## Michael Haumann

## List of Publications by Citations

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L-index

| #  | Paper   | IF         | Citations |
|----|---|------------|-----------|
| 85 | How oxygen attacks [FeFe] hydrogenases from photosynthetic organisms. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2009</b> , 106, 17331-6   | 11.5       | 260       |
| 84 | X-ray absorption spectroscopy to analyze nuclear geometry and electronic structure of biological metal centerspotential and questions examined with special focus on the tetra-nuclear manganese complex of oxygenic photosynthesis. <i>Analytical and Bioanalytical Chemistry</i> , <b>2003</b> , 376, 562 | 4.4<br>-83 | 241       |
| 83 | Synthetic manganeseBalcium oxides mimic the water-oxidizing complex of photosynthesis functionally and structurally. <i>Energy and Environmental Science</i> , <b>2011</b> , 4, 2400  | 35.4       | 238       |
| 82 | Recent developments in research on water oxidation by photosystem II. <i>Current Opinion in Chemical Biology</i> , <b>2012</b> , 16, 3-10   | 9.7        | 167       |
| 81 | Alternating electron and proton transfer steps in photosynthetic water oxidation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2012</b> , 109, 16035-40  | 11.5       | 147       |
| 80 | Eight steps preceding O-O bond formation in oxygenic photosynthesisa basic reaction cycle of the Photosystem II manganese complex. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>2007</b> , 1767, 472-83  | 4.6        | 147       |
| 79 | Extent and rate of proton release by photosynthetic water oxidation in thylakoids: electrostatic relaxation versus chemical production. <i>Biochemistry</i> , <b>1994</b> , 33, 864-72  | 3.2        | 134       |
| 78 | Electrostatics and proton transfer in photosynthetic water oxidation. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , <b>2002</b> , 357, 1407-17; discussion 1417-20  | 5.8        | 112       |
| 77 | Photosynthetic oxygen evolution: H/D isotope effects and the coupling between electron and proton transfer during the redox reactions at the oxidizing side of Photosystem II. <i>Photosynthesis Research</i> , <b>1997</b> , 51, 193-208   | 3.7        | 93        |
| 76 | Experimental and quantum chemical characterization of the water oxidation cycle catalysed by [Rull(damp)(bpy)(H2O)]2+. <i>Chemical Science</i> , <b>2012</b> , 3, 2576  | 9.4        | 88        |
| 75 | O2 reactions at the six-iron active site (H-cluster) in [FeFe]-hydrogenase. <i>Journal of Biological Chemistry</i> , <b>2011</b> , 286, 40614-23  | 5.4        | 74        |
| 74 | Tyrosine-Z in oxygen-evolving photosystem II: a hydrogen-bonded tyrosinate. <i>Biochemistry</i> , <b>1999</b> , 38, 1258-67   | 3.2        | 74        |
| 73 | From an FeP complex to FeP nanoparticles as efficient electrocatalysts for water-splitting. <i>Chemical Science</i> , <b>2018</b> , 9, 8590-8597  | 9.4        | 73        |
| 72 | Behavior of the Ru-bda Water Oxidation Catalyst Covalently Anchored on Glassy Carbon Electrodes. <i>ACS Catalysis</i> , <b>2015</b> , 5, 3422-3429  | 13.1       | 68        |
| 71 | Seven steps of alternating electron and proton transfer in photosystem II water oxidation traced by time-resolved photothermal beam deflection at improved sensitivity. <i>Journal of Physical Chemistry B</i> , <b>2015</b> , 119, 2677-89   | 3.4        | 64        |
| 70 | The structure of the active site H-cluster of [FeFe] hydrogenase from the green alga Chlamydomonas reinhardtii studied by X-ray absorption spectroscopy. <i>Biochemistry</i> , <b>2009</b> , 48, 5042-9   | 3.2        | 64        |
