**, 3 (23), 5115–5120.
171. Albracht, S. P. J.; Bertrand, P.; Bleijlevens, B.; Dole, F.; Guigliarelli, B.; Hagen, W. R.; Happe, R. P.; Lubitz, W.; Maroney, M. J.; Massanz, C.; Moura, J. J. G.; Pereira, A. S.; Pierik, A. J.; Sorgenfrei, O.; Stein, M.; Tavares, P. Spectroscopy - the Functional Puzzle. In *Hydrogen as a Fuel*; Cammack, R., Frey, M., Robson, R., Eds. Taylor & Francis: London and New York, **2001**; pp 110–158.
172. Teutloff, C.; Hofbauer, W.; Zech, S. G.; Stein, M.; Bittl, R.; Lubitz, W. High-Frequency EPR Studies on Cofactor Radicals in Photosystem I. *Appl. Magn. Reson.* **2001**, 21 (3–4), 363–379.
173. Müh, F.; Gardiner, A. T.; Witt, H.; Schulz, C.; Imhoff, R. J.; Cogdell, R. J.; Lubitz, W. Conserved Electronic Structure of the Primary Donor in Reaction Centers of Sulfur and Non-Sulfur Purple Bacteria, 12th International Congress on Photosynthesis, CSIRO Publishing, Australia: Brisbane, **2001**; S7-005.
174. Gardiner, A. T.; Kuglstatter, A.; Fritzsche, G.; Breton, J.; Nbedryk, E.; Lubitz, W. The Crystal Structure of the Rb. *sphaeroides* Zn²⁺ Reaction Centre Mutant HC-(M266), 12th International Congress on Photosynthesis, CSIRO Publishing, Australia: Brisbane, **2001**; S7-016.
175. Teutloff, C.; Bittl, R.; Stein, M.; Jordan, P.; Fromme, P.; Krauß, N.; Lubitz, W. Structure Based Analysis of the Magnetic Resonance Parameters of Phylloquinone Acceptor A₁ in PS I, 12th International Congress on Photosynthesis, CSIRO Publishing, Australia: Brisbane, **2001**; S6-030.
176. Witt, H.; Schlodder, E.; Teutloff, C.; Bordignon, E.; Carbonera, D.; Niklas, J.; Lubitz, W. Site-directed Mutagenesis of Thr A739 of Photosystem I in *Chlamydomonas reinhardtii* Alters Significantly the Excitonic and Electronic Coupling if the Primary Electron Donor P700, 12th International Congress on Photosynthesis, CSIRO Publishing, Australia: Brisbane, **2001**; S6-011.
177. Bleifuss, G.; Kolberg, M.; Pötsch, S.; Hofbauer, W.; Bittl, R.; Lubitz, W.; Gräslund, A.; Lassmann, G.; Lendzian, F. Tryptophan and Tyrosine Radicals in Ribonucleotide Reductase: A Comparative High-field EPR Study at 94 GHz. *Biochemistry* **2001**, 40 (50), 15362–15368.
178. Lubitz, W. Paramagnetic States of Photosynthetic Reaction Centers Studied by Advanced EPR Techniques. In *Advanced EPR Applied to Biosciences*; Kawamori, A., Ed. Kwansei Gakuin Univ. Press: Japan, **2002**; pp 117–123.
179. Kolberg, M.; Bleifuss, G.; Sjöberg, B. M.; Gräslund, A.; Lubitz, W.; Lendzian, F.; Lassmann, G. 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.* **2002**, 397 (1), 57–68.
180. Schenkl, S.; Spörlein, S.; Müh, F.; Witt, H.; Lubitz, W.; Zinth, W.; Wachtevilt, J. Selective Perturbation of the Second Electron Transfer Step in Mutant Bacterial Reaction Centers. *Biochim. Biophys. Acta, Bioenerg.* **2002**, 1554 (1–2), 36–47.
181. Sinnecker, S.; Koch, W.; Lubitz, W. Chlorophyll *a* Radical Ions: A Density Functional Study. *J. Phys. Chem. B* **2002**, 106 (20), 5281–5288.
182. Lubitz, W.; Lendzian, F.; Bittl, R. Radicals, Radical Pairs and Triplet States in Photosynthesis. *Acc. Chem. Res.* **2002**, 35 (5), 313–320.
183. Müh, F.; Lendzian, F.; Roy, M.; Williams, J. C.; Allen, J. P.; Lubitz, W. 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* **2002**, 106 (12), 3226–3236.
184. Lubitz, W.; Brecht, M.; Foerster, S.; Stein, M.; Higuchi, Y.; Friedrich, B. EPR and Theoretical Investigations of [NiFe] Hydrogenase: Insight into the Mechanism of Biological Hydrogen Conversion. In *EPR in the 21st Century: Basics and Applications to Material, Life and Earth Sciences*; Kawamori, A., Yamauchi, J., Ohta, H., Eds. Elsevier: **2002**; pp 437–445.
185. Buhrke, T.; Brecht, M.; Lubitz, W.; Friedrich, B. 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.* **2002**, 7 (7–8), 897–908.
186. Stein, M.; Lubitz, W. Quantum Chemical Calculations of [NiFe] Hydrogenase. *Curr. Opin. Chem. Biol.* **2002**, 6 (2), 243–249.
187. Kolberg, M.; Bleifuss, G.; Gräslund, A.; Sjöberg, B. M.; Lubitz, W.; Lendzian, F.; Lassmann, G. Protein Thiyl Radicals Directly Observed by EPR Spectroscopy. *Arch. Biochem. Biophys.* **2002**, 403 (1), 141–144.
188. Schnegg, A.; Fuhs, M.; Rohrer, M.; Lubitz, W.; Prisner, T. F.; Möbius, K. 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* **2002**, 106 (36), 9454–9462.
189. Witt, H.; Schlodder, E.; Teutloff, C.; Niklas, J.; Bordignon, E.; Carbonera, D.; Kohler, S.; Labahn, A.; Lubitz, W. Hydrogen bonding to P700: Site-directed mutagenesis of threonine A739 of photosystem I in *Chlamydomonas reinhardtii*. *Biochemistry* **2002**, 41 (27), 8557–8569.
190. Johnson, E. T.; Müh, F.; Nbedryk, E.; Williams, J. C.; Allen, J. P.; Lubitz, W.; Breton, J.; Parson, W. W. 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* **2002**, 106 (45), 11859–11869.
191. Lubitz, W. Pulse EPR and ENDOR Studies of Light-induced Radicals and Triplet States in Photosystem II of Oxygenic Photosynthesis. *Phys. Chem. Chem. Phys.* **2002**, 4 (22), 5539–5545.
192. Foerster, S.; Stein, M.; Brecht, M.; Ogata, H.; Higuchi, Y.; Lubitz, W. Single Crystal EPR Studies of the Reduced Active Site of [NiFe] Hydrogenase from *Desulfiovibrio vulgaris* Miyazaki F. *J. Am. Chem. Soc.* **2003**, 125 (1), 83–93.
193. Sarrou, J.; Isgandarova, S.; Kern, J.; Zouni, A.; Renger, G.; Lubitz, W.; Messinger, J. Nitric Oxide-induced Formation of the S-2 State in the Oxygen-evolving

- Complex of Photosystem II from *Synechococcus elongatus*. *Biochemistry* **2003**, 42 (4), 1016–1023.
194. Schäfer, K. O.; Bittl, R.; Lendzian, F.; Barynin, V.; Weyhermüller, T.; Wieghardt, K.; Lubitz, W. Multi-frequency EPR investigation of dimanganese catalase and related Mn(III)Mn(IV) Complexes. *J. Phys. Chem. B* **2003**, 107 (5), 1242–1250.
195. Lassmann, G.; Kolberg, M.; Bleifuss, G.; Gräslund, A.; Sjöberg, B. M.; Lubitz, W. Protein Thiyl Radicals in Disordered Systems: A Comparative EPR Study at Low Temperature. *Phys. Chem. Chem. Phys.* **2003**, 5 (11), 2442–2453.
196. Lubitz, W. Photochemical Processes in Photosynthesis Studied by Advanced Electron Paramagnetic Resonance Techniques. *Pure Appl. Chem.* **2003**, 75 (8), 1021–1030.
197. Lubitz, W.; Brecht, M.; Foerster, S.; van Gastel, M.; Stein, M. EPR and ENDOR Studies of [NiFe] Hydrogenase: Contributions to Understanding the Mechanism of Biological Hydrogen Conversion. In *Paramagnetic Resonance of Metallobiomolecules*; Telser, J., Ed. ACS Symposium Series, American Chemical Society: Washington, DC, **2003**; Vol. 858, pp 128–149.
198. Lendzian, F.; Bittl, R.; Telfer, A.; Lubitz, W. Hyperfine Structure of the Photoexcited Triplet State $^3P_{680}$ in Plant PS II Reaction Centres as Determined by Pulse ENDOR Spectroscopy. *Biochim. Biophys. Acta, Bioenerg.* **2003**, 1605 (1–3), 35–46.
199. Kammel, M.; Kern, J.; Lubitz, W.; Bittl, R. Photosystem II Single Crystals Studied by Transient EPR: The Light-induced Triplet State. *Biochim. Biophys. Acta, Bioenerg.* **2003**, 1605 (1–3), 47–54.
200. Plato, M.; Krauß, N.; Fromme, P.; Lubitz, W. Molecular Orbital Study of the Primary Electron Donor P700 of Photosystem I Based on a Recent X-ray Single Crystal Structure Analysis. *Chem. Phys.* **2003**, 294 (3), 483–499.
201. Müller, M. G.; Niklas, J.; Lubitz, W.; Holzwarth, A. R. 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. *Biophys. J.* **2003**, 85 (6), 3899–3922.
202. Fuchs, M. R.; Schnegg, A.; Plato, M.; Schulz, C.; Müh, F.; Lubitz, W.; Möbius, K. 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.* **2003**, 294 (3), 371–384.
203. Flores, M.; Isaacson, R. A.; Calvo, R.; Feher, G.; Lubitz, W. Probing Hydrogen Bonding to Quinone Anion Radicals by 1H and 2H ENDOR spectroscopy at 35 GHz. *Chem. Phys.* **2003**, 294 (3), 401–413.
204. Brecht, M.; van Gastel, M.; Buhrke, T.; Friedrich, B.; Lubitz, W. Direct Detection of a Hydrogen Ligand in the [NiFe] Center of the Regulatory H_2 -sensing Hydrogenase from *Ralstonia eutropha* in Its Reduced State by HYSCORE and ENDOR Spectroscopy. *J. Am. Chem. Soc.* **2003**, 125 (43), 13075–13083.
