Wolfgang Lubitz

List of Publications by Year in descending order

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394 papers 26,685 citations

83 h-index 139 g-index

405 all docs

405 docs citations

405 times ranked 11831 citing authors

#	Article	IF	Citations
1	Hydrogenases. Chemical Reviews, 2014, 114, 4081-4148.	23.0	1,653
2	Hydrogen:  An Overview. Chemical Reviews, 2007, 107, 3900-3903.	23.0	628
3	Biomimetic assembly and activation of [FeFe]-hydrogenases. Nature, 2013, 499, 66-69.	13.7	597
4	[NiFe] and [FeFe] Hydrogenases Studied by Advanced Magnetic Resonance Techniques. Chemical Reviews, 2007, 107, 4331-4365.	23.0	458
5	Biological Water Oxidation. Accounts of Chemical Research, 2013, 46, 1588-1596.	7.6	453
6	Electronic structure of the oxygen-evolving complex in photosystem II prior to O-O bond formation. Science, 2014, 345, 804-808.	6.0	432
7	Solar water-splitting into H2 and O2: design principles of photosystem II and hydrogenases. Energy and Environmental Science, 2008, 1, 15.	15.6	388
8	14N HYSCORE investigation of the H-cluster of [FeFe] hydrogenase: evidence for a nitrogen in the dithiol bridge. Physical Chemistry Chemical Physics, 2009, 11, 6592.	1.3	354
9	Two Interconvertible Structures that Explain the Spectroscopic Properties of the Oxygenâ€Evolving Complex of Photosystemâ€II in the S ₂ State. Angewandte Chemie - International Edition, 2012, 51, 9935-9940.	7.2	342
10	Spontaneous activation of [FeFe]-hydrogenases by an inorganic [2Fe] active site mimic. Nature Chemical Biology, 2013, 9, 607-609.	3.9	316
11	Metal oxidation states in biological water splitting. Chemical Science, 2015, 6, 1676-1695.	3.7	275
12	Theoretical Evaluation of Structural Models of the S ₂ State in the Oxygen Evolving Complex of Photosystem II: Protonation States and Magnetic Interactions. Journal of the American Chemical Society, 2011, 133, 19743-19757.	6.6	271
13	Hydrogens detected by subatomic resolution protein crystallography in a [NiFe] hydrogenase. Nature, 2015, 520, 571-574.	13.7	267
14	Energy and environment policy case for a global project on artificial photosynthesis. Energy and Environmental Science, 2013, 6, 695.	15.6	264
15	Direct Detection of a Hydrogen Ligand in the [NiFe] Center of the Regulatory H2-Sensing Hydrogenase fromRalstoniaeutrophain Its Reduced State by HYSCORE and ENDOR Spectroscopy. Journal of the American Chemical Society, 2003, 125, 13075-13083.	6.6	259
16	Detection of the Water-Binding Sites of the Oxygen-Evolving Complex of Photosystem II Using W-Band ¹⁷ O Electron–Electron Double Resonance-Detected NMR Spectroscopy. Journal of the American Chemical Society, 2012, 134, 16619-16634.	6.6	248
17	Electronic Structure of the Mn ₄ O <i>_x</i> Ca Cluster in the S _O and S ₂ States of the Oxygen-Evolving Complex of Photosystem II Based on Pulse ⁵⁵ Mn-ENDOR and EPR Spectroscopy. Journal of the American Chemical Society, 2007, 129, 13421-13435.	6.6	230
18	P700: the primary electron donor of photosystem I. Biochimica Et Biophysica Acta - Bioenergetics, 2001, 1507, 61-79.	0.5	225

