Mark A Iron

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2286219/publications.pdf

Version: 2024-02-01

		81839	102432
77	4,517	39	66
papers	citations	h-index	g-index

92	92	92	4638
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Iron-catalysed ring-opening metathesis polymerization of olefins and mechanistic studies. Nature Catalysis, 2022, 5, 494-502.	16.1	19
2	Theoretical estimates of equilibrium carbon and hydrogen isotope effects in microbial methane production and anaerobic oxidation of methane. Geochimica Et Cosmochimica Acta, 2021, 295, 237-264.	1.6	17
3	Noncovalent Bonding Caught in Action: From Amorphous to Cocrystalline Molecular Thin Films. ACS Nano, 2021, 15, 14643-14652.	7.3	2
4	Fluorophore spectroscopy in aqueous glycerol solution: the interactions of glycerol with the fluorophore. Photochemical and Photobiological Sciences, 2021, 20, 1397-1418.	1.6	1
5	The formyloxyl radical: electrophilicity, Câ€“H bond activation and anti-Markovnikov selectivity in the oxidation of aliphatic alkenes. Chemical Science, 2020, 11, 11584-11591.	3.7	2
6	Dynamic Interactions in Synthetic Receptors: A Guest Exchange Saturation Transfer Study. Chemistry - A European Journal, 2019, 25, 1687-1690.	1.7	11
7	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
8	Manganese Catalyzed Hydrogenation of Carbamates and Urea Derivatives. Journal of the American Chemical Society, 2019, 141, 12962-12966.	6.6	92
9	A Nanoscopic View of Photoinduced Charge Transfer in Organic Nanocrystalline Heterojunctions. Journal of Physical Chemistry C, 2019, 123, 25031-25041.	1.5	2
10	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchangeâ€“Correlation Functionals: The MOBH35 Benchmark Database. Journal of Physical Chemistry A, 2019, 123, 3761-3781.	1.1	104
11	Ultraslow isomerization in photoexcited gas-phase carbon cluster $${{m C}}_{10}^ -$$. Nature Communications, 2018, 9, 912.	5.8	10
12	Selfâ€Assembled Hybrid Materials Based on Organic Nanocrystals and Carbon Nanotubes. Advanced Materials, 2018, 30, 1705027.	11.1	22
13	Organic phototransistors based on perylene diimide nanocrystals lacking Ï€â€“Ï€ interactions. Journal of Materials Chemistry C, 2018, 6, 10597-10602.	2.7	12
14	The cationic dye basic orange 21 (BO21) as a potential fluorescent sensor. Photochemical and Photobiological Sciences, 2018, 17, 1417-1428.	1.6	6
15	Enolonium Speciesâ€”Umpoled Enolates. Angewandte Chemie - International Edition, 2017, 56, 2599-2603.	7.2	84
16	Enolonium Speciesâ€”Umpoled Enolates. Angewandte Chemie, 2017, 129, 2643-2647.	1.6	39
17	Evaluation of the Factors Impacting the Accuracy of ‹sup›13‹/sup›C NMR Chemical Shift Predictions using Density Functional Theoryâ€”The Advantage of Long-Range Corrected Functionals. Journal of Chemical Theory and Computation, 2017, 13, 5798-5819.	2.3	77
18	Mechanism of the Copper/TEMPOâ€Catalyzed Aerobic Oxidation of Alcohols. Chemistry - A European Journal, 2017, 23, 1368-1378.	1.7	45