| 69 | Room-Temperature Energy-Sampling KIX-ray Emission Spectroscopy of the Mn4Ca Complex of Photosynthesis Reveals Three Manganese-Centered Oxidation Steps and Suggests a Coordination Change Prior to O2 Formation <i>Biochemistry</i> <b>2016</b> , 55, 4197-211  | 3.2        | 55        |

| 68 | Protonation/reduction dynamics at the [4Fe-4S] cluster of the hydrogen-forming cofactor in [FeFe]-hydrogenases. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 3128-3140   | 3.6                | 54 |
|----|--|--------------------|----|
| 67 | Hydride binding to the active site of [FeFe]-hydrogenase. <i>Inorganic Chemistry</i> , <b>2014</b> , 53, 12164-77  | 5.1                | 53 |
| 66 | Time-resolved X-ray spectroscopy leads to an extension of the classical S-state cycle model of photosynthetic oxygen evolution. <i>Photosynthesis Research</i> , <b>2007</b> , 92, 327-43  | 3.7                | 52 |
| 65 | Electronic and molecular structures of the active-site H-cluster in [FeFe]-hydrogenase determined by site-selective X-ray spectroscopy and quantum chemical calculations. <i>Chemical Science</i> , <b>2014</b> , 5, 1187                          | -9 <del>2</del> 03 | 50 |
| 64 | Photosynthetic water oxidation at elevated dioxygen partial pressure monitored by time-resolved X-ray absorption measurements. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2008</b> , 105, 17384-9 | 11.5               | 46 |
| 63 | The Molecular Proceedings of Biological Hydrogen Turnover. <i>Accounts of Chemical Research</i> , <b>2018</b> , 51, 1755-1763  | 24.3               | 44 |
| 62 | Stepwise isotope editing of [FeFe]-hydrogenases exposes cofactor dynamics. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, 8454-9  | 11.5               | 42 |
| 61 | Proton-Coupled Reduction of the Catalytic [4Fe-4S] Cluster in [FeFe]-Hydrogenases. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 16503-16506  | 16.4               | 41 |
| 60 | Facilitated hydride binding in an Fe-Fe hydrogenase active-site biomimic revealed by X-ray absorption spectroscopy and DFT calculations. <i>Inorganic Chemistry</i> , <b>2007</b> , 46, 11094-105  | 5.1                | 41 |
| 59 | Intermediates in assembly by photoactivation after thermally accelerated disassembly of the manganese complex of photosynthetic water oxidation. <i>Biochemistry</i> , <b>2006</b> , 45, 14523-32  | 3.2                | 40 |
| 58 | The Manganese Complex of Oxygenic Photosynthesis Conversion of FiveCoordinated MnIII to SixCoordinated MnIV in the S2S3 Transition is Implied by XANES Simulations. <i>Physica Scripta</i> , <b>2005</b> , 844                                     | 2.6                | 40 |
| 57 | Reduction of unusual iron-sulfur clusters in the H2-sensing regulatory Ni-Fe hydrogenase from Ralstonia eutropha H16. <i>Journal of Biological Chemistry</i> , <b>2005</b> , 280, 19488-95   | 5.4                | 40 |
| 56 | Sequential and Coupled Proton and Electron Transfer Events in the S - Transition of Photosynthetic Water Oxidation Revealed by Time-Resolved X-ray Absorption Spectroscopy. <i>Biochemistry</i> , <b>2016</b> , 55, 6996-7004                      | 3.2                | 40 |
| 55 | Bridging Hydride at Reduced H-Cluster Species in [FeFe]-Hydrogenases Revealed by Infrared Spectroscopy, Isotope Editing, and Quantum Chemistry. <i>Journal of the American Chemical Society</i> , <b>2017</b> , 139, 12157-12160                   | 16.4               | 39 |
| 54 | Identification of a bis-molybdopterin intermediate in molybdenum cofactor biosynthesis in Escherichia coli. <i>Journal of Biological Chemistry</i> , <b>2013</b> , 288, 29736-45   | 5.4                | 39 |
| 53 | Structure of the molybdenum site in YedY, a sulfite oxidase homologue from Escherichia coli. <i>Inorganic Chemistry</i> , <b>2011</b> , 50, 741-8  | 5.1                | 38 |