#	Article	IF	CITATIONS
19	3-mm High-field EPR on semiquinone radical anions Q.cntdot related to photosynthesis and on the primary donor P.cntdot.+ and acceptor QA.cntdot in reaction centers of Rhodobacter sphaeroides R-26. The Journal of Physical Chemistry, 1993, 97, 7639-7647.	2.9	220
20	[NiFe] hydrogenases: A common active site for hydrogen metabolism under diverse conditions. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 986-1002.	0.5	219
21	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. Journal of the American Chemical Society, 2011, 133, 3635-3648.	6.6	211
22	A redox hydrogel protects hydrogenase from high-potential deactivation and oxygen damage. Nature Chemistry, 2014, 6, 822-827.	6.6	209
23	Single Crystal EPR Studies of the Reduced Active Site of [NiFe] Hydrogenase fromDesulfovibrio vulgarisMiyazaki F. Journal of the American Chemical Society, 2003, 125, 83-93.	6.6	196
24	Calculating the Electron Paramagnetic Resonance Parameters of Exchange Coupled Transition Metal Complexes Using Broken Symmetry Density Functional Theory:Â Application to a MnIII/MnIVModel Compound. Journal of the American Chemical Society, 2004, 126, 2613-2622.	6.6	194
25	Identification and Characterization of the "Superâ€Reduced―State of the Hâ€Cluster in [FeFe] Hydrogenase: A New Building Block for the Catalytic Cycle?. Angewandte Chemie - International Edition, 2012, 51, 11458-11462.	7.2	184
26	Ultrafast Transient Absorption Studies on Photosystem I Reaction Centers from Chlamydomonas reinhardtii. 1. A New Interpretation of the Energy Trapping and Early Electron Transfer Steps in Photosystem I. Biophysical Journal, 2003, 85, 3899-3922.	0.2	180
27	[NiFe] hydrogenases: structural and spectroscopic studies of the reaction mechanism. Dalton Transactions, 2009, , 7577.	1.6	179
28	55Mn Pulse ENDOR at 34 GHz of the S0and S2States of the Oxygen-Evolving Complex in Photosystem II. Journal of the American Chemical Society, 2005, 127, 2392-2393.	6.6	174
29	Structural adaptations of photosynthetic complex I enable ferredoxin-dependent electron transfer. Science, 2019, 363, 257-260.	6.0	162
30	Radicals, Radical Pairs and Triplet States in Photosynthesis. Accounts of Chemical Research, 2002, 35, 313-320.	7.6	161
31	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. Biochimica Et Biophysica Acta - Bioenergetics, 1993, 1183, 139-160.	0.5	159
32	A five-coordinate Mn(<scp>iv</scp>) intermediate in biological water oxidation: spectroscopic signature and a pivot mechanism for water binding. Chemical Science, 2016, 7, 72-84.	3.7	158
33	The Electronic Structure of the H-Cluster in the [FeFe]-Hydrogenase from <i>Desulfovibrio </i> desulfuricans: A Q-band ⁵⁷ Fe-ENDOR and HYSCORE Study. Journal of the American Chemical Society, 2007, 129, 11447-11458.	6.6	157
34	Direct Observation of an Iron-Bound Terminal Hydride in [FeFe]-Hydrogenase by Nuclear Resonance Vibrational Spectroscopy. Journal of the American Chemical Society, 2017, 139, 4306-4309.	6.6	155
35	Characterization of a unique [FeS] cluster in the electron transfer chain of the oxygen tolerant [NiFe] hydrogenase from <i>Aquifex aeolicus</i> . Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 6097-6102.	3.3	154
36	Water oxidation in photosystem II. Photosynthesis Research, 2019, 142, 105-125.	1.6	149