205. Fichtner, C.; van Gastel, M.; Lubitz, W. Wavelength Dependence of the Photoinduced Conversion of the Ni–C to the Ni–L Redox State in the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F. *Phys. Chem. Chem. Phys.* **2003**, 5 (24), 5507–5513.
206. Witt, H.; Bordignon, E.; Carbonera, D.; Dekker, J. P.; Karapetyan, N.; Teutloff, C.; Webber, A.; Lubitz, W.; Schlodder, E. Species-specific Differences of the Spectroscopic Properties of P700 - Analysis of the Influence of Nonconserved Amino Acid Residues by Site-directed Mutagenesis of Photosystem I from *Chlamydomonas reinhardtii*. *J. Biol. Chem.* **2003**, 278 (47), 46760–46771.
207. Van Gastel, M.; Lubitz, W.; Lassmann, G.; Neese, F. Electronic Structure of the Cysteine Thiyl Radical: A DFT and Correlated *ab initio* Study. *J. Am. Chem. Soc.* **2004**, 126 (7), 2237–2246.
208. Sinnecker, S.; Neese, F.; Noodleman, L.; Lubitz, W. 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.* **2004**, 126 (8), 2613–2622.
209. Sinnecker, S.; Reiher, E.; Neese, F.; Lubitz, W. Hydrogen Bond Geometries from Electron Paramagnetic Resonance and Electron–Nuclear Double Resonance Parameters: Density Functional Study of Quinone Radical Anion-Solvent Interactions. *J. Am. Chem. Soc.* **2004**, 126 (10), 3280–3290.
210. Teutloff, C.; Bittl, R.; Lubitz, W. Pulse ENDOR Studies on the Radical Pair $P_{700}^{++}A_1^{\bullet}$ and the Photoaccumulated Quinone Acceptor A_1^{\bullet} of Photosystem I. *Appl. Magn. Reson.* **2004**, 26 (1–2), 5–21.
211. Stein, M.; Lubitz, W. Relativistic DFT Calculation of the Reaction Cycle Intermediates of [NiFe] Hydrogenase: A Contribution to Understanding the Enzymatic Mechanism. *J. Inorg. Biochem.* **2004**, 98 (5), 862–877.
212. D’Amelio, N.; Gaggelli, E.; Mlynarz, P.; Molteni, E.; Valensin, G.; Lubitz, W. NMR Structural Model of the Interaction of Herbicides with the Photosynthetic Reaction Center from *Rhodobacter sphaeroides*. *ChemBioChem* **2004**, 5 (9), 1237–1244.
213. Pushkar, Y. N.; Stehlik, D.; van Gastel, M.; Lubitz, W. An EPR/ENDOR Study of the Asymmetric Hydrogen Bond Between the Quinone Electron Acceptor and the Protein Backbone in Photosystem I. *J. Mol. Struct.* **2004**, 700 (1–3), 233–241.
214. Koulougliotis, D.; Teutloff, C.; Sanakis, Y.; Lubitz, W.; Petrouleas, V. The $S_1Y_Z^{\bullet}$ Metalloradical Intermediate in Photosystem II: An X- and W-Band EPR Study. *Phys. Chem. Chem. Phys.* **2004**, 6 (20), 4859–4863.
215. Lubitz, W. EPR in Photosynthesis. In *Electron Paramagnetic Resonance. A Specialist Periodical Report*; Gilbert, B., Davies, M., Murphy, D., Eds. Royal Society of Chemistry: Cambridge, **2004**; Vol. 19 (5), pp 174–242.
216. Lassmann, G.; Schmidt, P. P.; Lubitz, W. An Advanced EPR Stopped-flow Apparatus Based on a Dielectric Ring Resonator. *J. Magn. Reson.* **2005**, 172 (2), 312–323.
217. Foerster, S.; van Gastel, M.; Brecht, M.; Lubitz, W. An Orientation-selected ENDOR and HYSCORE Study of the Ni–C Active State of *Desulfovibrio vulgaris* Miyazaki F Hydrogenase. *J. Biol. Inorg. Chem.* **2005**, 10 (1), 51–62.
218. Goenka, A.; Voordouw, J. K.; Lubitz, W.; Gärtner, W.; Voordouw, G. Construction of a [NiFe]-Hydrogenase Deletion Mutant of *Desulfovibrio vulgaris* Hildenborough. *Biochem. Soc. Trans.* **2005**, 33, 59–60.
219. Van Gastel, M.; Fichtner, C.; Neese, F.; Lubitz, W. EPR Experiments to Elucidate the Structure of the Ready and

- Unready States of the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F. *Biochem. Soc. Trans.* **2005**, *33*, 7–11.
220. Kolberg, M.; Logan, D. T.; Bleifuss, G.; Pötsch, S.; Sjöberg, B. M.; Gräslund, A.; Lubitz, W.; Lassmann, G. N.; Lendzian, F. A New Tyrosyl Radical on Phe²⁰⁸ as Ligand to the Diiron Center in *Escherichia coli* Ribonucleotide Reductase, Mutant R2-Y122H: Combined X-ray Diffraction and EPR/ENDOR Studies. *J. Biol. Chem.* **2005**, *280* (12), 11233–11246.
221. Holzwarth, A. R.; Müller, M. G.; Niklas, J.; Lubitz, W. Charge Recombination Fluorescence in Photosystem I Reaction Centers from *Chlamydomonas reinhardtii*. *J. Phys. Chem. B* **2005**, *109* (12), 5903–5911.
222. Kulik, L. V.; Epel, B.; Messinger, J.; Lubitz, W. Pulse EPR, ⁵⁵Mn-ENDOR and ELDOR-Detected NMR of the S₂-State of the Oxygen Evolving Complex in Photosystem II. *Photosynth. Res.* **2005**, *84* (1–3), 347–353.
223. Kulik, L. V.; Epel, B.; Lubitz, W.; Messinger, J. ⁵⁵Mn Pulse ENDOR at 34 GHz of the S₀ and S₂ States of the Oxygen-Evolving Complex in Photosystem II. *J. Am. Chem. Soc.* **2005**, *127* (8), 2392–2393.
224. Pogni, R.; Baratto, M. C.; Giansanti, S.; Teutloff, C.; Verdin, J.; Valderrama, B.; Lendzian, F.; Lubitz, W.; Vazquez-Duhalt, R.; Basosi, R. Tryptophan-based Radical in the Catalytic Mechanism of Versatile Peroxidase from *Bjerkandera adusta*. *Biochemistry* **2005**, *44* (11), 4267–4274.
225. Epel, B.; Schäfer, K. O.; Quentmeier, A.; Friedrich, C.; Lubitz, W. Multifrequency EPR Analysis of the Dimanganese Cluster of the Putative Sulfate Thiohydrolase SoxB of *Paracoccus pantotrophus*. *J. Biol. Inorg. Chem.* **2005**, *10* (6), 636–642.
226. Holzwarth, A. R.; Müller, M. G.; Niklas, J.; Witt, H.; Lubitz, W. A New Model for the Energy Transfer and Early Electron Transfer Processes in Photosystem I. In *Photosynthesis: Fundamental Aspects to Global Perspectives*; van der Est, A., Bruce, D., Eds. Int. Soc. Photosynth.: **2005**; pp 52–54.
227. Kulik, L. V.; Epel, B.; Lubitz, W.; Messinger, J. Q-band Pulse EPR and ⁵⁵Mn-ENDOR Studied of the S₀-State of the Oxygen Evolving Complex in Photosystem II. In *Photosynthesis: Fundamental Aspects to Global Perspectives*; van der Est, A., Bruce, D., Eds. Int. Soc. Photosynth.: **2005**; pp 380–382.
228. Sinnecker, S.; Neese, F.; Lubitz, W. Dimanganese Catalase-Spectroscopic Parameters from Broken-Symmetry Density Functional Theory of the Superoxidized Mn^{III}/Mn^{IV} State. *J. Biol. Inorg. Chem.* **2005**, *10* (3), 231–238.
229. Kulik, L. V.; Lubitz, W.; Messinger, J. Electron Spin-Lattice Relaxation of the S₀ State of the Oxygen-Evolving Complex in Photosystem II and of Dinuclear Manganese Model Complexes. *Biochemistry* **2005**, *44* (26), 9368–9374.
230. Petersen, J.; Geßner, C.; Fisher, K.; Mitchell, C. J.; Lowe, D. J.; Lubitz, W. Mn²⁺-Adenosine Nucleotide Complexes in the Presence of the Nitrogenase Iron-Protein: Detection of Conformational Rearrangements Directly at the Nucleotide Binding Site by EPR and 2D-ESEEM Spectroscopy. *Biochem. J.* **2005**, *391*, 527–539.
231. Teutloff, C.; Schäfer, K. O.; Sinnecker, S.; Barynin, V.; Bittl, R.; Wieghardt, K.; Lendzian, F.; Lubitz, W. High-Field EPR Investigations of Mn^{III}Mn^{IV} and Mn^{II}Mn^{III} States of Dimanganese Catalase and Related Model Systems. *Magn. Reson. Chem.* **2005**, *43*, S51–S64.
232. Lubitz, W. EPR Studies of the Primary Electron Donor P700 in Photosystem I. In *Photosystem I: The Light-Driven Plastocyanin: Ferredoxin Oxidoreductase*; Golbeck, J. H., Ed. Springer: Dordrecht, The Netherlands, **2006**; pp 245–269.
233. Holzwarth, A. R.; Müller, M. G.; Niklas, J.; Lubitz, W. Ultrafast Transient Absorption Studies on Photosystem I Reaction Centers from *Chlamydomonas reinhardtii*. 2: Mutations Near the P700 Reaction Center Chlorophylls Provide New Insight Into the Nature of the Primary Electron Donor. *Biophys. J.* **2006**, *90* (2), 552–565.
234. Van Gastel, M.; Stein, M.; Brecht, M.; Schröder, O.; Lendzian, F.; Bittl, R.; Ogata, H.; Higuchi, Y.; Lubitz, W. A Single-Crystal ENDOR and Density Functional Theory Study of the Oxidized States of the [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F. *J. Biol. Inorg. Chem.* **2006**, *11* (1), 41–51.
235. Biglino, D.; Schmidt, P. P.; Reijerse, E. J.; Lubitz, W. PELDOR Study on the Tyrosyl Radicals in the R2 Protein of Mouse Ribonucleotide Reductase. *Phys. Chem. Chem. Phys.* **2006**, *8* (1), 58–62.
