Djamaladdin G Musaev

List of Publications by Year
in descending order

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259	16,734	12303	19690
papers	citations	69 h-index	117 g-index

264	264	264	11947
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Fast Soluble Carbon-Free Molecular Water Oxidation Catalyst Based on Abundant Metals. Science, 2010, 328, 342-345.	6.0	1,354
2	Polyoxometalate water oxidation catalysts and the production of green fuel. Chemical Society Reviews, 2012, 41, 7572.	18.7	678
3	An Allâ€inorganic, Stable, and Highly Active Tetraruthenium Homogeneous Catalyst for Water Oxidation. Angewandte Chemie - International Edition, 2008, 47, 3896-3899.	7.2	559
4	Efficient Light-Driven Carbon-Free Cobalt-Based Molecular Catalyst for Water Oxidation. Journal of the American Chemical Society, 2011, 133, 2068-2071.	6.6	336
5	Homogeneous Light-Driven Water Oxidation Catalyzed by a Tetraruthenium Complex with All Inorganic Ligands. Journal of the American Chemical Society, 2009, 131, 7522-7523.	6.6	330
6	Site-selective and stereoselective functionalization of unactivated Câ€“H bonds. Nature, 2016, 533, 230-234.	13.7	313
7	A Diruthenium Catalyst for Selective, Intramolecular Allylic Câ€“H Amination: Reaction Development and Mechanistic Insight Gained through Experiment and Theory. Journal of the American Chemical Society, 2011, 133, 17207-17216.	6.6	281
8	Câ€“H activation. Nature Reviews Methods Primers, 2021, 1, .	11.8	277
9	An Exceptionally Fast Homogeneous Carbon-Free Cobalt-Based Water Oxidation Catalyst. Journal of the American Chemical Society, 2014, 136, 9268-9271.	6.6	260
10	Site-selective and stereoselective functionalization of non-activated tertiary Câ€“H bonds. Nature, 2017, 551, 609-613.	13.7	239
11	Decarbonylative organoboron cross-coupling of esters by nickel catalysis. Nature Communications, 2015, 6, 7508.	5.8	237
12	A Noble-Metal-Free, Tetra-nickel Polyoxotungstate Catalyst for Efficient Photocatalytic Hydrogen Evolution. Journal of the American Chemical Society, 2014, 136, 14015-14018.	6.6	213
13	Parameter Calibration of Transition-Metal Elements for the Spin-Polarized Self-Consistent-Charge Density-Functional Tight-Binding (DFTB) Method:â€‰ Sc, Ti, Fe, Co, and Ni. Journal of Chemical Theory and Computation, 2007, 3, 1349-1367.	2.3	208
14	Differentiating Homogeneous and Heterogeneous Water Oxidation Catalysis: Confirmation that [Co₄(H₂O)₂(Î±-PW₉O₃₄)₂]^{10â€“} Is a Molecular Water Oxidation Catalyst. Journal of the American Chemical Society, 2013, 135, 14110-14118.	6.6	196
15	A Density Functional Study of the Mechanism of the Diimineâ^'Nickel-Catalyzed Ethylene Polymerization Reaction. Journal of the American Chemical Society, 1997, 119, 367-374.	6.6	181
16	D₂-Symmetric Dirhodium Catalyst Derived from a 1,2,2-Triarylcyclopropanecarboxylate Ligand: Design, Synthesis and Application. Journal of the American Chemical Society, 2011, 133, 19198-19204.	6.6	180
17	Scope and Mechanistic Analysis of the Enantioselective Synthesis of Allenes by Rhodium-Catalyzed Tandem Ylide Formation/[2,3]-Sigmatropic Rearrangement between Donor/Acceptor Carbenoids and Propargylic Alcohols. Journal of the American Chemical Society, 2012, 134, 15497-15504.	6.6	177