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37	Ammonia binding to the oxygen-evolving complex of photosystem II identifies the solvent-exchangeable oxygen bridge (1½-oxo) of the manganese tetramer. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 15561-15566.	3.3	148
38	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. Biophysical Journal, 2006, 90, 552-565.	0.2	146
39	Membrane-Bound Hydrogenase I from the Hyperthermophilic Bacterium <i>Aquifex aeolicus</i> Enzyme Activation, Redox Intermediates and Oxygen Tolerance. Journal of the American Chemical Society, 2010, 132, 6991-7004.	6.6	145
40	The primary and secondary acceptors in bacterial photosynthesis III. Characterization of the quinone radicals Q A \hat{a}	0.6	142
41	Proton Coupled Electronic Rearrangement within the H-Cluster as an Essential Step in the Catalytic Cycle of [FeFe] Hydrogenases. Journal of the American Chemical Society, 2017, 139, 1440-1443.	6.6	142
42	Spectroelectrochemical Characterization of the Active Site of the [FeFe] Hydrogenase HydA1 from <i>Chlamydomonas reinhardtii Biochemistry, 2009, 48, 7780-7786.</i>	1.2	133
43	A Model of the [FeFe] Hydrogenase Active Site with a Biologically Relevant Azadithiolate Bridge: A Spectroscopic and Theoretical Investigation. Angewandte Chemie - International Edition, 2011, 50, 1439-1443.	7.2	130
44	Importance of the Protein Framework for Catalytic Activity of [FeFe]-Hydrogenases. Journal of Biological Chemistry, 2012, 287, 1489-1499.	1.6	129
45	A New Quantum Chemical Approach to the Magnetic Properties of Oligonuclear Transitionâ€Metal Complexes: Application to a Model for the Tetranuclear Manganese Cluster of Photosystem II. Chemistry - A European Journal, 2009, 15, 5108-5123.	1.7	123
46	Current Understanding of the Mechanism of Water Oxidation in Photosystem II and Its Relation to XFEL Data. Annual Review of Biochemistry, 2020, 89, 795-820.	5.0	123
47	The Crystal Structure of the [NiFe] Hydrogenase from the Photosynthetic Bacterium Allochromatium vinosum: Characterization of the Oxidized Enzyme (Ni-A State). Journal of Molecular Biology, 2010, 402, 428-444.	2.0	122
48	A Systematic Density Functional Study of the Zero-Field Splitting in Mn(II) Coordination Compounds. Inorganic Chemistry, 2008, 47, 134-142.	1.9	121
49	Structure of the oxygen-evolving complex of photosystem II: information on the S2 state through quantum chemical calculation of its magnetic properties. Physical Chemistry Chemical Physics, 2009, 11, 6788.	1.3	121
50	New Redox States Observed in [FeFe] Hydrogenases Reveal Redox Coupling Within the H-Cluster. Journal of the American Chemical Society, 2014, 136, 11339-11346.	6.6	121
51	Electronic Structure of Antiferromagnetically Coupled Dinuclear Manganese (MnIIIMnIV) Complexes Studied by Magnetic Resonance Techniques. Journal of the American Chemical Society, 1998, 120, 13104-13120.	6.6	120
52	Time-Resolved X-, K-, and W-Band EPR of the Radical Pair State of Photosystem I in Comparison with in Bacterial Reaction Centers. Journal of Physical Chemistry B, 1997, 101, 1437-1443.	1.2	118
53	Hydrogen Bond Geometries from Electron Paramagnetic Resonance and Electronâ^'Nuclear Double Resonance Parameters:  Density Functional Study of Quinone Radical Anionâ^'Solvent Interactions. Journal of the American Chemical Society, 2004, 126, 3280-3290.	6.6	118
54	ENDOR Studies of the Primary Donor Cation Radical in Mutant Reaction Centers of Rhodobacter sphaeroides with Altered Hydrogen-Bond Interactions. Biochemistry, 1995, 34, 8130-8143.	1,2	114

