# Maurice van Gastel

List of Publications by Year
in descending order

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|---|---|---|---|
| 89 papers | 3,478 citations | 147801 31 h-index | 155660 55 g-index |
| 89 all docs | 89 docs citations | 89 times ranked | 3464 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | [NiFe] and [FeFe] Hydrogenases Studied by Advanced Magnetic Resonance Techniques. Chemical Reviews, 2007, 107, 4331-4365. | 47.7 | 458 |
| 2 | 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. | 13.7 | 259 |
| 3 | Palladium-catalysed electrophilic aromatic Câ€“H fluorination. Nature, 2018, 554, 511-514. | 27.8 | 131 |
| 4 | 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. | 2.6 | 110 |
| 5 | Probing the Structure of a Water-Oxidizing Anodic Iridium Oxide Catalyst using Raman Spectroscopy. ACS Catalysis, 2016, 6, 8098-8105. | 11.2 | 104 |
| 6 | 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. | 2.6 | 103 |
| 7 | A Functional [NiFe]-Hydrogenase Model Compound That Undergoes Biologically Relevant Reversible Thiolate Protonation. Journal of the American Chemical Society, 2012, 134, 20745-20755. | 13.7 | 101 |
| 8 | Hydride bridge in [NiFe]-hydrogenase observed by nuclear resonance vibrational spectroscopy. Nature Communications, 2015, 6, 7890. | 12.8 | 96 |
| 9 | A Metalâ€“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. | 13.7 | 95 |
| 10 | Electronic Structure of a Formal Iron(0) Porphyrin Complex Relevant to CO<sub>2</sub> Reduction. Inorganic Chemistry, 2017, 56, 4745-4750. | 4.0 | 85 |
| 11 | An Intermediate Cobalt(IV) Nitrido Complex and its N-Migratory Insertion Product. Journal of the American Chemical Society, 2014, 136, 15072-15078. | 13.7 | 84 |
| 12 | H<sub>2</sub>O Activation for Hydrogenâ€Atom Transfer: Correct Structures and Revised Mechanisms. Angewandte Chemie - International Edition, 2012, 51, 3266-3270. | 13.8 | 72 |
| 13 | The active site for the water oxidising anodic iridium oxide probed through in situ Raman spectroscopy. Chemical Communications, 2017, 53, 12414-12417. | 4.1 | 68 |
| 14 | Crystalline Radicals Derived from Classical Nâ€Heterocyclic Carbenes. Angewandte Chemie - International Edition, 2018, 57, 4765-4768. | 13.8 | 57 |
| 15 | Theoretical Spectroscopy of the Ni<sup>II</sup> Intermediate States in the Catalytic Cycle and the Activation of [NiFe] Hydrogenases. ChemBioChem, 2013, 14, 1898-1905. | 2.6 | 56 |
| 16 | Nâ€Heterocyclic Carbene Analogues of Thiele and Chichibabin Hydrocarbons. Angewandte Chemie - International Edition, 2018, 57, 5838-5842. | 13.8 | 55 |
| 17 | Entropic Changes Control the Charge Separation Process in Triads Mimicking Photosynthetic Charge Separation. Journal of Physical Chemistry A, 2008, 112, 4215-4223. | 2.5 | 52 |
| 18 | Reactive Electrophilic O<sup>Iâ€™</sup> Species Evidenced in Highâ€Performance Iridium Oxohydroxide Water Oxidation Electrocatalysts. ChemSusChem, 2017, 10, 4786-4798. | 6.8 | 49 |

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|---|---|---|---|
| 19 | Electronic Structure and Spin Multiplicity of Iron Tetraphenylporphyrins in Their Reduced States as Determined by a Combination of Resonance Raman Spectroscopy and Quantum Chemistry. Inorganic Chemistry, 2018, 57, 2141-2148. | 4.0 | 48 |