18	Theoretical Insight into the Câ^'C Coupling Reactions of the Vinyl, Phenyl, Ethynyl, and Methyl Complexes of Palladium and Platinum. Organometallics, 2005, 24, 715-723.	1.1	164

#	Article	IF	Citations
19	Key Mechanistic Features of Ni-Catalyzed Câ€“H/Câ€“O Biaryl Coupling of Azoles and Naphthalen-2-yl Pivalates. Journal of the American Chemical Society, 2014, 136, 14834-14844.	6.6	164
20	Structural, Physicochemical, and Reactivity Properties of an All-Inorganic, Highly Active Tetraruthenium Homogeneous Catalyst for Water Oxidation. Journal of the American Chemical Society, 2009, 131, 17360-17370.	6.6	162
21	Key Mechanistic Features of Enantioselective Câ€“H Bond Activation Reactions Catalyzed by [(Chiral) Tj ETQq1 1 0.784314 rgBT /Ove 2012, 134, 1690-1698.	6.6	159
22	A Late-Transition Metal Oxo Complex: K7Na9[O=PtIV(H2O)L2], L = [PW9O34]9-. Science, 2004, 306, 2074-2077.	6.0	158
23	Theoretical Study of Substituent Effects in the Diimineâ€'M(II) Catalyzed Ethylene Polymerization Reaction Using the IMOMM Method. Journal of the American Chemical Society, 1998, 120, 1581-1587.	6.6	153
24	Mechanism of the Methane â†' Methanol Conversion Reaction Catalyzed by Methane Monooxygenase:â€‰ A Density Functional Study. Journal of the American Chemical Society, 1999, 121, 7249-7256.	6.6	152
25	Versatile reactivity of Pd-catalysts: mechanistic features of the mono-N-protected amino acid ligand and cesium-halide base in Pd-catalyzed Câ€“H bond functionalization. Chemical Society Reviews, 2014, 43, 5009-5031.	18.7	148
26	Molecular orbital study of H2 and CH4 activation on small metal clusters. I. Pt, Pd, Pt2, and Pd2. Journal of Chemical Physics, 1998, 108, 8418-8428.	1.2	136
27	Design of catalysts for site-selective and enantioselective functionalization of non-activated primary Câ€“H bonds. Nature Chemistry, 2018, 10, 1048-1055.	6.6	131
28	Effects of the Protein Environment on the Structure and Energetics of Active Sites of Metalloenzymes. ONIOM Study of Methane Monooxygenase and Ribonucleotide Reductase. Journal of the American Chemical Society, 2002, 124, 192-193.	6.6	124
29	Comparative Investigations of Cp*-Based Group 9 Metal-Catalyzed Direct Câ€“H Amination of Benzamides. Organometallics, 2014, 33, 4076-4085.	1.1	123
30	Theory Does Not Support an Osmaoxetane Intermediate in the Osmium-Catalyzed Dihydroxylation of Olefins. Journal of the American Chemical Society, 1996, 118, 11660-11661.	6.6	121
31	In situ probe of photocarrier dynamics in water-splitting hematite (Î±-Fe2O3) electrodes. Energy and Environmental Science, 2012, 5, 8923.	15.6	121
32	N2 Cleavage by Three-Coordinate Group 6 Complexes. W(III) Complexes Would Be Better Than Mo(III) Complexes. Journal of the American Chemical Society, 1995, 117, 12366-12367.	6.6	118
33	Molecular Orbital Study of the Mechanism of Platinum(0)-Catalyzed Alkene and Alkyne Diboration Reactions. Organometallics, 1997, 16, 1355-1364.	1.1	116
34	Rhodium-catalyzed enantioselective cyclopropanation of electron-deficient alkenes. Chemical Science, 2013, 4, 2844.	3.7	116
35	Ab Initio MO Study of the Full Cycle of Olefin Hydroformylation Catalyzed by a Rhodium Complex, RhH(CO)2(PH3)2. Organometallics, 1997, 16, 1065-1078.	1.1	115