#	Article	IF	Citations
19	Overcoming artificial broadening in Gd³⁺â€“Gd³⁺ distance distributions arising from dipolar pseudo-secular terms in DEER experiments. Physical Chemistry Chemical Physics, 2016, 18, 12847-12859.	1.3	28
20	Amplifying undetectable NMR signals to study hostâ€“guest interactions and exchange. Chemical Science, 2016, 7, 6905-6909.	3.7	29
21	Mechanistic Aspects of Arylâ€“Halide Oxidative Addition, Coordination Chemistry, and Ringâ€Walking by Palladium. Chemistry - A European Journal, 2015, 21, 16113-16125.	1.7	11
22	Design concept for Î±-hydrogen-substituted nitroxides. Nature Communications, 2015, 6, 6070.	5.8	26
23	A novel liquid organic hydrogen carrier system based on catalytic peptide formation and hydrogenation. Nature Communications, 2015, 6, 6859.	5.8	115
24	Synthesis and stability of cyclic Î±-hydrogen nitroxides. Organic and Biomolecular Chemistry, 2015, 13, 10726-10733.	1.5	14
25	Iron Dicarbonyl Complexes Featuring Bipyridineâ€Based PNN Pincer Ligands with Short Interpyridine Cï£¿C Bond Lengths: Innocent or Nonâ€Innocent Ligand?. Chemistry - A European Journal, 2014, 20, 4403-4413.	1.7	56
26	On the Innocence of Bipyridine Ligands: How Well Do DFT Functionals Fare for These Challenging Spin Systems?. Journal of Chemical Theory and Computation, 2014, 10, 220-235.	2.3	34
27	A Phosphine-Accelerated Ar_Fâ€“Chloride Bond Activation Process by Palladium. Organometallics, 2013, 32, 3074-3082.	1.1	3
28	Synthesis, Structures, and Dearomatization by Deprotonation of Iron Complexes Featuring Bipyridine-based PNN Pincer Ligands. Inorganic Chemistry, 2013, 52, 9636-9649.	1.9	53
29	Authorizing Multiple Chemical Passwords by a Combinatorial Molecular Keypad Lock. Journal of the American Chemical Society, 2013, 135, 15330-15333.	6.6	96
30	Activation of Nitriles by Metal Ligand Cooperation. Reversible Formation of Ketimido- and Enamido-Rhenium PNP Pincer Complexes and Relevance to Catalytic Design. Journal of the American Chemical Society, 2013, 135, 17004-17018.	6.6	110
31	Ru(0) and Ru(II) Nitrosyl Pincer Complexes: Structure, Reactivity, and Catalytic Activity. Inorganic Chemistry, 2013, 52, 11469-11479.	1.9	29
32	Anionic Nickel(II) Complexes with Doubly Deprotonated PNP Pincer-Type Ligands and Their Reactivity toward CO₂. Organometallics, 2013, 32, 300-308.	1.1	79
33	Platinum complexes of cationic ligands for the aerobic oxidation of â€œinertâ€•perfluoro-substituted alcohols. Chemical Communications, 2013, 49, 1720.	2.2	11
34	Medication Detection by a Combinatorial Fluorescent Molecular Sensor. Angewandte Chemie - International Edition, 2012, 51, 12477-12481.	7.2	72
35	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
36	Iron Borohydride Pincer Complexes for the Efficient Hydrogenation of Ketones under Mild, Baseâ€Free Conditions: Synthesis and Mechanistic Insight. Chemistry - A European Journal, 2012, 18, 7196-7209.	1.7	180

#	Article	IF	Citations
37	A New Mode of Activation of CO₂ by Metalâ€“Ligand Cooperation with Reversible Cï£¿C and Mï£¿O Bond Formation at Ambient Temperature. Chemistry - A European Journal, 2012, 18, 9194-9197.	1.7	125
38	On the Unexpected Stability of the Dianion of Perylene Diimide in Waterâ€”A Computational Study. Journal of Physical Chemistry A, 2011, 115, 2047-2056.	1.1	49
39	Synergism in Multicomponent Self-Propagating Molecular Assemblies. Langmuir, 2011, 27, 1319-1325.	1.6	14
40	A Dearomatized Anionic PNP Pincer Rhodium Complex: Câ€“H and Hâ€“H Bond Activation by Metalâ€“Ligand Cooperation and Inhibition by Dinitrogen. Organometallics, 2011, 30, 2721-2729.	1.1	64
41	Photoinduced Singlet Charge Transfer in a Ruthenium(II) Perylene-3,4:9,10-bis(dicarboximide) Complex. Journal of Physical Chemistry B, 2011, 115, 7533-7540.	1.2	36
42	Nitrenium ions as ligands for transition metals. Nature Chemistry, 2011, 3, 525-531.	6.6	97
43	Anionic d⁸ Alkyl Hydrides â€“ Selective Formation and Reactivity of Anionic cisâ€Pt^{II} Methyl Hydride. European Journal of Inorganic Chemistry, 2010, 2010, 1991-1999.	1.0	7
44	Designing Surfaceâ€Confined Coordination Oligomers. Chemistry - A European Journal, 2010, 16, 6744-6747.	1.7	13
45	Molecular Structureâ€“Function Relations of the Optical Properties and Dimensions of Gold Nanoparticle Assemblies. Angewandte Chemie - International Edition, 2010, 49, 1218-1221.	7.2	42
46	Nâˆ’H Activation of Amines and Ammonia by Ru via Metalâˆ’Ligand Cooperation. Journal of the American Chemical Society, 2010, 132, 8542-8543.	6.6	214
47	Cationic, Neutral, and Anionic PNP Pd^{II}and Pt^{II}Complexes: Dearomatization by Deprotonation and Double-Deprotonation of Pincer Systems. Inorganic Chemistry, 2010, 49, 1615-1625.	1.9	78
48	â€œLong-Rangeâ€•Metalâˆ’Ligand Cooperation in H₂ Activation and Ammonia-Promoted Hydride Transfer with a Rutheniumâˆ’Acridine Pincer Complex. Journal of the American Chemical Society, 2010, 132, 14763-14765.	6.6	129
49	Synthesis and Reactivity of an Iridium(I) Acetonyl PNP Complex. Experimental and Computational Study of Metalâˆ’Ligand Cooperation in Hâˆ’H and Câˆ’H Bond Activation via Reversible Ligand Dearomatization. Organometallics, 2010, 29, 3817-3827.	1.1	97
50	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
51	A Monolayer-Based Setup for Optical Amplification. ACS Applied Materials & Interfaces, 2010, 2, 7-10.	4.0	15
52	Electrochemical Characteristics of a Self-Propagating Molecular-Based Assembly. Journal of Physical Chemistry B, 2010, 114, 14283-14286.	1.2	27
53	Stepwise Assembly of Coordination-Based Metalâˆ’Organic Networks. Journal of the American Chemical Society, 2010, 132, 14554-14561.	6.6	57
54	Consecutive Thermal H ₂ and Light-Induced O ₂ Evolution from Water Promoted by a Metal Complex. Science, 2009, 324, 74-77.	6.0	448