| 20 | Electronic Structure of the Cysteine Thiyl Radical:â€‰ A DFT and Correlated ab Initio Study. Journal of the American Chemical Society, 2004, 126, 2237-2246. | 13.7 | 47 |
| 21 | Sulfide Protects [FeFe] Hydrogenases From O<sub>2</sub>. Journal of the American Chemical Society, 2018, 140, 9346-9350. | 13.7 | 47 |
| 22 | Computational study of the electronic structure and magnetic properties of the Niâ€“C state in [NiFe] hydrogenases including the second coordination sphere. Journal of Biological Inorganic Chemistry, 2012, 17, 1269-1281. | 2.6 | 46 |
| 23 | Characterization of one-electron oxidized copper(<scp>ii</scp>)-salophen-type complexes; effects of electronic and geometrical structures on reactivities. Dalton Transactions, 2014, 43, 2283-2293. | 3.3 | 45 |
| 24 | Openâ€Shell Complexes Containing Metalâ€“Germanium Triple Bonds. Angewandte Chemie - International Edition, 2012, 51, 789-793. | 13.8 | 44 |
| 25 | EPR study of the dinuclear active copper site of tyrosinase from Streptomyces antibioticus. FEBS Letters, 2000, 474, 228-232. | 2.8 | 40 |
| 26 | Zinc-Bacteriochlorophyllide Dimers in de Novo Designed Four-Helix Bundle Proteins. A Model System for Natural Light Energy Harvesting and Dissipation. Journal of the American Chemical Society, 2011, 133, 9526-9535. | 13.7 | 39 |
| 27 | Diphosphene radical cations and dications with a Ï€-conjugated C<sub>2</sub>P<sub>2</sub>C<sub>2</sub>-framework. Chemical Communications, 2019, 55, 10408-10411. | 4.1 | 36 |
| 28 | Spectroscopic Characterization of the Electronic Changes in the Active Site of Streptomyces antibioticus Tyrosinase upon Binding of Transition State Analogue Inhibitors. Journal of Biological Chemistry, 2003, 278, 7381-7389. | 3.4 | 34 |
| 29 | Wavelength dependence of the photo-induced conversion of the Niâ€“C to the Niâ€“L redox state in the [NiFe] hydrogenase of Desulfovibrio vulgaris Miyazaki F. Physical Chemistry Chemical Physics, 2003, 5, 5507-5513. | 2.8 | 33 |
| 30 | Electronâ^'Electron Double Resonance-Detected NMR to Measure Metal Hyperfine Interactions:â€‰<sup>61</sup>Ni in the Niâ^'B State of the [NiFe] Hydrogenase ofDesulfovibrio vulgarisMiyazaki F. Journal of the American Chemical Society, 2008, 130, 2402-2403. | 13.7 | 33 |
| 31 | Insights into the Chemistry of Transient Pâ€Chlorophosphanyl Complexes. Angewandte Chemie - International Edition, 2010, 49, 6894-6898. | 13.8 | 33 |
| 32 | Productive Alkyne Metathesis with â€œCanopy Catalystsâ€•Mandates Pseudorotation. Journal of the American Chemical Society, 2021, 143, 5643-5648. | 13.7 | 33 |
| 33 | 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. Journal of the American Chemical Society, 2007, 129, 15442-15443. | 13.7 | 31 |
| 34 | Cobalt Phosphino-Î±-Iminopyridine-Catalyzed Hydrofunctionalization of Alkenes: Catalyst Development and Mechanistic Analysis. Organometallics, 2016, 35, 2900-2914. | 2.3 | 31 |
| 35 | Diradical Character Enhancement by Spacing: Nâ€Heterocyclic Carbene Analogues of MÃ¼ller's Hydrocarbon. Chemistry - A European Journal, 2018, 24, 16537-16542. | 3.3 | 31 |
| 36 | Crystalline Divinyldiarsene Radical Cations and Dications. Angewandte Chemie - International Edition, 2019, 58, 17599-17603. | 13.8 | 31 |