36	Theoretical Studies of Ethylene Polymerization Reactions Catalyzed by Zirconium and Titanium Chelating Alkoxide Complexes. Journal of the American Chemical Society, 1997, 119, 7190-7196.	6.6	114

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37	Four-Coordinate Molybdenum Chalcogenide Complexes Relevant to Nitrous Oxide Nâ^'N Bond Cleavage by Three-Coordinate Molybdenum(III):Â Synthesis, Characterization, Reactivity, and Thermochemistry. Journal of the American Chemical Society, 1998, 120, 2071-2085.	6.6	113
38	Density Functional Study of the Mechanism of the Palladium(II)-Catalyzed Ethylene Polymerization Reaction. Organometallics, 1997, 16, 1933-1945.	1.1	109
39	Electron Transfer Dynamics in Semiconductorâ€"Chromophoreâ€"Polyoxometalate Catalyst Photoanodes. Journal of Physical Chemistry C, 2013, 117, 918-926.	1.5	108
40	An ab initio molecular orbital study of the mechanism of the rhodium(I)-catalyzed olefin hydroboration reaction. Journal of the American Chemical Society, 1994, 116, 10693-10702.	6.6	106
41	Theoretical Predictions and Single-Crystal Neutron Diffraction and Inelastic Neutron Scattering Studies on the Reaction of Dihydrogen with the Dinuclear Dinitrogen Complex of Zirconium [P2N2]Zr(Î¼-Î·2-N2)Zr[P2N2], P2N2= PhP(CH2SiMe2NSiMe2CH2)2PPh. Journal of the American Chemical Society, 1999, 121, 523-528.	6.6	106
42	Density Functional Study on Activation of ortho-CH Bond in Aromatic Ketone by Ru Complex. Role of Unusual Five-Coordinated d6 Metallacycle Intermediate with Agostic Interaction. Journal of the American Chemical Society, 1998, 120, 12692-12693.	6.6	105
43	Molecular Orbital and IMOMM Studies of the Chain Transfer Mechanisms of the Diimineâ^'M(II)-Catalyzed (M = Ni, Pd) Ethylene Polymerization Reaction. Organometallics, 1998, 17, 1850-1860.	1.1	105
44	The True Nature of the Di-iron(III) Î³-Keggin Structure in Water:Â Catalytic Aerobic Oxidation and Chemistry of an Unsymmetrical Trimer. Journal of the American Chemical Society, 2006, 128, 11268-11277.	6.6	105
45	Ab Initio Molecular Orbital Study of the Mechanism of H-H, C-H, N-H, O-H and Si-H Bond Activation on Transient Cyclopentadienylcarbonylrhodium. Journal of the American Chemical Society, 1995, 117, 799-805.	6.6	103
46	Theoretical Study on Bis(imino)pyridylâ^'Fe(II) Olefin Poly- and Oligomerization Catalysts. Dominance of Different Spin States in Propagation and Î²-Hydride Transfer Pathways. Organometallics, 2001, 20, 2007-2026.	1.1	102
47	Broadâ€Spectrum Liquidâ€•and Gasâ€Phase Decontamination of Chemical Warfare Agents by Oneâ€Dimensional Heteropolyniobates. Angewandte Chemie - International Edition, 2016, 55, 7403-7407.	7.2	101
48	Desymmetrization of cyclohexanes by site- and stereoselective Câ€"H functionalization. Nature, 2018, 564, 395-399.	13.7	100
49	Why Do Pt(PR3)2Complexes Catalyze the Alkyne Diboration Reaction, but Their Palladium Analogues Do Not? A Density Functional Study. Organometallics, 1998, 17, 742-751.	1.1	99
50	Vinylâ^'Vinyl Coupling on Late Transition Metals through Câ^'C Reductive Elimination Mechanism. A Computational Study. Journal of the American Chemical Society, 2002, 124, 2839-2852.	6.6	99
51	Catalytic Adaptive Recognition of Thiol (SH) and Selenol (SeH) Groups Toward Synthesis of Functionalized Vinyl Monomers. Journal of the American Chemical Society, 2012, 134, 6637-6649.	6.6	97