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55	Hybrid [FeFe]-Hydrogenases with Modified Active Sites Show Remarkable Residual Enzymatic Activity. Biochemistry, 2015, 54, 1474-1483.	1.2	113
56	Electronic structure of Q-A in reaction centers from Rhodobacter sphaeroides. I. Electron paramagnetic resonance in single crystals. Biophysical Journal, 1995, 69, 311-322.	0.2	112
57	Time-resolved W-band (95 GHz) EPR spectroscopy of Zn-substituted reaction centers of Rhodobacter sphaeroides R-26. Chemical Physics, 1995, 194, 361-370.	0.9	110
58	EPR Study of the Molecular and Electronic Structure of the Semiquinone Biradical QA-•QB-•in Photosynthetic Reaction Centers fromRhodobactersphaeroides. Journal of the American Chemical Society, 2000, 122, 7327-7341.	6.6	110
59	An orientation-selected ENDOR and HYSCORE study of the Ni-C active state of Desulfovibrio vulgaris Miyazaki F hydrogenase. Journal of Biological Inorganic Chemistry, 2005, 10, 51-62.	1.1	110
60	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. The Journal of Physical Chemistry, 1993, 97, 2015-2020.	2.9	109
61	Relativistic DFT Calculations of the Paramagnetic Intermediates of [NiFe] Hydrogenase. Implications for the Enzymatic Mechanism. Journal of the American Chemical Society, 2001, 123, 5839-5840.	6.6	109
62	Orientation and Electronic Structure of the Primary Donor Radical Cation in Photosystem I:  A Single Crystals EPR and ENDOR Study. Journal of Physical Chemistry B, 2001, 105, 1225-1239.	1.2	106
63	Isolation and first EPR characterization of the [FeFe]-hydrogenases from green algae. Biochimica Et Biophysica Acta - Bioenergetics, 2008, 1777, 410-416.	0.5	104
64	Intermediates in the Catalytic Cycle of [NiFe] Hydrogenase: Functional Spectroscopy of the Active Site. ChemPhysChem, 2010, 11, 1127-1140.	1.0	104
65	A single-crystal ENDOR and density functional theory study of the oxidized states of the [NiFe] hydrogenase from Desulfovibrio vulgaris Miyazaki F. Journal of Biological Inorganic Chemistry, 2006, 11, 41-51.	1.1	103
66	Electronic Structure of Neutral Tryptophan Radicals in Ribonucleotide Reductase Studied by EPR and ENDOR Spectroscopy. Journal of the American Chemical Society, 1996, 118, 8111-8120.	6.6	101
67	A Functional [NiFe]-Hydrogenase Model Compound That Undergoes Biologically Relevant Reversible Thiolate Protonation. Journal of the American Chemical Society, 2012, 134, 20745-20755.	6.6	101
68	In Situ EPR Study of the Redox Properties of CuO–CeO ₂ Catalysts for Preferential CO Oxidation (PROX). ACS Catalysis, 2016, 6, 3520-3530.	5.5	97
69	Recent developments in biological water oxidation. Current Opinion in Chemical Biology, 2016, 31, 113-119.	2.8	97
70	Hydride bridge in [NiFe]-hydrogenase observed by nuclear resonance vibrational spectroscopy. Nature Communications, 2015, 6, 7890.	5.8	96
71	Influence of the Axial Ligands on the Spectral Properties of P700 of Photosystem I:  A Study of Site-Directed Mutants. Biochemistry, 2000, 39, 13012-13025.	1.2	95
72	A Metal–Metal Bond in the Light-Induced State of [NiFe] Hydrogenases with Relevance to Hydrogen Evolution. Journal of the American Chemical Society, 2013, 135, 3915-3925.	6.6	95

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73	The [FeFe]â€hydrogenase maturase HydF from <i>Clostridium acetobutylicum</i> contains a CO and CN ^{â^'} ligated iron cofactor. FEBS Letters, 2010, 584, 638-642.	1.3	94
74	A Tyrosylâ^Dimanganese Coupled Spin System is the Native Metalloradical Cofactor of the R2F Subunit of the Ribonucleotide Reductase of Corynebacterium ammoniagenes. Journal of the American Chemical Society, 2010, 132, 11197-11213.	6.6	93
75	ENDOR Spectroscopy— A Promising Technique for Investigating the Structure of Organic Radicals. Angewandte Chemie International Edition in English, 1984, 23, 173-194.	4.4	92
76	Structure and function of [NiFe] hydrogenases. Journal of Biochemistry, 2016, 160, 251-258.	0.9	92
77	Comparative Study of Reaction Centers from Photosynthetic Purple Bacteria: Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Spectroscopy. Biochemistry, 1994, 33, 12077-12084.	1.2	90
78	Orientation-Resolving Pulsed Electron Dipolar High-Field EPR Spectroscopy on Disordered Solids:Â I. Structure of Spin-Correlated Radical Pairs in Bacterial Photosynthetic Reaction Centers. Journal of Physical Chemistry B, 2007, 111, 6245-6262.	1.2	90
79	Hydrogen Bonding to P700:  Site-Directed Mutagenesis of Threonine A739 of Photosystem I in Chlamydomonas reinhardtii,. Biochemistry, 2002, 41, 8557-8569.	1.2	88
80	Relativistic DFT calculation of the reaction cycle intermediates of [NiFe] hydrogenase: a contribution to understanding the enzymatic mechanism. Journal of Inorganic Biochemistry, 2004, 98, 862-877.	1.5	87
81	A Redox Hydrogel Protects the O ₂ â€Sensitive [FeFe]â€Hydrogenase from <i>Chlamydomonas reinhardtii</i> from Oxidative Damage. Angewandte Chemie - International Edition, 2015, 54, 12329-12333.	7.2	87
82	Spin State as a Marker for the Structural Evolution of Nature's Water-Splitting Catalyst. Inorganic Chemistry, 2016, 55, 488-501.	1.9	87
83	Fluid solution and solid-state electron nuclear double resonance studies of flavin model compounds and flavoenzymes. Journal of the American Chemical Society, 1984, 106, 737-746.	6.6	86
84	Effects of Hydrogen Bonding to a Bacteriochlorophyllâ^'Bacteriopheophytin Dimer in Reaction Centers fromRhodobacter sphaeroidesâ€. Biochemistry, 1996, 35, 6612-6619.	1.2	84
85	Radicals in solution studied by endor and triple resonance spectroscopy. Physics Reports, 1982, 87, 171-208.	10.3	83
86	Pulsed EPR Structure Analysis of Photosystem I Single Crystals: Localization of the Phylloquinone Acceptorâ€. Biochemistry, 1997, 36, 12001-12004.	1.2	82
87	Quantum chemical calculations of [NiFe] hydrogenase. Current Opinion in Chemical Biology, 2002, 6, 243-249.	2.8	81
88	The electronic structures of the S2 states of the oxygen-evolving complexes of photosystem II in plants and cyanobacteria in the presence and absence of methanol. Biochimica Et Biophysica Acta - Bioenergetics, 2011, 1807, 829-840.	0.5	81
89	Structural and Spectroscopic Features of Mixed Valent Fe ^{II} Fe ^I Complexes and Factors Related to the Rotated Configuration of Diiron Hydrogenase. Journal of the American Chemical Society, 2012, 134, 13089-13102.	6.6	81
90	Mechanism of Protection of Catalysts Supported in Redox Hydrogel Films. Journal of the American Chemical Society, 2015, 137, 5494-5505.	6.6	81