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| 37 | Electron Paramagnetic Resonance and Electron Nuclear Double Resonance Investigation of the Diradical Bis(Î±-iminopyridinato)zinc Complex. Inorganic Chemistry, 2009, 48, 2626-2632. | 4.0 | 29 |
| 38 | A Combined Spectroscopic and Computational Study on the Mechanism of Iron-Catalyzed Aminofunctionalization of Olefins Using Hydroxylamine Derived Nâ€“O Reagent as the â€œAminoâ€•Source and â€œOxidantâ€• Journal of the American Chemical Society, 2022, 144, 2637-2656. | 13.7 | 29 |
| 39 | Hydrogen Bonding Affects the [NiFe] Active Site of Desulfovibrio vulgaris Miyazaki F Hydrogenase:â€‰ A Hyperfine Sublevel Correlation Spectroscopy and Density Functional Theory Study. Journal of Physical Chemistry B, 2006, 110, 8142-8150. | 2.6 | 28 |
| 40 | Radical 4â€‹exo Cyclizations via Template Catalysis. Chemistry - A European Journal, 2012, 18, 2591-2599. | 3.3 | 25 |
| 41 | Mechanistic Implications for the Ni(I)-Catalyzed Kumada Cross-Coupling Reaction. Inorganics, 2017, 5, 78. | 2.7 | 25 |
| 42 | Nickel(<scp>ii</scp>) radical complexes of thiosemicarbazone ligands appended by salicylidene, aminophenol and aminothiophenol moieties. Dalton Transactions, 2015, 44, 12743-12756. | 3.3 | 24 |
| 43 | Structural and Spectroscopic Investigation of an Anilinosalen Cobalt Complex with Relevance to Hydrogen Production. Inorganic Chemistry, 2013, 52, 14428-14438. | 4.0 | 22 |
| 44 | A Manganese(IV)-Hydroperoxo Intermediate Generated by Protonation of the Corresponding Manganese(III)-Superoxo Complex. Journal of the American Chemical Society, 2020, 142, 10255-10260. | 13.7 | 22 |
| 45 | 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. Physical Chemistry Chemical Physics, 2015, 17, 16204-16212. | 2.8 | 21 |
| 46 | Mononuclear Manganese(III) Superoxo Complexes: Synthesis, Characterization, and Reactivity. Inorganic Chemistry, 2019, 58, 9756-9765. | 4.0 | 21 |
| 47 | An EPR/ENDOR study of the asymmetric hydrogen bond between the quinone electron acceptor and the protein backbone in Photosystem I. Journal of Molecular Structure, 2004, 700, 233-241. | 3.6 | 20 |
| 48 | Spin Density Distribution of the Excited Triplet State of Bacteriochlorophylls. Pulsed ENDOR and DFT Studies. Journal of Physical Chemistry B, 2009, 113, 6917-6927. | 2.6 | 20 |
| 49 | Radical-Based Epoxide Opening by Titanocenes. Inorganic Chemistry, 2013, 52, 11859-11866. | 4.0 | 20 |
| 50 | Electronic Structure of a Binuclear Nickel Complex of Relevance to [NiFe] Hydrogenase. Inorganic Chemistry, 2008, 47, 11688-11697. | 4.0 | 19 |
| 51 | Isolation of singlet carbene derived 2-phospha-1,3-butadienes and their sequential one-electron oxidation to radical cations and dications. Chemical Science, 2020, 11, 1975-1984. | 7.4 | 19 |
| 52 | Low-Temperature Pulsed EPR Study at 34 GHz of the Triplet States of the Primary Electron Donor P<sub>865</sub> and the Carotenoid in Native and Mutant Bacterial Reaction Centers of Rhodobacter sphaeroides. Biochemistry, 2007, 46, 14782-14794. | 2.5 | 18 |
| 53 | High surface area black TiO2 templated from ordered mesoporous carbon for solar driven hydrogen evolution. Microporous and Mesoporous Materials, 2018, 268, 162-169. | 4.4 | 18 |