52	Critical Effect of Phosphane Ligands on the Mechanism of Carbonâ€"Carbon Bond Formation Involving Palladium(II) Complexes: A Theoretical Investigation of Reductive Elimination from Squareâ€Planar and Tâ€Shaped Species. European Journal of Inorganic Chemistry, 2007, 2007, 5390-5399.	1.0	95
53	Visible-light-driven hydrogen evolution from water using a noble-metal-free polyoxometalate catalyst. Journal of Catalysis, 2013, 307, 48-54.	3.1	95
54	Rh₂(II,III) Catalysts with Chelating Carboxylate and Carboxamidate Supports: Electronic Structure and Nitrene Transfer Reactivity. Journal of the American Chemical Society, 2016, 138, 2327-2341.	6.6	95

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55	Metalâ^'Peroxo versus Metalâ^'Oxo Oxidants in Non-Heme Iron-Catalyzed Olefin Oxidations:Â Computational and Experimental Studies on the Effect of Water. Journal of the American Chemical Society, 2005, 127, 6548-6549.	6.6	94
56	Density Functional Study on Highly Ortho-Selective Addition of an Aromatic CH Bond to Olefins Catalyzed by a Ru(H)2(CO)(PR3)3Complex. Organometallics, 2000, 19, 2318-2329.	1.1	90
57	Dioxygen and Water Activation Processes on Multi-Ru-Substituted Polyoxometalates: Comparison with the â€œBlue-Dimerâ€•Water Oxidation Catalyst. Journal of the American Chemical Society, 2009, 131, 6844-6854.	6.6	88
58	Unusual31P Chemical Shielding Tensors in Terminal Phosphido Complexes Containing a Phosphorusâ^'Metal Triple Bond. Journal of the American Chemical Society, 1996, 118, 10654-10655.	6.6	87
59	Computational Study of the Aminolysis of Esters. The Reaction of Methylformate with Ammonia. Journal of Organic Chemistry, 2003, 68, 1496-1502.	1.7	87
60	Revisiting the Polyoxometalate-Based Late-Transition-Metal-Oxo Complexes: The â€œOxo Wallâ€•Stands. Inorganic Chemistry, 2012, 51, 7025-7031.	1.9	86
61	Theoretical Studies of the Factors Controlling Insertion Barriers for Olefin Polymerization by the Titanium-Chelating Bridged Catalysts. A Search for More Active New Catalysts. Organometallics, 1999, 18, 373-379.	1.1	83
62	Computational Insights into the Mechanism of Radical Generation in B12-Dependent Methylmalonyl-CoA Mutase. Journal of the American Chemical Society, 2006, 128, 1287-1292.	6.6	83
63	Synthesis and Characterization of a Metal-to-Polyoxometalate Charge Transfer Molecular Chromophore. Journal of the American Chemical Society, 2011, 133, 20134-20137.	6.6	81
64	A Palladium-Oxo Complex. Stabilization of This Proposed Catalytic Intermediate by an Encapsulating Polytungstate Ligand. Journal of the American Chemical Society, 2005, 127, 11948-11949.	6.6	79
65	Understanding the Reactivity of Pd⁰/PR₃-Catalyzed Intermolecular C(sp³)â€“H Bond Arylation. Journal of the American Chemical Society, 2013, 135, 14206-14214.	6.6	77
66	Long lived charge separation in iridium(iii)-photosensitized polyoxometalates: synthesis, photophysical and computational studies of organometallicâ€“redox tunable oxide assemblies. Chemical Science, 2013, 4, 1737.	3.7	75
67	Broadâ€Spectrum Liquidâ€•and Gasâ€Phase Decontamination of Chemical Warfare Agents by Oneâ€Dimensional Heteropolyniobates. Angewandte Chemie, 2016, 128, 7529-7533.	1.6	75