| 52 | Sulfido and cysteine ligation changes at the molybdenum cofactor during substrate conversion by formate dehydrogenase (FDH) from Rhodobacter capsulatus. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 3260-71                                    | 5.1                | 37 |
| 51 | Electronic structure of an [FeFe] hydrogenase model complex in solution revealed by X-ray absorption spectroscopy using narrow-band emission detection. <i>Journal of the American Chemical Society</i> 2012, 134, 14142-57                        | 16.4               | 34 |

| 50 | Specific loss of the extrinsic 18 KDa protein from photosystem II upon heating to 47 degrees C causes inactivation of oxygen evolution likely due to Ca release from the Mn-complex. <i>Photosynthesis Research</i> , <b>2005</b> , 84, 231-7  | 3.7  | 34 |
|----|--|------|----|
| 49 | Effective intermediate-spin iron in O-transporting heme proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2017</b> , 114, 8556-8561  | 11.5 | 32 |
| 48 | The Molybdenum Active Site of Formate Dehydrogenase Is Capable of Catalyzing C-H Bond Cleavage and Oxygen Atom Transfer Reactions. <i>Biochemistry</i> , <b>2016</b> , 55, 2381-9  | 3.2  | 32 |
| 47 | Rapid X-ray photoreduction of dimetal-oxygen cofactors in ribonucleotide reductase. <i>Journal of Biological Chemistry</i> , <b>2013</b> , 288, 9648-9661  | 5.4  | 29 |
| 46 | Hydrogen and oxygen trapping at the H-cluster of [FeFe]-hydrogenase revealed by site-selective spectroscopy and QM/MM calculations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>2018</b> , 1859, 28-41   | 4.6  | 27 |
| 45 | Site-selective X-ray spectroscopy on an asymmetric model complex of the [FeFe] hydrogenase active site. <i>Inorganic Chemistry</i> , <b>2012</b> , 51, 4546-59   | 5.1  | 27 |
| 44 | Carboxylate shifts steer interquinone electron transfer in photosynthesis. <i>Journal of Biological Chemistry</i> , <b>2011</b> , 286, 5368-74   | 5.4  | 27 |
| 43 | Bridging-hydride influence on the electronic structure of an [FeFe] hydrogenase active-site model complex revealed by XAES-DFT. <i>Dalton Transactions</i> , <b>2013</b> , 42, 7539-54   | 4.3  | 26 |
| 42 | Biomimetic [2Fe-2S] clusters with extensively delocalized mixed-valence iron centers. <i>Angewandte Chemie - International Edition</i> , <b>2015</b> , 54, 12506-10  | 16.4 | 25 |
| 41 | The structure of the Ni-Fe site in the isolated HoxC subunit of the hydrogen-sensing hydrogenase from Ralstonia eutropha. <i>FEBS Letters</i> , <b>2005</b> , 579, 4287-91   | 3.8  | 25 |
| 40 | KEX-ray Emission Spectroscopy on the Photosynthetic Oxygen-Evolving Complex Supports Manganese Oxidation and Water Binding in the S State. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 10424-10430  | 5.1  | 24 |
| 39 | Light-driven hydrogen evolution catalyzed by a cobaloxime catalyst incorporated in a MIL-101(Cr) metal-organic framework. <i>Sustainable Energy and Fuels</i> , <b>2018</b> , 2, 1148-1152   | 5.8  | 23 |
| 38 | Lyophilization protects [FeFe]-hydrogenases against O2-induced H-cluster degradation. <i>Scientific Reports</i> , <b>2015</b> , 5, 13978   | 4.9  | 23 |
| 37 | Abrupt versus Gradual Spin-Crossover in Fe(II)(phen)2(NCS)2 and Fe(III)(dedtc)3 Compared by X-ray Absorption and Emission Spectroscopy and Quantum-Chemical Calculations. <i>Inorganic Chemistry</i> , <b>2015</b> , 54, 11606-24  | 5.1  | 22 |
| 36 | Behavior of Ru-bda Water-Oxidation Catalysts in Low Oxidation States. <i>Chemistry - A European Journal</i> , <b>2018</b> , 24, 12838-12847  | 4.8  | 22 |
| 35 | A novel BioXAS technique with sub-millisecond time resolution to track oxidation state and structural changes at biological metal centers. <i>Journal of Synchrotron Radiation</i> , <b>2005</b> , 12, 35-44   | 2.4  | 22 |