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91	Photosystem II single crystals studied by EPR spectroscopy at 94 GHz: The tyrosine radical YFormula. Proceedings of the National Academy of Sciences of the United States of America, 2001, 98, 6623-6628.	3.3	79
92	Reaction Coordinate Leading to H ₂ Production in [FeFe]-Hydrogenase Identified by Nuclear Resonance Vibrational Spectroscopy and Density Functional Theory. Journal of the American Chemical Society, 2017, 139, 16894-16902.	6.6	78
93	Structure, ligands and substrate coordination of the oxygen-evolving complex of photosystem II in the S2 state: a combined EPR and DFT study. Physical Chemistry Chemical Physics, 2014, 16, 11877.	1.3	77
94	Enhancing hydrogen production of microalgae by redirecting electrons from photosystem I to hydrogenase. Energy and Environmental Science, 2014, 7, 3296-3301.	15.6	77
95	Inhibition of the [NiFe] hydrogenase from Desulfovibrio vulgaris Miyazaki F by carbon monoxide: An FTIR and EPR spectroscopic study. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 304-313.	0.5	76
96	Relationship between the oxidation potential and electron spin density of the primary electron donor in reaction centers from Rhodobacter sphaeroides. Proceedings of the National Academy of Sciences of the United States of America, 1997, 94, 13582-13587.	3.3	75
97	A Structural Model for the Charge Separated State in Photosystem I from the Orientation of the Magnetic Interaction Tensors. Journal of Physical Chemistry B, 2000, 104, 9728-9739.	1.2	75
98	ENDOR and ESEEM of the 15N labelled radical cations of chlorophyll a and the primary donor P700 in photosystem I. Chemical Physics, 1995, 194, 419-432.	0.9	74
99	Lightâ€Induced Excited Spin State Trapping in an Exchangeâ€Coupled Nitroxideâ€Copper(II)â€Nitroxide Cluster. Angewandte Chemie - International Edition, 2008, 47, 6897-6899.	7.2	74
100	EPR and ENDOR characterization of semiquinone anion radicals related to photosynthesis. Magnetic Resonance in Chemistry, 1995, 33, S81-S93.	1.1	72
101	DFT calculations of the electronic structure of the paramagnetic states Ni-A, Ni-B and Ni-C of [NiFe] hydrogenase. Physical Chemistry Chemical Physics, 2001, 3, 2668-2675.	1.3	72
102	A gas breathing hydrogen/air biofuel cell comprising a redox polymer/hydrogenase-based bioanode. Nature Communications, 2018, 9, 4715.	5.8	71
103	Molecular orbital investigation of dimer formations of bacteriochlorophyll a. Model configurations for the primary donor of photosynthesis. Chemical Physics, 1986, 107, 185-196.	0.9	69
104	Spectroscopic Investigations of [FeFe] Hydrogenase Maturated with [⁵⁷ Fe ₂ (adt)(CN) ₂ (CO) ₄] ^{2–} . Journal of the American Chemical Society, 2015, 137, 8998-9005.	6.6	69
105	Atomic-Scale Explanation of O ₂ Activation at the Au–TiO ₂ Interface. Journal of the American Chemical Society, 2018, 140, 18082-18092.	6.6	69
106	A solution ENDOR sensitivity study of various nuclei in organic radicals. The Journal of Physical Chemistry, 1981, 85, 1202-1219.	2.9	68
107	Geometry of the Hydrogen Bonds to the Primary Quinone		