236. Flores, M.; Isaacson, R.; Abresch, E.; Calvo, R.; Lubitz, W.; Feher, G. Protein–Cofactor Interactions in Bacterial Reaction Centers from *Rhodobacter sphaeroides* R-26: I. Identification of the ENDOR Lines Associated with the Hydrogen Bonds to the Primary Quinone Q_A^{•−}. *Biophys. J.* **2006**, *90* (9), 3356–3362.
237. Goenka Agrawal, A.; van Gastel, M.; Gärtner, W.; Lubitz, W. 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* **2006**, *110* (15), 8142–8150.
238. Epel, B.; Niklas, J.; Sinnecker, S.; Zimmermann, H.; Lubitz, W. Phylloquinone and Related Radical Anions Studied by Pulse Electron Nuclear Double Resonance Spectroscopy at 34 GHz and Density Functional Theory. *J. Phys. Chem. B* **2006**, *110* (23), 11549–11560.
239. Fichtner, C.; Laurich, C.; Bothe, E.; Lubitz, W. Spectroelectrochemical Characterization of the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F. *Biochemistry* **2006**, *45* (32), 9706–9716.
240. Vincent, K. A.; Belsey, N. A.; Lubitz, W.; Armstrong, F. A. Rapid and Reversible Reactions of [NiFe]-hydrogenases with Sulfide. *J. Am. Chem. Soc.* **2006**, *128* (23), 7448–7449.
241. Mennenga, A.; Gärtner, W.; Lubitz, W.; Görner, H. Effects of Noncovalently Bound Quinones on the Ground and Triplet States of Zinc Chlorins in Solution and Bound to *de novo* Synthesized Peptides. *Phys. Chem. Chem. Phys.* **2006**, *8* (46), 5444–5453.
242. Sinnecker, S.; Flores, M.; Lubitz, W. 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.* **2006**, *8* (48), 5659–5670.
243. Epel, B.; Niklas, J.; Antonkine, M. L.; Lubitz, W. Absolute Signs of Hyperfine Coupling Constants as Determined

- by Pulse ENDOR of Polarized Radical Pairs. *Appl. Magn. Reson.* **2006**, 30 (3–4), 311–327.
244. Reijerse, E.; Schmidt, P. P.; Klishin, G.; Lubitz, W. A CW and Pulse EPR Spectrometer Operating at 122 and 244 GHz Using a Quasi-optical Bridge and a Cryogen-free 12 T Superconducting Magnet. *Appl. Magn. Reson.* **2007**, 31 (3–4), 611–626.
245. Schnegg, A.; Dubinskii, A. A.; Fuchs, M. R.; Grishin, Y. A.; Kirilina, E. P.; Lubitz, W.; Plato, M.; Savitsky, A.; Möbius, K. High-Field EPR, ENDOR and ELDOR on Bacterial Photosynthetic Reaction Centers. *Appl. Magn. Reson.* **2007**, 31 (1–2), 59–98.
246. Lubitz, W.; van Gestel, M.; Gärtner, W. Nickel Iron Hydrogenases. *Met. Ions Life Sci.* **2007**, 2, 279–322.
247. Flores, M.; Isaacson, R.; Abresch, E.; Calvo, R.; Lubitz, W.; Feher, G. Protein–Cofactor Interactions in Bacterial Reaction Centers from *Rhodobacter sphaeroides* R-26: II. Geometry of the Hydrogen Bonds to the Primary Quinone Q_A^{\bullet} by ^1H and ^2H ENDOR Spectroscopy. *Biophys. J.* **2007**, 92 (2), 671–682.
248. Schröder, O.; Bleijlevens, B.; de Jongh, T. E.; Chen, Z. J.; Li, T. S.; Fischer, J.; Förster, J.; Friedrich, C. G.; Bagley, K. A.; Albracht, S. P. J.; Lubitz, W. Characterization of a Cyanobacterial-like Uptake [NiFe] Hydrogenase: EPR and FTIR Spectroscopic Studies of the Enzyme from *Acidithiobacillus ferrooxidans*. *J. Biol. Inorg. Chem.* **2007**, 12 (2), 212–233.
249. Savitsky, A.; Dubinskii, A. A.; Flores, M.; Lubitz, W.; Möbius, K. 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* **2007**, 111 (22), 6245–6262.
250. Reijerse, E. J.; Sommerhalter, M.; Hellwig, P.; Quentmeier, A.; Rother, D.; Laurich, C.; Bothe, E.; Lubitz, W.; Friedrich, C. G. The Unusual Redox Centers of SoxXA, a Novel *c*-type Heme-enzyme Essential for Chemotrophic Sulfur-oxidation of *Paracoccus pantotrophus*. *Biochemistry* **2007**, 46 (26), 7804–7810.
251. Kulik, L. V.; Epel, B.; Lubitz, W.; Messinger, J. Electronic Structure of the $\text{Mn}_4\text{O}_x\text{Ca}$ Cluster in the S_0 and S_2 States of the Oxygen-Evolving Complex of Photosystem II Based on Pulse ^{55}Mn ENDOR and EPR Spectroscopy. *J. Am. Chem. Soc.* **2007**, 129, 13421–13435.
252. Silakov, A.; Reijerse, E. J.; Albracht, S. P. J.; Hatchikian, E. C.; Lubitz, W. The Electronic Structure of the H-Cluster in the [FeFe]-Hydrogenase from *Desulfovibrio desulfuricans*: A Q-band ^{57}Fe ENDOR and HYSCORE Study. *J. Am. Chem. Soc.* **2007**, 129, 11447–11458.
253. Lubitz, W.; Reijerse, E.; van Gestel, M. [NiFe] and [FeFe] Hydrogenases Studied by Advanced Magnetic Resonance Techniques. *Chem. Rev.* **2007**, 107 (10), 4331–4365.
254. Lubitz, W.; Tumas, W. Hydrogen: An Overview. *Chem. Rev.* **2007**, 107 (10), 3900–3903.
255. Monien, B. H.; Drepper, F.; Sommerhalter, M.; Lubitz, W.; Haehnel, W. Detection of Heme Oxygenase Activity in a Library of Four-Helix Bundle Proteins: Toward the *de novo* Synthesis of Functional Heme Proteins. *J. Mol. Biol.* **2007**, 371 (3), 739–753.
256. Marchanka, A.; Paddock, M.; Lubitz, W.; van Gestel, M. Low-Temperature Pulsed EPR Study at 34 GHz of the Triplet States of the Primary Electron Donor P_{865} and the Carotenoid in Native and Mutant Bacterial Reaction Centers of *Rhodobacter sphaeroides*. *Biochemistry* **2007**, 46 (51), 14782–14794.
257. Niklas, J.; Schulte, T.; Prakash, S.; van Gestel, M.; Hofmann, E.; Lubitz, W. 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.* **2007**, 129 (50), 15442–15443.
258. Mennenga, A.; Gärtner, W.; Lubitz, W. Interaction of Heme- and Chlorophyll-Based Cofactors with *de novo* Synthesized Peptides. In: Peptides 2006, Proceedings 29th European Peptide Symposium, Gdansk, Poland, Kenes International, Geneva, Switzerland, **2007**, pp 388–389.
259. Zein, S.; Duboc, C.; Lubitz, W.; Neese, F. A Systematic Density Functional Study of the Zero-field Splitting in Mn(II) Coordination Compounds. *Inorg. Chem.* **2008**, 47 (1), 134–142.
260. Denysenkov, V. P.; Biglino, D.; Lubitz, W.; Prisner, T. F.; Bennati, M. Structure of the Tyrosyl Biradical in Mouse R2 Ribonucleotide Reductase from High-Field PELDOR. *Angew. Chem., Int. Ed.* **2008**, 47 (7), 1224–1227.
261. Su, J. H.; Lubitz, W.; Messinger, J. Probing Mode and Site of Substrate Water Binding to the Oxygen-Evolving Complex in the S_2 State of Photosystem II by ^{17}O -HYSCORE Spectroscopy. *J. Am. Chem. Soc.* **2008**, 130 (3), 786–787. Correction published: *J. Am. Chem. Soc.* **2011**, 133, 12317.
262. Zein, S.; Kulik, L. V.; Yano, J.; Kern, J.; Pushkar, Y.; Zouni, A.; Yachandra, V. K.; Lubitz, W.; Neese, F.; Messinger, J. Focusing the View on Nature's Water-Splitting Catalyst. *Philos. Trans. R. Soc., B* **2008**, 363 (1494), 1167–1177.
263. Niklas, J.; Prakash, S.; Schulte, T.; van Gestel, M.; Hofmann, E.; Lubitz, W. 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. In *Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis*; Allen, J. F., Golbeck, J. H., Osmond, B., Eds. Springer: Dordrecht, The Netherlands, **2008**; pp 291–294.
264. Marchanka, A.; Lubitz, W.; Paddock, M.; van Gestel, M. Triplet States in Photosynthetic Reaction Centers of *Rb. sphaeroides*. In *Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis*; Allen, J. F., Golbeck, J. H., Osmond, B., Eds. Springer: Dordrecht, The Netherlands, **2008**; pp 133–136.
265. Antonkine, M. L.; Breitenstein, C.; Epel, B.; Bill, E.; Gärtner, W.; Lubitz, W. *De Novo* Peptides Modeling the Binding Sites of [4Fe-4S] Clusters in Photosystem I. In *Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis*; Allen, J. F., Golbeck, J. H., Osmond, B., Eds. Springer: Dordrecht, The Netherlands, **2008**; pp 1257–1260.
266. Su, J. H.; Lubitz, W.; Messinger, J. Substrate Water Bound to the S_2 -State of the $\text{Mn}_4\text{O}_x\text{Ca}$ Cluster in Photosystem II Studied by Advanced Pulse EPR Spectroscopy. In *Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis*; Allen, J. F., Golbeck, J. H., Osmond, B., Eds. Springer: Dordrecht, The Netherlands, **2008**; pp 503–507.

267. Flores, M.; Savitsky, A.; Abresch, E. C.; Lubitz, W.; Möbius, K. Structure of Radical Pairs $D^{+\bullet}Q_A^{\bullet}$ in Bacterial Photosynthetic Reaction Centers Cooled to Cryogenic Temperatures in the Dark and Under Illumination: A High-Field EPR/PELDOR Study. In *Photosynthesis. Energy from the Sun: 14th International Congress on Photosynthesis*; Allen, J. F., Golbeck, J. H., Osmond, B., Eds. Springer: Dordrecht, The Netherlands, **2008**; pp 59–63.