#	Article	IF	Citations
55	Valenceâ€“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
56	Positive Constructs: Charges Localized on Surface-Confined Organometallic Oligomers. Chemistry of Materials, 2009, 21, 4676-4684.	3.2	25
57	Long-Range Through-Bond Heteronuclear Communication in Platinum Complexes. Inorganic Chemistry, 2009, 48, 4021-4030.	1.9	5
58	Metalâ€“ligand cooperation in the trans addition of dihydrogen to a pincer Ir(i) complex: a DFT study. Dalton Transactions, 2009, , 9433.	1.6	111
59	Density Functional Theory in Transition-Metal Chemistry:â€‰ Relative Energies of Low-Lying States of Iron Compounds and the Effect of Spatial Symmetry Breaking. Journal of Chemical Theory and Computation, 2008, 4, 307-315.	2.3	86
60	Stable Aromatic Dianion in Water. Journal of Physical Chemistry B, 2008, 112, 8855-8858.	1.2	105
61	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
62	Competitive Câˆ’I versus Câˆ’CN Reductive Elimination from a Rh^{III}Complex. Selectivity is Controlled by the Solvent. Journal of the American Chemical Society, 2008, 130, 14374-14375.	6.6	42
63	Proton Walk in the Aqueous Platinum Complex [TpPtMeCO] via a Sticky Ïƒ-Methane Ligand. Chemistry - A European Journal, 2007, 13, 2812-2823.	1.7	13
64	Benchmark Study of DFT Functionals for Late-Transition-Metal Reactionsâ€. Journal of Physical Chemistry A, 2006, 110, 709-716.	1.1	223
65	?-Accepting-Pincer Rhodium Complexes: An Unusual Coordination Mode of PCP-Type Systems. Chemistry - A European Journal, 2005, 11, 2319-2326.	1.7	47
66	NLO Properties of Metallabenzene-Based Chromophores:Â A Time-Dependent Density Functional Study. Journal of Physical Chemistry A, 2005, 109, 5454-5462.	1.1	44
67	Platinum Stilbazoles:Â Ring-Walking Coupled with Arylâˆ’Halide Bond Activation. Journal of the American Chemical Society, 2005, 127, 9322-9323.	6.6	60
68	sp3 Câ€“H and sp2 Câ€“H agostic ruthenium complexes: a combined experimental and theoretical study. Inorganica Chimica Acta, 2004, 357, 1854-1864.	1.2	49
69	Thermodynamic Properties of C1and C2Bromo Compounds and Radicals. A Relativistic ab Initio Study. Journal of Physical Chemistry A, 2004, 108, 7752-7761.	1.1	31
70	A Computational Foray into the Formation and Reactivity of Metallabenzenes. Journal of the American Chemical Society, 2004, 126, 11699-11710.	6.6	149
71	Cycloaddition Reactions of Metalloaromatic Complexes of Iridium and Rhodium:Â A Mechanistic DFT Investigation. Journal of the American Chemical Society, 2003, 125, 11702-11709.	6.6	53
72	Metallabenzene versus Cp Complex Formation:Â A DFT Investigation. Journal of the American Chemical Society, 2003, 125, 13020-13021.	6.6	71

#	Article	IF	Citations
73	Catalytic Reduction of Acetone by [(bpy)Rh]+:Â A Theoretical Mechanistic Investigation and Insight into Cooperativity Effects in This System. Journal of the American Chemical Society, 2003, 125, 11430-11441.	6.6	19
74	Heats of Formation of Alkali Metal and Alkaline Earth Metal Oxides and Hydroxides:â€‰ Surprisingly Demanding Targets for High-Level ab Initio Procedures. Journal of Physical Chemistry A, 2003, 107, 5617-5630.	1.1	76
75	Alkali and alkaline earth metal compounds: coreâ€”valence basis sets and importance of subvalence correlation. Molecular Physics, 2003, 101, 1345-1361.	0.8	103
76	Mechanistic aspects of acetone addition to metalloaromatic complexes of iridium: a DFT investigationElectronic supplementary information (ESI) available: selected geometric data, calculated structures of all complexes and full computational details. See http://www.rsc.org/suppdata/cc/b2/b210622a/.. Chemical Communications, 2003, , 132-133.	2.2	32
77	TpPtMe(H)2:Â Why Is There H/D Scrambling of the Methyl Group but Not Methane Loss?. Journal of the American Chemical Society, 2002, 124, 7041-7054.	6.6	63