

# Mark A Iron

## List of Publications by Year in descending order

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77  
papers

4,517  
citations

81839

39  
h-index

102432

66  
g-index

92  
all docs

92  
docs citations

92  
times ranked

4638  
citing authors

#	ARTICLE	IF	CITATIONS
1	Consecutive Thermal H <sub>2</sub> and Light-Induced O <sub>2</sub> Evolution from Water Promoted by a Metal Complex. <i>Science</i> , 2009, 324, 74-77.	6.0	448
2	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactions. <i>Journal of Physical Chemistry A</i> , 2006, 110, 709-716.	1.1	223
3	N <sup>+</sup> H Activation of Amines and Ammonia by Ru via Metal-Ligand Cooperation. <i>Journal of the American Chemical Society</i> , 2010, 132, 8542-8543.	6.6	214
4	Iron Borohydride Pincer Complexes for the Efficient Hydrogenation of Ketones under Mild, Base-Free Conditions: Synthesis and Mechanistic Insight. <i>Chemistry - A European Journal</i> , 2012, 18, 7196-7209.	1.7	180
5	A Computational Foray into the Formation and Reactivity of Metallabenzenes. <i>Journal of the American Chemical Society</i> , 2004, 126, 11699-11710.	6.6	149
6	Long-Range Metal-Ligand Cooperation in H <sub>2</sub> Activation and Ammonia-Promoted Hydride Transfer with a Ruthenium-Acridine Pincer Complex. <i>Journal of the American Chemical Society</i> , 2010, 132, 14763-14765.	6.6	129
7	A New Mode of Activation of CO <sub>2</sub> by Metal-Ligand Cooperation with Reversible C≡C and M-O Bond Formation at Ambient Temperature. <i>Chemistry - A European Journal</i> , 2012, 18, 9194-9197.	1.7	125
8	A novel liquid organic hydrogen carrier system based on catalytic peptide formation and hydrogenation. <i>Nature Communications</i> , 2015, 6, 6859.	5.8	115
9	Metal-Ligand cooperation in the trans addition of dihydrogen to a pincer Ir(i) complex: a DFT study. <i>Dalton Transactions</i> , 2009, , 9433.	1.6	111
10	Activation of Nitriles by Metal Ligand Cooperation. Reversible Formation of Ketimido- and Enamido-Rhenium PNP Pincer Complexes and Relevance to Catalytic Design. <i>Journal of the American Chemical Society</i> , 2013, 135, 17004-17018.	6.6	110
11	Stable Aromatic Dianion in Water. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8855-8858.	1.2	105
12	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange-Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3761-3781.	1.1	104
13	Alkali and alkaline earth metal compounds: core-valence basis sets and importance of subvalence correlation. <i>Molecular Physics</i> , 2003, 101, 1345-1361.	0.8	103
14	Synthesis and Reactivity of an Iridium(I) Acetylonyl PNP Complex. Experimental and Computational Study of Metal-Ligand Cooperation in H <sup>+</sup> H and C <sup>+</sup> H Bond Activation via Reversible Ligand Dearomatization. <i>Organometallics</i> , 2010, 29, 3817-3827.	1.1	97
15	Nitrenium ions as ligands for transition metals. <i>Nature Chemistry</i> , 2011, 3, 525-531.	6.6	97
16	Authorizing Multiple Chemical Passwords by a Combinatorial Molecular Keypad Lock. <i>Journal of the American Chemical Society</i> , 2013, 135, 15330-15333.	6.6	96
17	Manganese Catalyzed Hydrogenation of Carbamates and Urea Derivatives. <i>Journal of the American Chemical Society</i> , 2019, 141, 12962-12966.	6.6	92
18	Density Functional Theory in Transition-Metal Chemistry: Relative Energies of Low-Lying States of Iron Compounds and the Effect of Spatial Symmetry Breaking. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 307-315.	2.3	86