268. Flores, M.; Goenka Agrawal, A.; van Gestel, M.; Gärtner, W.; Lubitz, W. Electron–Electron Double Resonance-Detected NMR to Measure Metal Hyperfine Interactions: ^{61}Ni in the Ni–B State of the [NiFe] Hydrogenase of *Desulfovibrio vulgaris* Miyazaki F. *J. Am. Chem. Soc.* **2008**, 130 (8), 2402–2403.
269. Kamp, C.; Silakov, A.; Winkler, M.; Reijerse, E. J.; Lubitz, W.; Happe, T. Isolation and First EPR Characterization of the [FeFe]-Hydrogenases from Green Algae. *Biochim. Biophys. Acta* **2008**, 1777 (5), 410–416.
270. Fedin, M.; Ovcharenko, V.; Sagdeev, R.; Reijerse, E.; Lubitz, W.; Bagryanskaya, E. Light-Induced Excited Spin State Trapping in an Exchange-Coupled Nitroxide-Copper(II)-Nitroxide Cluster. *Angew. Chem., Int. Ed.* **2008**, 47 (36), 6897–6899.
271. Koay, M. S.; Antonkine, M. L.; Gärtner, W.; Lubitz, W. Modeling Low-Potential $[\text{Fe}_4\text{S}_4]$ Clusters in Proteins. *Chem. Biodiversity* **2008**, 5 (8), 1571–1587.
272. Kellers, P.; Ogata, H.; Lubitz, W. Purification, Crystallization and Preliminary X-ray Analysis of the Membrane-bound [NiFe] Hydrogenase from *Allochrochromatium vinosum*. *Acta Crystallogr.* **2008**, F64, 719–722.
273. Lubitz, W.; Reijerse, E. J.; Messinger, J. Solar Water-Splitting into H_2 and O_2 : Design Principles of Photosystem II and Hydrogenases. *Energy Environ. Sci.* **2008**, 1 (1), 15–31.
274. Brogioni, B.; Biglino, D.; Sinicropi, A.; Reijerse, E. J.; Giardina, P.; Sannia, G.; Lubitz, W.; Basosi, R.; Pogni, R. Characterization of Radical Intermediates in Laccase-Mediator Systems. A Multifrequency EPR, ENDOR and DFT/PCM Investigation. *Phys. Chem. Chem. Phys.* **2008**, 10 (48), 7284–7292.
275. Ogata, H.; Goenka Agrawal, A.; Kaur, A. P.; Goddard, R.; Gärtner, W.; Lubitz, W. Purification, Crystallization and Preliminary X-ray Analysis of Adenylylsulfate Reductase from *Desulfovibrio vulgaris* Miyazaki F. *Acta Crystallogr.* **2008**, F64, 1010–1012.
276. Van Gestel, M.; Shaw, J. L.; Blake, A. J.; Flores, M.; Schröder, M.; McMaster, J.; Lubitz, W. Electronic Structure of a Binuclear Nickel Complex of Relevance to [NiFe] Hydrogenase. *Inorg. Chem.* **2008**, 47 (24), 11688–11697.
277. Van Gestel, M.; Lubitz, W. EPR Investigation of [NiFe] Hydrogenases. In *High Resolution EPR: Applications to Metalloenzymes and Metals in Medicine*; Hanson, G. R., Berliner, L. J., Eds. Springer: **2009**; pp 441–470.
278. Allen, J. P.; Cordova, J. M.; Jolley, C. C.; Murray, T. A.; Schneider, J. W.; Woodbury, N. W.; Williams, J. C.; Niklas, J.; Klihm, G.; Reus, M.; Lubitz, W. EPR, ENDOR, and Special TRIPLE measurements of $\text{P}^{+\bullet}$ in Wild Type and Modified Reaction Centers from *Rb. sphaeroides*. *Photosynth. Res.* **2009**, 99 (1), 1–10.
279. Silakov, A.; Wenk, B.; Reijerse, E.; Albracht, S. P. J.; Lubitz, W. Spin Distribution of the H-Cluster in the H_{ox} -CO State of the [FeFe] Hydrogenase from *Desulfovibrio desulfuricans*: HYSCORE and ENDOR Study of ^{14}N and ^{13}C Nuclear Interactions. *J. Biol. Inorg. Chem.* **2009**, 14 (2), 301–313.
280. Van Gestel, M.; Lu, C. C.; Wieghardt, K.; Lubitz, W. Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Investigation of the Diradical Bis(α -Iminopyridinato)Zinc Complex. *Inorg. Chem.* **2009**, 48 (6), 2626–2632.
281. Kulik, L. V.; Lubitz, W. Electron–Nuclear Double Resonance. *Photosynth. Res.* **2009**, 102 (2–3), 391–401.
282. Reijerse, E. J.; Silakov, A.; Lubitz, W. In Search of Nonfossil Fuels. Understanding the Active Site of [FeFe] Hydrogenase: Basis for a Biohydrogen Technology. In *The Treasures of Eureka. Volume 1. Electron Paramagnetic Resonance. From Fundamental Research to Pioneering Applications & Zavoisky Award*; Salikhov, K. M., Ed. AXAS Publishing Ltd.: Wellington, New Zealand, **2009**; Vol. 1, pp 166–167.
283. Messinger, J.; Kulik, L. V.; Lubitz, W. Mastering Sustainable Energy. Light-induced Water-splitting in Nature: Electronic Structure of the Manganese Cluster in Photosystem II. In *The Treasures of Eureka. Volume 1. Electron Paramagnetic Resonance. From Fundamental Research to Pioneering Applications & Zavoisky Award*; Salikhov, K. M., Ed. AXAS Publishing Ltd.: Wellington, New Zealand, **2009**; Vol. 1, pp 164–165.
284. Feher, G.; Lubitz, W.; Möbius, K. The Most Important Biochemical Process on Earth. EPR and ENDOR of Primary Reactants in Bacterial Photosynthesis. In *The Treasures of Eureka. Volume 1. Electron Paramagnetic Resonance. From Fundamental Research to Pioneering Applications & Zavoisky Award*; Salikhov, K. M., Ed. AXAS Publishing Ltd.: Wellington, New Zealand, **2009**; Vol. 1, pp 158–159.
285. Antonkine, M. L.; Koay, M. S.; Epel, B.; Breitenstein, C.; Gupta, O.; Gärtner, W.; Bill, E.; Lubitz, W. Synthesis and Characterization of *de novo* Designed Peptides Modeling the Binding Sites of $[\text{4Fe-4S}]$ Clusters in Photosystem I. *Biochim. Biophys. Acta, Bioenerg.* **2009**, 1787 (8), 995–1008.
286. Conlan, B.; Cox, N.; Su, J. H.; Hillier, W.; Messinger, J.; Lubitz, W.; Dutton, P. L.; Wydrzynski, T. Photocatalytic Oxidation of a Di-Nuclear Manganese Centre in an Engineered Bacterioferritin ‘Reaction Centre’. *Biochim. Biophys. Acta, Bioenerg.* **2009**, 1787 (9), 1112–1121.
287. Pantazis, D. A.; Orto, M.; Petrenko, T.; Zein, S.; Bill, E.; Lubitz, W.; Messinger, J.; Neese, F. 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.* **2009**, 15 (20), 5108–5123.
288. Marchanka, A.; Lubitz, W.; van Gestel, M. Spin Density Distribution of the Excited Triplet State of Bacteriochlorophylls. Pulsed ENDOR and DFT Studies. *J. Phys. Chem. B* **2009**, 113 (19), 6917–6927.
289. Silakov, A.; Wenk, B.; Reijerse, E.; Lubitz, W. ^{14}N HYSCORE Investigation of the H-Cluster of [FeFe] Hydrogenase: Evidence for a Nitrogen in the Dithiol Bridge. *Phys. Chem. Chem. Phys.* **2009**, 11 (31), 6592–6599.

290. Niklas, J.; Epel, B.; Antonkine, M. L.; Sinnecker, S.; Pandelia, M. E.; Lubitz, W. Electronic Structure of the Quinone Radical Anion $A_1^{\bullet-}$ of Photosystem I Investigated by Advanced Pulse EPR and ENDOR Techniques. *J. Phys. Chem. B* **2009**, 113 (30), 10367–10379.
291. Ogata, H.; Lubitz, W.; Higuchi, Y. [NiFe] Hydrogenases: Structural and Spectroscopic Studies of the Reaction Mechanism. *Dalton Trans.* **2009**, (37), 7577–7587.
292. Fedin, M. V.; Veber, S. L.; Romanenko, G. V.; Ovcharenko, V. I.; Sagdeev, R. Z.; Klihm, G.; Reijerse, E.; Lubitz, W.; Bagryanskaya, E. G. 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.* **2009**, 11 (31), 6654–6663.
293. Pandelia, M. E.; Ogata, H.; Currell, L. J.; Flores, M.; Lubitz, W. Probing Intermediates in the Activation Cycle of [NiFe] Hydrogenase by Infrared Spectroscopy: The Ni–SI₁ State and its Light Sensitivity. *J. Biol. Inorg. Chem.* **2009**, 14 (8), 1227–1241.
294. Pantazis, D. A.; Orio, M.; Petrenko, T.; Zein, S.; Lubitz, W.; Messinger, J.; Neese, F. 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.* **2009**, 11 (31), 6788–6798.
295. Silakov, A.; Kamp, C.; Reijerse, E.; Happe, T.; Lubitz, W. Spectroelectrochemical Characterization of the Active Site of the [FeFe] Hydrogenase HydA1 from *Chlamydomonas reinhardtii*. *Biochemistry* **2009**, 48 (33), 7780–7786.
296. Ogata, H.; Stolle, P.; Stehr, M.; Auling, G.; Lubitz, W. Crystallization and Preliminary X-ray Analysis of the Small Subunit (R2F) of Native Ribonucleotide Reductase from *Corynebacterium ammoniagenes*. *Acta Crystallogr.* **2009**, F65, 878–880.
297. Kellers, P.; Pandelia, M. E.; Currell, L. J.; Görner, H.; Lubitz, W. 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.* **2009**, 11 (39), 8680–8683.
298. Millo, D.; Pandelia, M. E.; Utesch, T.; Wisitruangsakul, N.; Mroginski, M. A.; Lubitz, W.; Hildebrandt, P.; Zebger, I. Spectroelectrochemical Study of the [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F in Solution and Immobilized on Biocompatible Gold Surfaces. *J. Phys. Chem. B* **2009**, 113 (46), 15344–15351.