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109	Charge Recombination Fluorescence in Photosystem I Reaction Centers from Chlamydomonas reinhardtii. Journal of Physical Chemistry B, 2005, 109, 5903-5911.	1.2	66
110	A tunable general purpose Q-band resonator for CW and pulse EPR/ENDOR experiments with large sample access and optical excitation. Journal of Magnetic Resonance, 2012, 214, 237-243.	1.2	66
111	Species-specific Differences of the Spectroscopic Properties of P700. Journal of Biological Chemistry, 2003, 278, 46760-46771.	1.6	65
112	In vivo liquid solution ENDOR and TRIPLE resonance of bacterial photosynthetic reaction centers of Rhodopseudomonas sphaeroides R-26. Journal of the American Chemical Society, 1981, 103, 4635-4637.	6.6	64
113	Transient EPR spectroscopy of the charge separated state P+Qâ^' in photosynthetic reaction centers. Comparison of Zn-substituted Rhodobacter sphaeroides R-26 and Photosystem I. Biochimica Et Biophysica Acta - Bioenergetics, 1993, 1142, 23-35.	0.5	64
114	Differences in the binding of the primary quinone receptor in Photosystem I and reaction centres of Rhodobacter sphaeroides-R26 studied with transient EPR spectroscopy. Chemical Physics, 1995, 194, 349-359.	0.9	64
115	g- and A-Tensor Calculations in the Zero-Order Approximation for Relativistic Effects of Ni Complexes and Ni(CO)3H as Model Complexes for the Active Center of [NiFe]-Hydrogenase. Journal of Physical Chemistry A, 2001, 105, 416-425.	1.1	64
116	Probing hydrogen bonding to quinone anion radicals by 1H and 2H ENDOR spectroscopy at 35 GHz. Chemical Physics, 2003, 294, 401-413.	0.9	64
117	Spectroscopic Characterization of the Bridging Amine in the Active Site of [FeFe] Hydrogenase Using Isotopologues of the H-Cluster. Journal of the American Chemical Society, 2015, 137, 12744-12747.	6.6	64
118	ESR, ENDOR and TRIPLE resonance studies of the primary donor radical cation P960+• in the photosynthetic bacterium Rhodopseudomonas viridis. Chemical Physics Letters, 1988, 148, 377-385.	1.2	63
119	The First State in the Catalytic Cycle of the Water-Oxidizing Enzyme: Identification of a Water-Derived $\hat{l}^{1}\!\!/4$ -Hydroxo Bridge. Journal of the American Chemical Society, 2017, 139, 14412-14424.	6.6	63
120	Spectroscopic and Computational Evidence that [FeFe] Hydrogenases Operate Exclusively with CO-Bridged Intermediates. Journal of the American Chemical Society, 2020, 142, 222-232.	6.6	63
121	2D ESEEM of the 15N-Labeled Radical Cations of Bacteriochlorophyll a and of the Primary Donor in Reaction Centers of Rhodobacter sphaeroides. The Journal of Physical Chemistry, 1995, 99, 436-448.	2.9	62
122	Single crystal EPR studies of the oxidized active site of [NiFe] hydrogenase from Desulfovibrio vulgaris Miyazaki F. Journal of Biological Inorganic Chemistry, 2000, 5, 36-44.	1.1	62
123	Structure of the Tyrosyl Biradical in Mouse R2 Ribonucleotide Reductase from Highâ€Field PELDOR. Angewandte Chemie - International Edition, 2008, 47, 1224-1227.	7.2	62
124	Artificial Photosynthesis for Solar Fuels – an Evolving Research Field within AMPEA, a Joint Programme of the European Energy Research Alliance. Green, 2013, 3, .	0.4	62
125	Pigmentâ^'Protein Interactions in Bacterial Reaction Centers and Their Influence on Oxidation Potential and Spin Density Distribution of the Primary Donor. Journal of Physical Chemistry B, 2002, 106, 3226-3236.	1.2	61
126	Dimanganese catalaseâ€"spectroscopic parameters from broken-symmetry density functional theory of the superoxidized MnIII/MnIV state. Journal of Biological Inorganic Chemistry, 2005, 10, 231-238.	1.1	61