| 54 | A singlet ground state for a cobalt(<scp>ii</scp>)â€“anilinosalen radical complex. Chemical Communications, 2014, 50, 4924-4926. | 4.1 | 17 |

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| 55 | Solvent-Controlled CO<sub>2</sub> Reduction by a Triphosâ€“Iron Hydride Complex. Organometallics, 2019, 38, 289-299. | 2.3 | 17 |
| 56 | An Unusal Case of Facile Nonâ€Đegenerate Pï£¿C Bond Making and Breaking. Chemistry - an Asian Journal, 2012, 7, 1708-1712. | 3.3 | 16 |
| 57 | Spectroscopic and Quantum Chemical Study of the Ni(PPh2NC6H4CH2P(O)(OEt)22)2 Electrocatalyst for Hydrogen Production with Emphasis on the NiI Oxidation State. Journal of Physical Chemistry C, 2014, 118, 2350-2360. | 3.1 | 16 |
| 58 | Spontaneous Siâ€“C bond cleavage in (Triphos<sup>Si</sup>)-nickel complexes. Dalton Transactions, 2017, 46, 907-917. | 3.3 | 16 |
| 59 | Deoxygenation of Coordinated Oxaphosphiranes: A New Route to Pï£¾C Doubleâ€Bond Systems. Chemistry - A European Journal, 2012, 18, 9780-9783. | 3.3 | 15 |
| 60 | Hydrogen evolution in [NiFe] hydrogenases and related biomimetic systems: similarities and differences. Physical Chemistry Chemical Physics, 2016, 18, 24681-24692. | 2.8 | 15 |
| 61 | Spectroscopic and Theoretical Study on Siloxy-Based Molybdenum and Tungsten Alkylidyne Catalysts for Alkyne Metathesis. ACS Catalysis, 2021, 11, 9086-9101. | 11.2 | 15 |
| 62 | Combined Spectroscopic and Electrochemical Detection of a Ni<sup>I</sup>â‹…â‹…â‹…Hï£¿N Bonding Interaction with Relevance to Electrocatalytic H<sub>2</sub> Production. Chemistry - A European Journal, 2015, 21, 10338-10347. | 3.3 | 14 |
| 63 | Isolation of singlet carbene derived 2-arsa-1,3-butadiene radical cations and dications. Chemical Communications, 2020, 56, 3575-3578. | 4.1 | 14 |
| 64 | The effect of spin polarization on zero field splitting parameters in paramagnetic Ï€-electron molecules. Journal of Chemical Physics, 2009, 131, 124111. | 3.0 | 13 |
| 65 | EPR and Quantum Chemical Investigation of a Bioinspired Hydrogenase Model with a Redox-Active Ligand in the First Coordination Sphere. Organometallics, 2015, 34, 995-1000. | 2.3 | 13 |
| 66 | Zero-Field Splitting of the Lowest Excited Triplet States of C<sub>60</sub> and C<sub>70</sub> and Benzene. Journal of Physical Chemistry A, 2010, 114, 10864-10870. | 2.5 | 12 |
| 67 | Monomeric and Dimeric Conformation of the Vinculin Tail Five-Helix Bundle in Solution Studied by EPR Spectroscopy. Biophysical Journal, 2011, 101, 1772-1780. | 0.5 | 12 |
| 68 | Electronic Structure of the Lowest Triplet State of Flavin Mononucleotide. Journal of Physical Chemistry A, 2012, 116, 10090-10098. | 2.5 | 12 |
| 69 | Copper(II)-Coordinated Î±-Azophenols: Effect of the Metal-Ion Geometry on Phenoxyl/Phenolate Oxidation Potential and Reactivity. European Journal of Inorganic Chemistry, 2014, 2014, 4263-4267. | 2.0 | 12 |
| 70 | Metalloradical Cations and Dications Based on Divinyldiphosphene and Divinyldiarsene Ligands. Chemistry - A European Journal, 2021, 27, 5803-5809. | 3.3 | 12 |