299. Van der Est, A.; Pushkar, Y.; Karyagina, I.; Fonovic, B.; Dudding, T.; Niklas, J.; Lubitz, W.; Golbeck, J. H. Incorporation of 2,3-Disubstituted-1,4-Naphthoquinones into the A₁ Binding Site of Photosystem I Studied by EPR and ENDOR Spectroscopy. *Appl. Magn. Reson.* **2010**, 37 (1–4), 65–83.
300. Pandelia, M. E.; Ogata, H.; Currell, L. J.; Flores, M.; Lubitz, W. Inhibition of the [NiFe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F by Carbon Monoxide: An FTIR and EPR Spectroscopic Study. *Biochim. Biophys. Acta, Bioenerg.* **2010**, 1797 (2), 304–313.
301. Niklas, J.; Gupta, O.; Epel, B.; Lubitz, W.; Antonkine, M. L. Investigation of the Stationary and Transient $A_1^{\bullet-}$ Radical in Trp → Phe Mutants of Photosystem I. *Appl. Magn. Reson.* **2010**, 38 (2), 187–203.
302. Czech, I.; Silakov, A.; Lubitz, W.; Happe, T. The [FeFe]-Hydrogenase Maturase HydF from *Clostridium acetobutylicum* Contains a CO and CN[−] Ligated Iron Cofactor. *FEBS Lett.* **2010**, 584 (3), 638–642.
303. Saggiu, M.; Teutloff, C.; Ludwig, M.; Brecht, M.; Pandelia, M. E.; Lenz, O.; Friedrich, B.; Lubitz, W.; Hildebrandt, P.; Lendzian, F.; Bittl, R. 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.* **2010**, 12 (9), 2139–2148.
304. Pandelia, M. E.; Ogata, H.; Lubitz, W. Intermediates in the Catalytic Cycle of [NiFe] Hydrogenase: Functional Spectroscopy of the Active Site. *ChemPhysChem* **2010**, 11 (6), 1127–1140.
305. Grzyb, J.; Xu, F.; Weiner, L.; Reijerse, E. J.; Lubitz, W.; Nanda, V.; Noy, D. De Novo Design of a Non-Natural Fold for an Iron–Sulfur Protein: α -Helical Coiled-Coil with a Four-Iron Four-Sulfur Cluster Binding Site in its Central Core. *Biochim. Biophys. Acta, Bioenerg.* **2010**, 1797 (3), 406–413.
306. Pandelia, M. E.; Fourmond, V.; Tron-Infossi, P.; Lojou, E.; Bertrand, P.; Léger, C.; Giudici-Orticoni, M. T.; Lubitz, W. Membrane-Bound Hydrogenase I from the Hyperthermophilic Bacterium *Aquifex aeolicus*: Enzyme Activation, Redox Intermediates and Oxygen Tolerance. *J. Am. Chem. Soc.* **2010**, 132 (20), 6991–7004.
307. Marchanka, A.; Savitsky, A.; Lubitz, W.; Möbius, K.; van Gastel, M. 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* **2010**, 114, 14364–14372.
308. Stolle, P.; Barckhausen, O.; Oehlmann, W.; Knobbe, N.; Vogt, C.; Pierik, A. J.; Cox, N.; Schmidt, P. P.; Reijerse, E.; Lubitz, W.; Auling, G. Homologous Expression of the *nrdf* Gene of *Corynebacterium ammoniagenes* Strain ATCC 6872 Generates a Manganese–Metallocofactor (R2F) and a Stable Tyrosyl Radical (Y[•]) involved in Ribonucleotide Reductase Reduction. *FEBS J.* **2010**, 277 (23), 4849–4862.
309. Cox, N.; Ogata, H.; Stolle, P.; Reijerse, E.; Auling, G.; Lubitz, W. 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.* **2010**, 132 (32), 11197–11213.
310. Pandelia, M. E.; Infossi, P.; Giudici-Orticoni, M. T.; Lubitz, W. The Oxygen-Tolerant Hydrogenase I from *Aquifex aeolicus* Weakly Interacts with Carbon Monoxide: An Electrochemical and Time-Resolved FTIR Study. *Biochemistry* **2010**, 49 (41), 8873–8881.
311. Ogata, H.; Kellers, P.; Lubitz, W. The Crystal Structure of the [NiFe] Hydrogenase from the Photosynthetic Bacterium *Allochrocatium vinosum*: Characterization of the Oxidized Enzyme (Ni-A State). *J. Mol. Biol.* **2010**, 402 (2), 428–444.
312. Ogata, H.; Shomura, Y.; Goenka Agrawal, A.; Pal Kaur, A.; Gärtner, W.; Higuchi, Y.; Lubitz, W. Purification, Crystallization and Preliminary X-ray Analysis of the Dissimilatory Sulfite Reductase from *Desulfovibrio*

- vulgaris Miyazaki F. *Acta Crystallogr.* **2010**, F66 (11), 1470–1472.
313. Silakov, A.; Shaw, J. L.; Reijerse, E. J.; Lubitz, W. Advanced Electron Paramagnetic Resonance and Density Functional Theory Study of a {2Fe3S} Cluster Mimicking the Active Site of [FeFe] Hydrogenase. *J. Am. Chem. Soc.* **2010**, 132 (49), 17578–17587.
314. Flores, M.; Savitsky, A.; Paddock, M. L.; Abresch, E. C.; Dubinskii, A. A.; Okamura, M. Y.; Lubitz, W.; Möbius, K. 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* **2010**, 114 (50), 16894–16901.
315. Kulon, K.; Lubitz, W.; Antonkine, M. L. Modeling the Binding Site of a Linear [3Fe-4S] Cluster, In *10th European Biological Inorganic Chemistry Conference EUROBI 10*; Kessissoglou, D., Salifoglou, T., Eds. MEDIMOND: Pianoro (Bologna), 2010; pp 39–42.
316. Busch, A. W. U.; Reijerse, E. J.; Lubitz, W.; Hofmann, E.; Frankenberg-Dinkel, N. Radical Mechanism of Cyanophage Phycoerythrobilin Synthase (PebS). *Biochem. J.* **2011**, 433, 469–476.
317. Drew, S. C.; Reijerse, E. J.; Quentmeier, A.; Rother, D.; Friedrich, C. G.; Lubitz, W. Spectroscopic Characterization of the Molybdenum Cofactor of the Sulfane Dehydrogenase SoxCD from *Paracoccus pantotrophus*. *Inorg. Chem.* **2010**, 50 (2), 409–411.
318. Erdem, Ö. F.; Schwartz, L.; Stein, M.; Silakov, A.; Kaur-Ghumaan, S.; Huang, P.; Ott, S.; Reijerse, E. J.; Lubitz, W. A Model of the [FeFe] Hydrogenase Active Site with a Biologically Relevant Azadithiolate Bridge: A Spectroscopic and Theoretical Investigation. *Angew. Chem., Int. Ed.* **2011**, 50 (6), 1439–1443.
319. Millo, D.; Hildebrandt, P.; Pandelia, M. E.; Lubitz, W.; Zebger, I. SEIRA Spectroscopy of the Electrochemical Activation of an Immobilized [NiFe] Hydrogenase under Turnover and Non-Turnover Conditions. *Angew. Chem., Int. Ed.* **2011**, 50 (11), 2632–2634.
320. Silakov, A.; Reijerse, E. J.; Lubitz, W. Unraveling the Electronic Properties of the Photoinduced States of the H-Cluster in the [FeFe] Hydrogenase from *D. desulfuricans*. *Eur. J. Inorg. Chem.* **2011**, 2011 (7), 1056–1066.
321. Greco, C.; Silakov, A.; Bruschi, M.; Ryde, U.; De Gioia, L.; Lubitz, W. 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.* **2011**, 2011 (7), 1043–1049.
322. Cox, N.; Rapatskiy, L.; Su, J. H.; Pantazis, D. A.; Sugiura, M.; Kulik, L. V.; Dorlet, P.; Rutherford, A. W.; Neese, F.; Boussac, A.; Lubitz, W.; Messinger, J. Effect of Ca^{2+}/Sr^{2+} Substitution on the Electronic Structure of the Oxygen-evolving Complex of Photosystem II: A Combined Multifrequency EPR, ^{55}Mn -ENDOR, and DFT Study of the S_2 State. *J. Am. Chem. Soc.* **2011**, 133 (10), 3635–3648. Correction published: *J. Am. Chem. Soc.* **2011**, 133 (35), 14149.
323. Pandelia, M. E.; Nitschke, W.; Infossi, P.; Giudici-Orticoni, M. T.; Bill, E.; Lubitz, W. Characterization of a Unique [FeS] Cluster in the Electron Transfer Chain of the Oxygen Tolerant [NiFe] Hydrogenase from *Aquifex aeolicus*. *Proc. Natl. Acad. Sci. U.S.A.* **2011**, 108 (15), 6097–6102.
324. Su, J. H.; Cox, N.; Ames, W.; Pantazis, D. A.; Rapatskiy, L.; Lohmiller, T.; Kulik, L. V.; Dorlet, P.; Rutherford, A. W.; Neese, F.; Boussac, A.; Lubitz, W.; Messinger, J. The Electronic Structures of the S_2 States of the Oxygen-evolving Complexes of Photosystem II in Plants and Cyanobacteria in the Presence and Absence of Methanol. *Biochim. Biophys. Acta, Bioenerg.* **2011**, 1807 (7), 829–840.
325. Cohen-Ofri, I.; van Gestel, M.; Grzyb, J.; Brandis, A.; Pinkas, I.; Lubitz, W.; Noy, D. 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.* **2011**, 133, 9526–9535.
326. Sedoud, A.; Cox, N.; Sugiura, M.; Lubitz, W.; Boussac, A.; Rutherford, A. W. 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* **2011**, 50, 6012–6021.
327. Hoppe, A.; Pandelia, M. E.; Gärtner, W.; Lubitz, W. $[Fe_4S_4]^-$ and $[Fe_3S_4]$ -Cluster Formation in Synthetic Peptides. *Biochim. Biophys. Acta, Bioenerg.* **2011**, 1807, 1414–1422.
328. Busch, A. W. U.; Reijerse, E. J.; Lubitz, W.; Frankenberg-Dinkel, N.; Hofmann, E. Structural and Mechanistic Insight into the Ferredoxin-Mediated two Electron Reduction of Bilins. *Biochem. J.* **2011**, 439, 257–264.