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19	Enolonium Species—Umpoled Enolates. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 2599-2603.	7.2	84
20	Anionic Nickel(II) Complexes with Doubly Deprotonated PNP Pincer-Type Ligands and Their Reactivity toward CO <sub>2</sub> . <i>Organometallics</i> , 2013, 32, 300-308.	1.1	79
21	Cationic, Neutral, and Anionic PNP Pd <sup>II</sup> and Pt <sup>II</sup> Complexes: Dearomatization by Deprotonation and Double-Deprotonation of Pincer Systems. <i>Inorganic Chemistry</i> , 2010, 49, 1615-1625.	1.9	78
22	Evaluation of the Factors Impacting the Accuracy of <sup>13</sup> C NMR Chemical Shift Predictions using Density Functional Theory—The Advantage of Long-Range Corrected Functionals. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5798-5819.	2.3	77
23	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides: Surprisingly Demanding Targets for High-Level ab Initio Procedures. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5617-5630.	1.1	76
24	Medication Detection by a Combinatorial Fluorescent Molecular Sensor. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 12477-12481.	7.2	72
25	Metallabenzene versus Cp Complex Formation: A DFT Investigation. <i>Journal of the American Chemical Society</i> , 2003, 125, 13020-13021.	6.6	71
26	A Dearomatized Anionic PNP Pincer Rhodium Complex: C—H and H—H Bond Activation by Metal—Ligand Cooperation and Inhibition by Dinitrogen. <i>Organometallics</i> , 2011, 30, 2721-2729.	1.1	64
27	TpPtMe(H) <sub>2</sub> : Why Is There H/D Scrambling of the Methyl Group but Not Methane Loss?. <i>Journal of the American Chemical Society</i> , 2002, 124, 7041-7054.	6.6	63
28	Platinum Stilbazoles: Ring-Walking Coupled with Aryl—Halide Bond Activation. <i>Journal of the American Chemical Society</i> , 2005, 127, 9322-9323.	6.6	60
29	Stepwise Assembly of Coordination-Based Metal—Organic Networks. <i>Journal of the American Chemical Society</i> , 2010, 132, 14554-14561.	6.6	57
30	Iron Dicarbonyl Complexes Featuring Bipyridine-Based PNN Pincer Ligands with Short Interpyridine C—C Bond Lengths: Innocent or Non-Innocent Ligand?. <i>Chemistry - A European Journal</i> , 2014, 20, 4403-4413.	1.7	56
31	Cycloaddition Reactions of Metalloaromatic Complexes of Iridium and Rhodium: A Mechanistic DFT Investigation. <i>Journal of the American Chemical Society</i> , 2003, 125, 11702-11709.	6.6	53
32	Synthesis, Structures, and Dearomatization by Deprotonation of Iron Complexes Featuring Bipyridine-based PNN Pincer Ligands. <i>Inorganic Chemistry</i> , 2013, 52, 9636-9649.	1.9	53
33	sp <sup>3</sup> C—H and sp <sup>2</sup> C—H agostic ruthenium complexes: a combined experimental and theoretical study. <i>Inorganica Chimica Acta</i> , 2004, 357, 1854-1864.	1.2	49
34	On the Unexpected Stability of the Dianion of Perylene Diimide in Water—A Computational Study. <i>Journal of Physical Chemistry A</i> , 2011, 115, 2047-2056.	1.1	49
35	π-Accepting-Pincer Rhodium Complexes: An Unusual Coordination Mode of PCP-Type Systems. <i>Chemistry - A European Journal</i> , 2005, 11, 2319-2326.	1.7	47
36	Mechanism of the Copper/TEMPO-Catalyzed Aerobic Oxidation of Alcohols. <i>Chemistry - A European Journal</i> , 2017, 23, 1368-1378.	1.7	45