| 34 | Photosynthetic water oxidation under flashing light. Oxygen release, proton release and absorption transients in the near ultraviolet 🖟 comparison between thylakoids and a reaction-centre core preparation. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>1993</b> , 1183, 210-214 | 4.6  | 22 |
| 33 | Geometry of the Catalytic Active Site in [FeFe]-Hydrogenase Is Determined by Hydrogen Bonding and Proton Transfer. <i>ACS Catalysis</i> , <b>2019</b> , 9, 9140-9149   | 13.1 | 21 |

| 32 | Stoichiometric Formation of an Oxoiron(IV) Complex by a Soluble Methane Monooxygenase Type Activation of O at an Iron(II)-Cyclam Center. <i>Journal of the American Chemical Society</i> , <b>2020</b> , 142, 5924-5                                  | 5928 <sup>4</sup> | 19 |  |
|----|---|-------------------|----|--|
| 31 | A Crystallographic and Mo K-Edge XAS Study of Molybdenum Oxo Bis-, Mono-, and Non-Dithiolene Complexes First-Sphere Coordination Geometry and Noninnocence of Ligands. <i>European Journal of Inorganic Chemistry</i> , <b>2011</b> , 2011, 4387-4399 | 2.3               | 19 |  |
| 30 | Effect of exchange of the cysteine molybdenum ligand with selenocysteine on the structure and function of the active site in human sulfite oxidase. <i>Biochemistry</i> , <b>2013</b> , 52, 8295-303  | 3.2               | 18 |  |
| 29 | The Escherichia coli Periplasmic Aldehyde Oxidoreductase Is an Exceptional Member of the Xanthine Oxidase Family of Molybdoenzymes. <i>ACS Chemical Biology</i> , <b>2016</b> , 11, 2923-2935   | 4.9               | 17 |  |
| 28 | Axial Ligation and Redox Changes at the Cobalt Ion in Cobalamin Bound to Corrinoid Iron-Sulfur Protein (CoFeSP) or in Solution Characterized by XAS and DFT. <i>PLoS ONE</i> , <b>2016</b> , 11, e0158681   | 3.7               | 17 |  |
| 27 | Spontaneous Si-C bond cleavage in (Triphos)-nickel complexes. <i>Dalton Transactions</i> , <b>2017</b> , 46, 907-917  | 4.3               | 14 |  |
| 26 | Protonation State of MnFe and FeFe Cofactors in a Ligand-Binding Oxidase Revealed by X-ray Absorption, Emission, and Vibrational Spectroscopy and QM/MM Calculations. <i>Inorganic Chemistry</i> , <b>2016</b> , 55, 9869-9885                        | 5.1               | 14 |  |
| 25 | Differential Protonation at the Catalytic Six-Iron Cofactor of [FeFe]-Hydrogenases Revealed by Fe Nuclear Resonance X-ray Scattering and Quantum Mechanics/Molecular Mechanics Analyses. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 4000-4013     | 5.1               | 14 |  |
| 24 | Structural differences of oxidized iron-sulfur and nickel-iron cofactors in O2-tolerant and O2-sensitive hydrogenases studied by X-ray absorption spectroscopy. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>2015</b> , 1847, 162-170    | 4.6               | 13 |  |
| 23 | Light-driven formation of manganese oxide by todays photosystem II supports evolutionarily ancient manganese-oxidizing photosynthesis. <i>Nature Communications</i> , <b>2020</b> , 11, 6110  | 17.4              | 13 |  |
| 22 | O-Tolerant H Activation by an Isolated Large Subunit of a [NiFe] Hydrogenase. <i>Biochemistry</i> , <b>2018</b> , 57, 5339-5349   | 3.2               | 11 |  |
| 21 | Temperature Dependence of Structural Dynamics at the Catalytic Cofactor of [FeFe]-hydrogenase. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 16474-16488   | 5.1               | 10 |  |
| 20 | Protein-protein complex formation affects the Ni-Fe and Fe-S centers in the H2-sensing regulatory hydrogenase from Ralstonia eutropha H16. <i>ChemPhysChem</i> , <b>2010</b> , 11, 1297-306   | 3.2               | 10 |  |
| 19 | Cofactor X of photosynthetic water oxidation: electron transfer, proton release, and electrogenic behaviour in chloride-depleted Photosystem II. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>1997</b> , 1321, 47-60                     | 4.6               | 8  |  |