329. Cox, N.; Ames, W.; Epel, B.; Kulik, L. V.; Rapatskiy, L.; Neese, F.; Messinger, J.; Wieghardt, K.; Lubitz, W. Electronic Structure of a Weakly Antiferromagnetically Coupled $Mn^{II}Mn^{III}$ Model Relevant to Manganese Proteins: A Combined EPR, ^{55}Mn -ENDOR, and DFT Study. *Inorg. Chem.* **2011**, 50 (17), 8238–8251.
330. Ames, W.; Pantazis, D. A.; Krewald, V.; Cox, N.; Messinger, J.; Lubitz, W.; Neese, F. Theoretical Evaluation of Structural Models of the S_2 State in the Oxygen Evolving Complex of Photosystem II: Protonation States and Magnetic Interactions. *J. Am. Chem. Soc.* **2011**, 133 (49), 19743–19757.
331. Veber, S. L.; Fedin, M. V.; Maryunina, K. Y.; Potapov, A.; Goldfarb, D.; Reijerse, E.; Lubitz, W.; Sagdeev, R. Z.; Ovcharenko, V. I.; Bagryanskaya, E. G. Temperature-Dependent Exchange Interaction in Molecular Magnets $Cu(hfac)_2L^R$ Studied by EPR: Methodology and Interpretations. *Inorg. Chem.* **2011**, 50 (20), 10204–10212.
332. Savitsky, A.; Dubinskii, A. A.; Zimmermann, H.; Lubitz, W.; Möbius, K. 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* **2011**, 115 (41), 11950–11963.
333. Möbius, K.; Lubitz, W.; Savitsky, A. Photo-Induced Electron Spin Polarization in Chemical and Biological Reactions: Probing Structure and Dynamics of Transient Intermediates by Multifrequency EPR Spectroscopy. *J. Magn. Reson.* **2011**, 41, 113–143.
334. Reijerse, E.; Lendzian, F.; Isaacson, R.; Lubitz, W. A Tunable General Purpose Q-Band Resonator for CW and Pulse EPR/ENDOR Experiments With Large

- Sample Access and Optical Excitation. *J. Magn. Reson.* **2012**, 214, 237–243.
335. Pandelia, M. E.; Infossi, P.; Stein, M.; Giudici-Orticoni, M. T.; Lubitz, W. 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.* **2012**, 48 (6), 823–825.
336. Lubitz, W.; Ogata, H.; Reijerse, E.; Higuchi, Y. Structure and Function of Hydrogenase Enzymes. In *Molecular Solar Fuels*; Wydrzynski, T. J., Hillier, W., Eds. The Royal Society of Chemistry: Cambridge, UK, **2012**; RSC Energy and Environment Series, pp 288–325.
337. Knoerzer, P.; Silakov, A.; Foster, C. E.; Armstrong, F. A.; Lubitz, W.; Happe, T. The Importance of the Protein Framework for the Catalytic Activity of [FeFe]-Hydrogenases. *J. Biol. Chem.* **2012**, 287, 1489–1499.
338. Mula, S.; Savitsky, A.; Möbius, K.; Lubitz, W.; Golbeck, J. H.; Mamedov, M. D.; Semenov, A. Y.; van der Est, A. Incorporation of a High Potential Quinone Reveals that Electron Transfer in Photosystem I Becomes Highly Asymmetric at Low Temperature. *Photochem. Photobiol. Sci.* **2012**, 11 (6), 946–956.
339. Grzyb, J.; Xu, F.; Nanda, V.; Luczkowska, R.; Reijerse, E.; Lubitz, W.; Noy, D. Empirical and Computational Design of Iron–Sulfur Cluster Proteins. *Biochim. Biophys. Acta, Bioenerg.* **2012**, 1817 (8), 1256–1262.
340. Lohmiller, T.; Cox, N.; Su, H.; Messinger, J.; Lubitz, W. 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 22–27 August 2010, Beijing*; Kuang, T., Lu, C., Zhang, L., Eds. Springer: **2012**; pp 239–243.
341. Adamska, A.; Silakov, A.; Lambert, C.; Rüdiger, O.; Happe, T.; Reijerse, E.; Lubitz, W. 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.* **2012**, 51 (46), 11458–11462.
342. Shafaat, H. S.; Weber, K.; Petrenko, T.; Neese, F.; Lubitz, W. Key Hydride Vibrational Modes in [NiFe] Hydrogenase Model Compounds Studied by Resonance Raman Spectroscopy and Density Functional Calculations. *Inorg. Chem.* **2012**, 51 (21), 11787–11797.
343. Pantazis, D. A.; Ames, W.; Cox, N.; Lubitz, W.; Neese, F. Two Interconvertible Structures that Explain the Spectroscopic Properties of the Oxygen-Evolving Complex of Photosystem II in the S₂ State. *Angew. Chem., Int. Ed.* **2012**, 51 (39), 9935–9940.
344. Pandelia, M. E.; Lubitz, W.; Nitschke, W. Evolution and Diversification of Group 1 [NiFe] Hydrogenases. Is there a Phylogenetic Marker for O₂-tolerance? *Biochim. Biophys. Acta, Bioenerg.* **2012**, 1817 (9), 1565–1575.
345. Lohmiller, T.; Cox, N.; Su, J. H.; Messinger, J.; Lubitz, W. The Basic Properties of the Electronic Structure of the Oxygen-evolving Complex of Photosystem II are not Perturbed by Ca²⁺ Removal. *J. Biol. Chem.* **2012**, 287 (29), 24721–24733.
346. Rapatskiy, L.; Cox, N.; Savitsky, A.; Ames, W. M.; Sander, J.; Nowaczyk, M. M.; Rögner, M.; Boussac, A.; Neese, F.; Messinger, J.; Lubitz, W. Detection of the Water Binding Sites of the Oxygen-Evolving Complex of Photosystem II Using W-Band ¹⁷O ELDOR-Detected NMR Spectroscopy. *J. Am. Chem. Soc.* **2012**, 134 (40), 16619–16634.
347. Flores, M.; Okamura, M. Y.; Niklas, J.; Pandelia, M. E.; Lubitz, W. Pulse Q-Band EPR and ENDOR Spectroscopies of the Photochemically Generated Monoprotonated Benzosemiquinone Radical in Frozen Alcoholic Solution. *J. Phys. Chem. B* **2012**, 116 (30), 8890–8900.
348. Hsieh, C. H.; Erdem, Ö. F.; Harman, S. D.; Singleton, M. L.; Reijerse, E. J.; Lubitz, W.; Popescu, C. V.; Reibenspies, J. H.; Brothers, S. M.; Hall, M. B.; Darensbourg, M. Y. 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.* **2012**, 134 (31), 13089–13102.
349. Silakov, A.; Olsen, M. T.; Sproules, S.; Reijerse, E. J.; Rauchfuss, T. B.; Lubitz, W. EPR/ENDOR, Mössbauer, and Quantum-Chemical Investigations of Diiron Complexes Mimicking the Active Oxidized State of [FeFe]-Hydrogenase. *Inorg. Chem.* **2012**, 51 (15), 8617–8628.
350. Tretyakov, E. V.; Tolstikov, S. E.; Suvorova, A. O.; Polushkin, A. V.; Romanenko, G. V.; Bogomyakov, A. S.; Veber, S. L.; Fedin, M. V.; Stass, D. V.; Reijerse, E.; Lubitz, W.; Zueva, E. M.; Ovcharenko, V. I. Crucial Role of Paramagnetic Ligands for Magnetostructural Anomalies in "Breathing Crystals". *Inorg. Chem.* **2012**, 51 (17), 9385–9394.
351. Karnahl, M.; Tschierlei, S.; Erdem, Ö. F.; Pullen, S.; Santoni, M. P.; Reijerse, E.; Lubitz, W.; Ott, S. Mixed-valence [Fe^IFe^{II}] Hydrogenase Active Site Model Complexes Stabilized by a Bidentate Carborane bis Phosphine Ligand. *Dalton Trans.* **2012**, 41, 12468–12477.
352. Kampa, M.; Lubitz, W.; van Gastel, M.; Neese, F. 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.* **2012**, 17 (8), 1269–1281.
353. Weber, K.; Krämer, T.; Shafaat, H. S.; Weyhermüller, T.; Bill, E.; van Gastel, M.; Neese, F.; Lubitz, W. A Functional [NiFe]-Hydrogenase Model Compound That Undergoes Biologically Relevant Reversible Thiolate Protonation. *J. Am. Chem. Soc.* **2012**, 134 (51), 20745–20755.
354. Cox, N.; Lubitz, W. Molecular Concepts of Water Splitting: Nature's Approach. In *Chemical Energy Storage*; Schlögl, R., Ed. Walter de Gruyter GmbH: Berlin/Boston, **2013**; pp 185–224.
355. Cox, N.; Lubitz, W. Molecular Concepts of Water Splitting: Nature's Approach. *Green* **2013**, 3 (5–6), 235–263.
356. Pandelia, M. E.; Bykov, D.; Izsak, R.; Infossi, P.; Giudici-Orticoni, M. T.; Bill, E.; Neese, F.; Lubitz, W. Electronic Structure of the Unique [4Fe-3S] Cluster in O₂-Tolerant Hydrogenases Characterized by ⁵⁷Fe Mössbauer and EPR Spectroscopy. *Proc. Natl. Acad. Sci. U.S.A.* **2013**, 110 (2), 483–488.
357. Lubitz, W.; Ogata, H. Hydrogenases, Structure and Function. In *The Encyclopedia of Biological Chemistry*; Lennarz, W. J., Lane, M. D., Eds. Academic Press: Waltham, MA, **2013**; pp 562–567.

358. Kamali, S.; Wang, H.; Mitra, D.; Ogata, H.; Lubitz, W.; Manor, B. C.; Rauchfuss, T. B.; Byrne, D.; Bonnefoy, V.; Jenney Jr., F. E.; Adams, M. W. W.; Yoda, Y.; Alp, E. E.; Zhao, J.; Cramer, S. P. 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.* **2013**, *52* (2), 724–728.
359. Savitsky, A.; Grishin, Y.; Rakhmatullin, R.; Reijerse, E.; Lubitz, W. An Improved Coupling Design for High-frequency TE₀₁₁ Electron Paramagnetic Resonance Cavities. *Rev. Sci. Instrum.* **2013**, *84*, 014704, DOI: 10.1063/1.4788735.
360. Shafaat, H. S.; Rüdiger, O.; Ogata, H.; Lubitz, W. [NiFe] Hydrogenases: A Common Active Site for Hydrogen Metabolism Under Diverse Conditions. *Biochim. Biophys. Acta, Bioenerg.* **2013**, 1827 (8–9), 986–1002.