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127	Spectroelectrochemical Study of the [NiFe] Hydrogenase from Desulfovibrio vulgaris Miyazaki F in Solution and Immobilized on Biocompatible Gold Surfaces. Journal of Physical Chemistry B, 2009, 113, 15344-15351.	1.2	61
128	Direct Comparison of the Performance of a Bioâ€inspired Synthetic Nickel Catalyst and a [NiFe]â€Hydrogenase, Both Covalently Attached to Electrodes. Angewandte Chemie - International Edition, 2015, 54, 12303-12307.	7.2	61
129	Time-resolved EPR of the radical pair P865+.QAâ^'. in bacterial reaction centers. Observations of transient nutations, quantum beats and envelope modulation effects. Chemical Physics Letters, 1994, 226, 349-358.	1.2	60
130	Pulsed EPR measurement of the distance between P680 +· and QA Ⱂ· in photosystem II. FEBS Letters, 1997, 414, 454-456.	1.3	60
131	Multifrequency EPR Investigation of Dimanganese Catalase and Related Mn(III)Mn(IV) Complexes. Journal of Physical Chemistry B, 2003, 107, 1242-1250.	1.2	60
132	De novo design of a non-natural fold for an iron–sulfur protein: Alpha-helical coiled-coil with a four-iron four-sulfur cluster binding site in its central core. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 406-413.	0.5	60
133	Observation of the FeCN and FeCO Vibrations in the Active Site of [NiFe] Hydrogenase by Nuclear Resonance Vibrational Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 724-728.	7.2	60
134	Artificial photosynthesis: understanding water splitting in nature. Interface Focus, 2015, 5, 20150009.	1.5	60
135	Transient EPR spectroscopy of perdeuterated Zn-substituted reaction centres of Rhodobacter sphaeroides R-26. Chemical Physics Letters, 1993, 212, 561-568.	1,2	59
136	W-band ELDOR-detected NMR (EDNMR) spectroscopy as a versatile technique for the characterisation of transition metal–ligand interactions. Molecular Physics, 2013, 111, 2788-2808.	0.8	59
137	Molecular orbital study of the primary electron donor P700 of photosystem I based on a recent X-ray single crystal structure analysis. Chemical Physics, 2003, 294, 483-499.	0.9	58
138	Redox active iron nitrosyl units in proton reduction electrocatalysis. Nature Communications, 2014, 5, 3684.	5.8	58
139	Electron Spinâ^'Lattice Relaxation of the SO State of the Oxygen-Evolving Complex in Photosystem II and of Dinuclear Manganese Model Complexes. Biochemistry, 2005, 44, 9368-9374.	1.2	57
140	Electronic structure of the unique [4Fe-3S] cluster in O ₂ -tolerant hydrogenases characterized by ⁵⁷ Fe Mössbauer and EPR spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 483-488.	3.3	57
141	Electronic Structure of a Transient Histidine Radical in Liquid Aqueous Solution:Â EPR Continuous-Flow Studies and Density Functional Calculations. Journal of Physical Chemistry A, 1999, 103, 1283-1290.	1.1	56
142	The Basic Properties of the Electronic Structure of the Oxygen-evolving Complex of Photosystem II Are Not Perturbed by Ca2+ Removal. Journal of Biological Chemistry, 2012, 287, 24721-24733.	1.6	56
143	Theoretical Spectroscopy of the Ni ^{II} Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenases. ChemBioChem, 2013, 14, 1898-1905.	1.3	56
144	Models of the Ni-L and Ni-SI _a States of the [NiFe]-Hydrogenase Active Site. Inorganic Chemistry, 2016, 55, 419-431.	1.9	56

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145	Intercluster Redox Coupling Influences Protonation at the H-cluster in [FeFe] Hydrogenases. Journal of the American Chemical Society, 2017, 139, 15122-15134.	6.6	56
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