| 18 | Protonation and Sulfido versus Oxo Ligation Changes at the Molybdenum Cofactor in Xanthine Dehydrogenase (XDH) Variants Studied by X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , <b>2017</b> , 56, 2165-2176                            | 5.1               | 7  |  |
| 17 | Spectroscopical Investigations on the Redox Chemistry of [FeFe]-Hydrogenases in the Presence of Carbon Monoxide. <i>Molecules</i> , <b>2018</b> , 23,   | 4.8               | 7  |  |
| 16 | A Pseudotetrahedral Terminal Oxoiron(IV) Complex: Mechanistic Promiscuity in C-H Bond Oxidation Reactions. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 6752-6756   | 16.4              | 7  |  |
| 15 | Identification of YdhV as the First Molybdoenzyme Binding a Bis-Mo-MPT Cofactor in Escherichia coli. <i>Biochemistry</i> , <b>2019</b> , 58, 2228-2242  | 3.2               | 6  |  |

| 14 | Anion Binding and Oxidative Modification at the Molybdenum Cofactor of Formate Dehydrogenase from Studied by X-ray Absorption Spectroscopy. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 214-225  | 5.1  | 6 |
|----|---|------|---|
| 13 | Electronic and molecular structure relations in diiron compounds mimicking the [FeFe]-hydrogenase active site studied by X-ray spectroscopy and quantum chemistry. <i>Dalton Transactions</i> , <b>2017</b> , 46, 12544-12557   | 4.3  | 5 |
| 12 | Simulation of XANES Spectra for ProteinBound Metal Centers Analysis of Linear Dichroism Data. <i>Physica Scripta</i> , <b>2005</b> , 859  | 2.6  | 5 |
| 11 | Operando tracking of oxidation-state changes by coupling electrochemistry with time-resolved X-ray absorption spectroscopy demonstrated for water oxidation by a cobalt-based catalyst film. <i>Analytical and Bioanalytical Chemistry</i> , <b>2021</b> , 413, 5395-5408 | 4.4  | 5 |
| 10 | 5 Metal centers in hydrogenase enzymes studied by X-ray spectroscopy  |      | 4 |
| 9  | Protonengekoppelte Reduktion des katalytischen [4Fe-4S]-Zentrums in [FeFe]-Hydrogenasen. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 16728-16732  | 3.6  | 4 |
| 8  | [FeFe]-hydrogenase maturation: H-cluster assembly intermediates tracked by electron paramagnetic resonance, infrared, and X-ray absorption spectroscopy. <i>Journal of Biological Inorganic Chemistry</i> , <b>2020</b> , 25, 777-788                                     | 3.7  | 3 |
| 7  | A bioinspired oxoiron(IV) motif supported on a NS macrocyclic ligand. <i>Chemical Communications</i> , <b>2021</b> , 57, 2947-2950  | 5.8  | 3 |
| 6  | A Pseudotetrahedral Terminal Oxoiron(IV) Complex: Mechanistic Promiscuity in CH Bond Oxidation Reactions. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 6826-6830   | 3.6  | 2 |
| 5  | Ligand binding at the A-cluster in full-length or truncated acetyl-CoA synthase studied by X-ray absorption spectroscopy. <i>PLoS ONE</i> , <b>2017</b> , 12, e0171039  | 3.7  | 1 |
| 4  | Fate of oxygen species from O activation at dimetal cofactors in an oxidase enzyme revealed by Fe nuclear resonance X-ray scattering and quantum chemistry. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , <b>2019</b> , 1860, 148060                             | 4.6  | 1 |
| 3  | Bimetallic Mn, Fe, Co, and Ni Sites in a Four-Helix Bundle Protein: Metal Binding, Structure, and Peroxide Activation. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 17498-17508   | 5.1  | 1 |
| 2  | Light-driven formation of high-valent manganese oxide by photosystem II supports evolutionary role in early bioenergetics   |      | 1 |
| 1  | Tryptophan regulates zinc stores <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2022</b> , 119, e2117807119  | 11.5 | O |