361. Faunce, T. A.; Lubitz, W.; Rutherford, A. W.; MacFarlane, D.; Moore, G. F.; Yang, P.; Nocera, D. G.; Moore, T. A.; Gregory, D. H.; Fukuzumi, S.; Yoon, K. B.; Armstrong, F. A.; Wasielewski, M. R.; Styring, S. Energy and Environment Policy Case for a Global Project on Artificial Photosynthesis. *Energy Environ. Sci.* **2013**, *6*, 695–698.
362. Lubitz, W.; Cox, N. Wie Pflanzen Wasser spalten. *Spektrum der Wissenschaften* **2013**, *9*, 34–43.
363. Lohmiller, T.; Ames, W.; Lubitz, W.; Cox, N.; Misra, S. K. EPR Spectroscopy and the Electronic Structure of the Oxygen-Evolving Complex of Photosystem II. *Appl. Magn. Reson.* **2013**, *44*, 691–720.
364. He, C.; Nishikawa, K.; Erdem, Ö. F.; Reijerse, E.; Ogata, H.; Lubitz, W.; Knipp, M. Complexes of Ferriheme Nitrophorin 4 with Low-Molecular Weight Thiol(ate)s Occurring in Blood Plasma. *J. Inorg. Biochem.* **2013**, *122*, 38–48.
365. Kampa, M.; Pandelia, M. E.; Lubitz, W.; van Gastel, M.; Neese, F. A Metal–Metal Bond in the Light-induced State of [NiFe] Hydrogenases with Relevance to Hydrogen Evolution. *J. Am. Chem. Soc.* **2013**, *135* (10), 3915–3925.
366. Cox, N.; Pantazis, D. A.; Neese, F.; Lubitz, W. Biological Water Oxidation. *Acc. Chem. Res.* **2013**, *46* (7), 1588–1596.
367. Berggren, G.; Adamska, A.; Lambert, C.; Simmons, T. R.; Esselborn, J.; Atta, M.; Gambarelli, S.; Mousca, J. M.; Reijerse, E.; Lubitz, W.; Happe, T.; Artero, V.; Fontecave, M. Biomimetic Assembly and Activation of [FeFe]-Hydrogenases. *Nature* **2013**, *499* (7456), 66–69.
368. Thapper, A.; Styring, S.; Saraccao, G.; Rutherford, A. W.; Robert, B.; Magnuson, A.; Lubitz, W.; Llobet, A.; Kurz, P.; Holzwarth, A. R.; Fiechter, S.; de Groot, H.; Campagna, S.; Braun, A.; Bergacol, H.; Vincent, A. Artificial Photosynthesis for Solar Fuels - an Evolving Research Field within AMPEA, a Joint Programme of the European Energy Research Alliance. *Green* **2013**, *3* (1), 43–57.
369. Savitsky, A.; Niklas, J.; Golbeck, J. H.; Möbius, K.; Lubitz, W. Orientation Resolving Dipolar High-Field EPR Spectroscopy on Disordered Solids: II. Structure of Spin-Correlated Radical Pairs in Photosystem I. *J. Phys. Chem. B* **2013**, *117* (38), 11184–11199.
370. Krämer, T.; Kampa, M.; Lubitz, W.; van Gastel, M.; Neese, F. Theoretical Spectroscopy of the Ni^{II} Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenase. *ChemBioChem* **2013**, *14* (14), 1898–1905.
371. Riethausen, J.; Rüdiger, O.; Gärtner, W.; Lubitz, W.; Shafaat, H. S. Spectroscopic and Electrochemical Characterization of the [NiFeSe] Hydrogenase from *Desulfovibrio vulgaris* Miyazaki F: Reversible Redox Behavior and Interactions Between Electron Transfer Centers. *ChemBioChem* **2013**, *14* (14), 1714–1719.
372. Griesse, J. J.; Roos, K.; Cox, N.; Shafaat, H. S.; Branca, R. M. M.; Lehtio, J.; Gräslund, A.; Lubitz, W.; Siegbahn, P. E. M.; Högbom, M. Direct Observation of Structurally Encoded Metal Discrimination and Ether Bond Formation in a Heterodinuclear Metalloprotein. *Proc. Natl. Acad. Sci. U.S.A.* **2013**, *110* (43), 17189–17194.
373. Pérez Navarro, M.; Ames, W. M.; Nilsson, H.; Lohmiller, T.; Pantazis, D. A.; Rapatskiy, L.; Nowaczyk, M. M.; Neese, F.; Boussac, A.; Messinger, J.; Lubitz, W.; Cox, N. Ammonia Binding to the Oxygen-Evolving Complex of Photosystem II Identifies the Solvent-Exchangeable μ -oxo of the Manganese Tetramer. *Proc. Natl. Acad. Sci. U.S.A.* **2013**, *110* (39), 15561–15566.
374. Molitor, B.; Stassen, M.; Modi, A.; El-Mashtoly, S. F.; Laurich, C.; Lubitz, W.; Dawson, J. H.; Rother, M.; Frankenberg-Dinkel, N. A Heme-Based Redox Sensor in the Methanogenic Archaeon *Methanosarcina acetivorans*. *J. Biol. Chem.* **2013**, *288*, 18458–18472.
375. Esselborn, J.; Lambert, C.; Adamska-Venkatesh, A.; Simmons, T.; Berggren, G.; Noth, J.; Siebel, J.; Hemschemeier, A.; Artero, V.; Reijerse, E.; Fontecave, M.; Lubitz, W.; Happe, T. Spontaneous Activation of the [FeFe]-Hydrogenases by an Inorganic [2Fe] Active Site Mimic. *Nat. Chem. Biol.* **2013**, *9*, 607–609.
376. Cox, N.; Lubitz, W.; Savitsky, A. W-Band ELDOR-Detected NMR (EDNMR) Spectroscopy as a Versatile Technique for the Characterization of Transition Metal–Ligand Interactions. *Mol. Phys.* **2013**, *111* (18–19), 2788–2808.
377. Möbius, K.; Lubitz, W.; Savitsky, A. High-Field EPR on Membrane Proteins - Crossing the Gap to NMR. *Prog. Nucl. Magn. Reson. Spectrosc.* **2013**, *75*, 1–49.
378. Erdem, Ö. F.; Stein, M.; Kaur-Ghumaan, S.; Reijerse, E. J.; Ott, S.; Lubitz, W. Effect of Cyanide Ligands on the Electronic Structure of [FeFe] Hydrogenase Active Site Model Complexes with an Azadithiolate Ligand. *Chem. Eur. J.* **2013**, *19* (43), 14566–14572.
379. Gutiérrez Sanz, O.; Marques, M.; Pereira, I. A. C.; de Lacey, A. L.; Lubitz, W.; Rüdiger, O. Orientation and Function of a Membrane Bound Enzyme Monitored by Electrochemical Surface Enhanced Infrared Absorption Spectroscopy. *J. Phys. Chem. Lett.* **2013**, *4*, 2794–2798.
380. Wang, H.; Ogata, H.; Lubitz, W.; Cramer, S. P. A Dynamic View of [NiFe] Hydrogenase by Means of Nuclear Resonance Vibrational Spectroscopy. *Spring-8 Res. Front.* **2012** **2013**, 80–81.
381. Weber, K.; Heise, I.; Weyhermüller, T.; Lubitz, W. Synthesis and Characterization of Nickel Compounds with Tetradentate Thiolate-Thioether Ligands as Precursors for [NiFe]-Hydrogenase Models. *Eur. J. Inorg. Chem.* **2014**, 148–155.
382. Ogata, H.; Decaneto, E.; Grossman, M.; Havenith, M.; Sagi, I.; Lubitz, W.; Knipp, M. Crystallization and Preliminary X-ray Crystallographic Analysis of the

- Catalytic Domain of Membrane Type 1 Matrix Metalloproteinase. *Acta Crystallogr.* **2014**, F70, 232–235.
383. Malferrari, M.; Nalepa, A.; Venturoli, G.; Francia, F.; Lubitz, W.; Möbius, K.; Savitsky, A. 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.* **2014**, 16 (21), 9831–9848.
384. Marchanka, A.; Lubitz, W.; Plato, M.; van Gestel, M. Comparative ENDOR Study at 34 GHz of the Triplet State of the Primary Donor in Bacterial Reaction Centers of *Rb. sphaeroides* and *Bl. viridis*. *Photosynth. Res.* **2014**, 120 (1–2), 99–111.
385. Lubitz, W.; Ogata, H.; Rüdiger, O.; Reijerse, E. Hydrogenases. *Chem. Rev.* **2014**, 114 (8), 4081–4148.
386. Nalepa, A.; Möbius, K.; Lubitz, W.; Savitsky, A. High-Field ELDOR-Detected NMR Study of a Nitroxide Radical in Disordered Solids: Toward Characterization of Heterogeneity of Microenvironments in Spin-Labeled Systems. *J. Magn. Reson.* **2014**, 242, 203–213.
387. Lohmiller, T.; Krewald, V.; Pérez Navarro, M.; Retegan, M.; Rapatskiy, L.; Nowaczyk, M. M.; Boussac, A.; Neese, F.; Lubitz, W.; Pantazis, D. A.; Cox, N. Structure, Ligands and Substrate Coordination of the Oxygen-Evolving Complex of Photosystem II in the S_2 State: A Combined EPR and DFT Study. *Phys. Chem. Chem. Phys.* **2014**, 16 (24), 11877–11892.
388. Retegan, M.; Cox, N.; Lubitz, W.; Neese, F.; Pantazis, D. The First Tyrosyl Radical Intermediate Formed in the S_2 – S_3 Transition of Photosystem II. *Phys. Chem. Chem. Phys.* **2014**, 16 (24), 11901–11910.
389. Hsieh, C.-H.; Ding, S.; Erdem, Ö. F.; Crouthers, D. J.; Liu, T.; McCrory, C. C. L.; Lubitz, W.; Popescu, C. V.; Reibenspies, J. H.; Hall, M. B.; Darensbourg, M. Y. Redox active iron nitrosyl units in proton reduction electrocatalysis. *Nat. Commun.* **2014**, 5, 3684, DOI: 10.1038/ncomms4684.
390. Weber, K.; Erdem, Ö. F.; Bill, E.; Weyhermüller, T.; Lubitz, W. Modeling the Active Site of [NiFe]-Hydrogenases and the [NiFe_u] Subsite of the H-Cluster of Carbon Monoxide Dehydrogenases: Iron(II) Low Spin vs Iron(II) High Spin. *Inorg. Chem.* **2014**, 53 (12), 6329–6337.