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37	NLO Properties of Metallabenzene-Based Chromophores: A Time-Dependent Density Functional Study. <i>Journal of Physical Chemistry A</i> , 2005, 109, 5454-5462.	1.1	44
38	Competitive C <sup>1</sup> versus C <sup>N</sup> Reductive Elimination from a Rh <sup>III</sup> Complex. Selectivity is Controlled by the Solvent. <i>Journal of the American Chemical Society</i> , 2008, 130, 14374-14375.	6.6	42
39	Molecular Structure-Function Relations of the Optical Properties and Dimensions of Gold Nanoparticle Assemblies. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1218-1221.	7.2	42
40	Enolonium Species-Unpoled Enolates. <i>Angewandte Chemie</i> , 2017, 129, 2643-2647.	1.6	39
41	Photoinduced Singlet Charge Transfer in a Ruthenium(II) Perylene-3,4:9,10-bis(dicarboximide) Complex. <i>Journal of Physical Chemistry B</i> , 2011, 115, 7533-7540.	1.2	36
42	On the Innocence of Bipyridine Ligands: How Well Do DFT Functionals Fare for These Challenging Spin Systems?. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 220-235.	2.3	34
43	Mechanistic aspects of acetone addition to metalloaromatic complexes of iridium: a DFT investigation. Electronic supplementary information (ESI) available: selected geometric data, calculated structures of all complexes and full computational details. See <a href="http://www.rsc.org/suppdata/cc/b2/b210622a/">http://www.rsc.org/suppdata/cc/b2/b210622a/</a> . <i>Chemical Communications</i> , 2003, 132-133.	2.2	32
44	Thermodynamic Properties of C1 and C2 Bromo Compounds and Radicals. A Relativistic ab Initio Study. <i>Journal of Physical Chemistry A</i> , 2004, 108, 7752-7761.	1.1	31
45	Ru(0) and Ru(II) Nitrosyl Pincer Complexes: Structure, Reactivity, and Catalytic Activity. <i>Inorganic Chemistry</i> , 2013, 52, 11469-11479.	1.9	29
46	Amplifying undetectable NMR signals to study host-guest interactions and exchange. <i>Chemical Science</i> , 2016, 7, 6905-6909.	3.7	29
47	Overcoming artificial broadening in Gd <sup>3+</sup> -Gd <sup>3+</sup> distance distributions arising from dipolar pseudo-secular terms in DEER experiments. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12847-12859.	1.3	28
48	Electrochemical Characteristics of a Self-Propagating Molecular-Based Assembly. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14283-14286.	1.2	27
49	Design concept for $\pm$ -hydrogen-substituted nitroxides. <i>Nature Communications</i> , 2015, 6, 6070.	5.8	26
50	Positive Constructs: Charges Localized on Surface-Confined Organometallic Oligomers. <i>Chemistry of Materials</i> , 2009, 21, 4676-4684.	3.2	25
51	Self-Assembled Hybrid Materials Based on Organic Nanocrystals and Carbon Nanotubes. <i>Advanced Materials</i> , 2018, 30, 1705027.	11.1	22
52	Catalytic Reduction of Acetone by [(bpy)Rh] <sup>+</sup> : A Theoretical Mechanistic Investigation and Insight into Cooperativity Effects in This System. <i>Journal of the American Chemical Society</i> , 2003, 125, 11430-11441.	6.6	19
53	Iron-catalysed ring-opening metathesis polymerization of olefins and mechanistic studies. <i>Nature Catalysis</i> , 2022, 5, 494-502.	16.1	19
54	Theoretical estimates of equilibrium carbon and hydrogen isotope effects in microbial methane production and anaerobic oxidation of methane. <i>Geochimica Et Cosmochimica Acta</i> , 2021, 295, 237-264.	1.6	17