| 71 | Sterically Stabilized End-On Superoxocopper(II) Complexes and Mechanistic Insights into Their Reactivity with Oâ€“H, Nâ€“H, and Câ€“H Substrates. Journal of the American Chemical Society, 2021, 143, 19731-19747. | 13.7 | 12 |
| 72 | EPR and ENDOR Study of the Frozen Ammoniated Electron at Low Alkali-Metal Concentrations. Journal of Physical Chemistry A, 2011, 115, 1939-1945. | 2.5 | 11 |

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|---|---|---|---|
| 73 | Photoinduced Charge Separation in an Organic Donorâ€“Acceptor Hybrid Molecule. Journal of Physical Chemistry B, 2011, 115, 13526-13533. | 2.6 | 11 |
| 74 | Isolation of a Homoleptic Non-oxo Mo(V) Alkoxide Complex: Synthesis, Structure, and Electronic Properties of Penta-tert-Butoxymolybdenum. Journal of the American Chemical Society, 2020, 142, 16392-16402. | 13.7 | 11 |
| 75 | EPR and ENDOR Studies of [NiFe] Hydrogenase: Contributions to Understanding the Mechanism of Biological Hydrogen Conversion. ACS Symposium Series, 2003, , 128-149. | 0.5 | 10 |
| 76 | Converged Structural and Spectroscopic Properties for Refined QM/MM Models of Azurin. Inorganic Chemistry, 2021, 60, 7399-7412. | 4.0 | 10 |
| 77 | Raman Spectroscopy as a Method to Investigate Catalytic Intermediates: CO<sub>2</sub> Reducing [Re(Cl)(bpy-R)(CO)<sub>3</sub>] Catalyst. Journal of Physical Chemistry A, 2016, 120, 7465-7474. | 2.5 | 9 |
| 78 | Spectroscopic and Quantum Chemical Investigation of Benzene-1,2-dithiolate-Coordinated Diiron Complexes with Relevance to Dinitrogen Activation. Inorganic Chemistry, 2019, 58, 5111-5125. | 4.0 | 9 |
| 79 | Structural Features of the Unready Ni-A State of [NiFe] Hydrogenase Revealed by X-Ray Crystallography and EPR Spectroscopy. Applied Magnetic Resonance, 2010, 37, 207-218. | 1.2 | 8 |
| 80 | Finding the Reactive Electron in Paramagnetic Systems: A Critical Evaluation of Accuracies for EPR Spectroscopy and Density Functional Theory Using 1,3,5-Triphenyl Verdazyl Radical as a Testcase. Applied Magnetic Resonance, 2015, 46, 117-139. | 1.2 | 8 |
| 81 | Where Is the Fluoro Wall?: A Quantum Chemical Investigation. Inorganic Chemistry, 2020, 59, 1556-1565. | 4.0 | 7 |
| 82 | EPR Investigation of [NiFe] Hydrogenases. Biological Magnetic Resonance, 2009, , 441-470. | 0.4 | 7 |
| 83 | Comparative ENDOR study at 34ÂGHz of the triplet state of the primary donor in bacterial reaction centers of Rb. sphaeroides and Bl. viridis. Photosynthesis Research, 2014, 120, 99-111. | 2.9 | 6 |
| 84 | Crystalline Divinyldiarsene Radical Cations and Dications. Angewandte Chemie, 2019, 131, 17763-17767. | 2.0 | 6 |
| 85 | Pulsed EPR spectroscopy. Photosynthesis Research, 2009, 102, 367-373. | 2.9 | 5 |
| 86 | What are the structural features of the active site that define binuclear copper proteins function?. Micron, 2004, 35, 143-145. | 2.2 | 4 |
| 87 | Reversed Freeze Quench Method near the Solvent Phase Transition. Journal of Physical Chemistry A, 2012, 116, 3899-3906. | 2.5 | 3 |
| 88 | Synthesis, Reactivity, and Electronic Structure of a Bioinspired Heterobimetallic [Ni(Î¼-S<sub>2</sub>)Fe] Complex with Disulfur Monoradical character. Organometallics, 2014, 33, 3154-3162. | 2.3 | 3 |
| 89 | Triplet States in Photosynthetic Reaction Centers of Rb. sphaeroides. , 2008, , 133-136. | | 0 |