391. Plumeré, N.; Rüdiger, O.; Oughli, A. A.; Williams, R.; Vivekananthan, J.; Pöller, S.; Schuhmann, W.; Lubitz, W. A Redox Hydrogel Protects Hydrogenase from High-potential Deactivation and Oxygen Damage. *Nat. Chem.* **2014**, 6 (9), 822–827.
392. Adamska-Venkatesh, A.; Krawietz, D.; Siebel, J.; Weber, K.; Happe, T.; Reijerse, E.; Lubitz, W. New Redox States Observed in [FeFe] Hydrogenases Reveal Redox Coupling within the H-Cluster. *J. Am. Chem. Soc.* **2014**, 136 (32), 11339–11346.
393. Rumpel, S.; Siebel, J. F.; Farès, C.; Duan, J.; Reijerse, E.; Happe, T.; Lubitz, W.; Winkler, M. Enhancing Hydrogen Production of Microalgae by Redirecting Electrons from Photosystem I to Hydrogenase. *Energy Environ. Sci.* **2014**, 7 (10), 3296–3301.
394. Cox, N.; Retegan, M.; Neese, F.; Pantazis, D. A.; Boussac, A.; Lubitz, W. Electronic Structure of the Oxygen-Evolving Complex in Photosystem II Prior to O–O Bond Formation. *Science* **2014**, 345 (6198), 804–808.
395. Shafaat, H. S.; Griesse, J. J.; Pantazis, D. A.; Roos, K.; Andersson, C. S.; Popović-Bijelić, A.; Gräslund, A.; Siegbahn, P. E. M.; Neese, F.; Lubitz, W.; Högbom, M.; Cox, N. Electronic Structural Flexibility of Heterobimetallic Mn/Fe Cofactors: R2lox and R2c Proteins. *J. Am. Chem. Soc.* **2014**, 136 (38), 13399–13409.
396. Pantazis, D. A.; Cox, N.; Lubitz, W.; Neese, F. Oxygen-evolving Photosystem II. In *Encyclopedia of Inorganic and Bioinorganic Chemistry*; John Wiley & Sons Inc.: **2014**; pp 1–13.
397. Ogata, H.; Lubitz, W. Protein Crystallography Using Free-Electron Lasers: Water Oxidation in Photosynthesis. *Angew. Chem., Int. Ed.* **2014**, 53 (48), 13007–13008.
398. Vondracek, H.; Dielmann-Gessner, J.; Lubitz, W.; Knipp, M.; Havenith, M. THz Absorption Spectroscopy of Solvated β -lactoglobulin. *J. Chem. Phys.* **2014**, 141 (22), 22D534.
399. Ogata, H.; Nishikawa, K.; Lubitz, W. Hydrogens Detected by Subatomic Resolution Protein Crystallography in a [NiFe] Hydrogenase. *Nature* **2015**, 520, 571–574.
400. Möbius, K.; Savitsky, A.; Nalepa, A.; Malferrari, M.; Francia, F.; Lubitz, W.; Venturoli, G. The Magic of Disaccharide Glass Matrices for Protein Function as Decoded by High-Field EPR and FTIR Spectroscopy. *Appl. Magn. Reson.* **2015**, 46 (4), 435–464.
401. Kiesel, S.; Wätzlich, D.; Lange, C.; Reijerse, E.; Bröcker, M. J.; Rüdiger, W.; Lubitz, W.; Scheer, H.; Moser, J.; Jahn, D. Iron–Sulfur Cluster-Dependent Catalysis of Chlorophyllide a Oxidoreductase from *Roseobacter denitrificans*. *J. Biol. Chem.* **2015**, 290 (2), 1141–1154.
402. Decaneto, E.; Abbruzzetti, S.; Heise, I.; Lubitz, W.; Viappiani, C.; Knipp, M. A Caged Substrate Peptide for Matrix Metalloproteinases. *Photochem. Photobiol. Sci.* **2015**, 14 (2), 300–307.
403. Krewald, V.; Retegan, M.; Cox, N.; Messinger, J.; Lubitz, W.; DeBeer, S.; Neese, F.; Pantazis, D. Metal Oxidation States in Biological Water Splitting. *Chem. Sci.* **2015**, 6 (3), 1676–1695.
404. Adamska-Venkatesh, A.; Simmons, T. R.; Siebel, J. F.; Artero, V.; Fontecave, M.; Reijerse, E.; Lubitz, W. Artificially Maturated [FeFe] Hydrogenase from *Chlamydomonas reinhardtii*: A HYSORE and ENDOR Study of a Non-Natural H-cluster. *Phys. Chem. Chem. Phys.* **2015**, 17 (7), 5421–5430.
405. Siebel, J. F.; Adamska-Venkatesh, A.; Weber, K.; Rumpel, S.; Reijerse, E. J.; Lubitz, W. Hybrid [FeFe]-hydrogenases with Modified Active Sites Show Remarkable Residual Enzymatic Activity. *Biochemistry* **2015**, 54 (7), 1474–1483.
406. Möbius, K.; Plato, M.; Klihm, G.; Laurich, C.; Savitsky, A.; Lubitz, W.; Szyszko, B.; Stepien, M.; Latos-Grazynski, L. Möbius-Hückel Topology Switching in an Expanded Porphyrin Cation Radical as Studied by EPR and ENDOR Spectroscopy. *Phys. Chem. Chem. Phys.* **2015**, 17 (9), 6644–6652.
407. Cox, N.; Pantazis, D. A.; Neese, F.; Lubitz, W. Artificial Photosynthesis: Understanding Water Splitting in Nature. *Interface Focus* **2015**, 5 (3), 20150009, <http://dx.doi.org/10.1098/rsfs.2015.0009>.
408. He, C.; Howes, B. D.; Smulevich, G.; Rumpel, S.; Reijerse, E. J.; Lubitz, W.; Cox, N.; Knipp, M. Nitrite

- Dismutase Reaction Mechanism: Kinetic and Spectroscopic Investigation of the Interaction between Nitrophenol and Nitrite. *J. Am. Chem. Soc.* **2015**, 137 (12), 4141–4150.
409. Fourmond, V.; Stapf, S.; Li, H.; Buesen, D.; Birrell, J. A.; Rüdiger, O.; Lubitz, W.; Schuhmann, W.; Plumeré, N.; Léger, C. Mechanism of Protection of Catalysts Supported in Redox Hydrogel Films. *J. Am. Chem. Soc.* **2015**, 137 (16), 5494–5505.
410. Rodriguez-Macià, P.; Dutta, A.; Lubitz, W.; Shaw, W.; Rüdiger, O. Direct Comparison of the Performance of a Bioinspired Synthetic Nickel Catalyst and a [NiFe]-Hydrogenase, Both Covalently Attached to Electrodes. *Angew. Chem., Int. Ed.* **2015**, 54 (42), 12303–12307.
411. Oughli, A. A.; Conzuelo, F.; Winkler, M.; Happe, T.; Lubitz, W.; Schuhmann, W.; Rüdiger, O.; Plumeré, N. A Redox Hydrogel Protects the O₂-Sensitive [FeFe]-Hydrogenase from *Chlamydomonas reinhardtii* from Oxidative Damage. *Angew. Chem., Int. Ed.* **2015**, 54 (42), 12329–12333.
412. Rumpel, S.; Siebel, J. F.; Diallo, M.; Farès, C.; Reijerse, E.; Lubitz, W. Structural Insight into the Complex of Ferredoxin and [FeFe] Hydrogenase from *Chlamydomonas reinhardtii*. *ChemBioChem* **2015**, 16 (11), 1663–1669.
413. Roncaroli, F.; Bill, E.; Friedrich, B.; Lenz, O.; Lubitz, W.; Pandelia, M.-E. Cofactor Composition and Function of a H₂-sensing Regulatory Hydrogenase as Revealed by Mössbauer and EPR Spectroscopy. *Chem. Sci.* **2015**, 6 (8), 4495–4507.
414. Barilone, J. L.; Ogata, H.; Lubitz, W.; van Gastel, M. 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.* **2015**, 17, 16204–16212.
415. Weber, K.; Weyhermüller, T.; Bill, E.; Erdem, Ö. F.; Lubitz, W. Design and Characterization of Phosphine Iron Hydrides: Toward Hydrogen-Producing Catalysts. *Inorg. Chem.* **2015**, 54 (14), 6928–6937.
416. Gilbert-Wilson, R.; Siebel, J. F.; Adamska-Venkatesh, A.; Pham, C. C.; Reijerse, E.; Wang, H.; Cramer, S. P.; Lubitz, W.; Rauchfuss, T. B. Spectroscopic Investigations of [FeFe] Hydrogenase Maturated with [⁵⁷Fe₂(adt)-(CN)₂(CO)₄]²⁻. *J. Am. Chem. Soc.* **2015**, 137 (28), 8998–9005.
417. Ogata, H.; Krämer, T.; Wang, H.; Schilter, D.; Pelmentschikov, V.; van Gastel, M.; Neese, F.; Rauchfuss, T. B.; Gee, L. B.; Scott, A. D.; Yoda, Y.; Tanaka, Y.; Lubitz, W.; Cramer, S. P. Hydride Bridge in [NiFe]-Hydrogenase Observed by Nuclear Resonance Vibrational Spectroscopy. *Nat. Commun.* **2015**, 6, 7890, doi: 10.1038/ncomms8890.
418. Cox, N.; Nalepa, A.; Pandelia, M.-E.; Lubitz, W.; Savitsky, A. Double-Resonance EPR Techniques for the Study of Metallobiomolecules. In *Methods in Enzymology*; Qin, P. Z., Warncke, K., Eds. Elsevier: Oxford, **2015**, doi: 10.1016/bs.mie.2015.08.016.
419. Chambers, G. M.; Huynh, M. T.; Hammes-Schiffer, S.; Rauchfuss, T. B.; Reijerse, E.; Lubitz, W. Models of the Ni-L and Ni-SI_a States of the [NiFe]-Hydrogenase Active Site. *Inorg. Chem.* **2015**, doi: 10.1021/acs.inorgchem.5b01662.
420. Adamska-Venkatesh, A.; Roy, S.; Siebel, J. F.; Simmons, T. R.; Fontecave, M.; Artero, V.; Reijerse, E.; Lubitz, W. Spectroscopic Characterization of the Bridging Amine in the Active Site of [FeFe] Hydrogenase Using Isotopologues of the H-Cluster. *J. Am. Chem. Soc.* **2015**, doi: 10.1021/jacs.5b06240.