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55	A Monolayer-Based Setup for Optical Amplification. ACS Applied Materials & Interfaces, 2010, 2, 7-10.	4.0	15
56	Synergism in Multicomponent Self-Propagating Molecular Assemblies. Langmuir, 2011, 27, 1319-1325.	1.6	14
57	Palladium-Catalyzed Cross-Coupling Reactions with Fluorinated Substrates: Mechanistic Insights into the Undesired Hydrodehalogenation of Aryl Halides. Organometallics, 2012, 31, 1271-1274.	1.1	14
58	Synthesis and stability of cyclic $\hat{\pm}$ -hydrogen nitroxides. Organic and Biomolecular Chemistry, 2015, 13, 10726-10733.	1.5	14
59	Proton Walk in the Aqueous Platinum Complex [TpPtMeCO] via a Sticky $\hat{f}$ -Methane Ligand. Chemistry - A European Journal, 2007, 13, 2812-2823.	1.7	13
60	Designing Surface-Confined Coordination Oligomers. Chemistry - A European Journal, 2010, 16, 6744-6747.	1.7	13
61	Activation of Molecular Oxygen by a Dioxygenase Pathway by a Ruthenium Bis-bipyridine Compound with a Proximal Selenium Site. Journal of the American Chemical Society, 2010, 132, 517-523.	6.6	13
62	Organic phototransistors based on perylene diimide nanocrystals lacking $\hat{\epsilon}$ - $\hat{\epsilon}$ interactions. Journal of Materials Chemistry C, 2018, 6, 10597-10602.	2.7	12
63	Valence-Bond Order (VBO): A New Approach to Modeling Reactive Potential Energy Surfaces for Complex Systems, Materials, and Nanoparticles. Journal of Chemical Theory and Computation, 2009, 5, 594-604.	2.3	11
64	Platinum complexes of cationic ligands for the aerobic oxidation of $\hat{\epsilon}$ -perfluoro-substituted alcohols. Chemical Communications, 2013, 49, 1720.	2.2	11
65	Mechanistic Aspects of Aryl-Halide Oxidative Addition, Coordination Chemistry, and Ring-Walking by Palladium. Chemistry - A European Journal, 2015, 21, 16113-16125.	1.7	11
66	Dynamic Interactions in Synthetic Receptors: A Guest Exchange Saturation Transfer Study. Chemistry - A European Journal, 2019, 25, 1687-1690.	1.7	11
67	Cost-effective density functional theory (DFT) calculations of equilibrium isotopic fractionation in large organic molecules. Physical Chemistry Chemical Physics, 2019, 21, 17555-17570.	1.3	11
68	Ultraslow isomerization in photoexcited gas-phase carbon cluster $\hat{\hat{m}}_{C}_{10}^{\hat{\hat{m}}}$ . Nature Communications, 2018, 9, 912.	5.8	10
69	Tight-Binding Configuration Interaction (TBCI): A Noniterative Approach to Incorporating Electrostatics into Tight Binding. Journal of Chemical Theory and Computation, 2008, 4, 804-818.	2.3	9
70	Anionic $d^{8}$ Alkyl Hydrides - Selective Formation and Reactivity of Anionic $\hat{\hat{Pt}}^{II}$ Methyl Hydride. European Journal of Inorganic Chemistry, 2010, 2010, 1991-1999.	1.0	7
71	The cationic dye basic orange 21 (BO21) as a potential fluorescent sensor. Photochemical and Photobiological Sciences, 2018, 17, 1417-1428.	1.6	6
72	Long-Range Through-Bond Heteronuclear Communication in Platinum Complexes. Inorganic Chemistry, 2009, 48, 4021-4030.	1.9	5

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73	A Phosphine-Accelerated Ar<sub>F</sub>-Chloride Bond Activation Process by Palladium. <i>Organometallics</i> , 2013, 32, 3074-3082.	1.1	3
74	A Nanoscopic View of Photoinduced Charge Transfer in Organic Nanocrystalline Heterojunctions. <i>Journal of Physical Chemistry C</i> , 2019, 123, 25031-25041.	1.5	2
75	The formyloxyl radical: electrophilicity, C-H bond activation and anti-Markovnikov selectivity in the oxidation of aliphatic alkenes. <i>Chemical Science</i> , 2020, 11, 11584-11591.	3.7	2
76	Noncovalent Bonding Caught in Action: From Amorphous to Cocrystalline Molecular Thin Films. <i>ACS Nano</i> , 2021, 15, 14643-14652.	7.3	2
77	Fluorophore spectroscopy in aqueous glycerol solution: the interactions of glycerol with the fluorophore. <i>Photochemical and Photobiological Sciences</i> , 2021, 20, 1397-1418.	1.6	1