68	Flexible Reaction Pocket on Bulky Diphosphineâ€“Ir Complex Controls Regioselectivity in para-Selective Câ€“H Borylation of Arenes. ACS Catalysis, 2016, 6, 7536-7546.	5.5	73
69	Density Functional Study on the Mechanism of Palladium(0)-Catalyzed Thioboration Reaction of Alkynes. Differences between Pd(0) and Pt(0) Catalysts and between Thioboration and Diboration. Organometallics, 1998, 17, 1383-1392.	1.1	72
70	Terminal Gold-Oxo Complexes. Journal of the American Chemical Society, 2007, 129, 11118-11133.	6.6	72
71	Factors Impacting the Mechanism of the Mono-N-Protected Amino Acid Ligand-Assisted and Directing-Group-Mediated Câ€“H Activation Catalyzed by Pd(II) Complex. ACS Catalysis, 2015, 5, 830-840.	5.5	72
72	Catalyst-Controlled Selective Functionalization of Unactivated Câ€“H Bonds in the Presence of Electronically Activated Câ€“H Bonds. Journal of the American Chemical Society, 2018, 140, 12247-12255.	6.6	68

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73	Molecular Orbital Study of H2and CH4Activation on Small Metal Clusters. 2. Pd3and Pt3. Journal of Physical Chemistry A, 1998, 102, 6373-6384.	1.1	67
74	Water splitting with polyoxometalate-treated photoanodes: enhancing performance through sensitizer design. Chemical Science, 2015, 6, 5531-5543.	3.7	67
75	Computational studies of reaction mechanisms of methane monooxygenase and ribonucleotide reductase. Journal of Computational Chemistry, 2002, 23, 59-76.	1.5	63
76	Computational Modeling of Di-Transition-Metal-Substituted Î³-Keggin Polyoxometalate Anions. Structural Refinement of the Protonated Divacant Lacunary Silicodecatungstate. Inorganic Chemistry, 2004, 43, 7702-7708.	1.9	63
77	Ab initio molecular orbital study of the molecular and electronic structure of FeCH+2 and of the reaction mechanism of FeCH+2+H2. Journal of Chemical Physics, 1994, 101, 10697-10707.	1.2	61
78	Ab initio study of the molecular and electronic structure of CoCH2+ and of the reaction mechanism of methylenecobalt(1+) + hydrogen. The Journal of Physical Chemistry, 1993, 97, 11435-11444.	2.9	59
79	Molecular Orbital Study of the Reaction Mechanism of Sc+with Methane. Comparison of the Reactivity of Early and Late First-Row Transition Metal Cations and Their Carbene Complexes. The Journal of Physical Chemistry, 1996, 100, 11600-11609.	2.9	59
80	Computational Studies of Tungsten-Catalyzedendo-Selective Cycloisomerization of 4-Pentyn-1-ol. Journal of the American Chemical Society, 2002, 124, 4149-4157.	6.6	59
81	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. Journal of Catalysis, 2017, 350, 56-63.	3.1	59
82	Cu-Catalyzed aromatic Câ€“H imidation with N-fluorobenzenesulfonimide: mechanistic details and predictive models. Chemical Science, 2017, 8, 988-1001.	3.7	57
83	Insights into the Mechanism of Selective Olefin Epoxidation Catalyzed by [Î³-(SiO4)W10O32H4]4-. A Computational Study. Inorganic Chemistry, 2006, 45, 5703-5709.	1.9	56
84	Factors Controlling Stability and Reactivity of Dimeric Pd(II) Complexes in Câ€“H Functionalization Catalysis. ACS Catalysis, 2016, 6, 829-839.	5.5	56
85	Ab initio molecular orbital study of the electronic and geometric structure of methylenerhodium(1+) and the reaction mechanism: RhCH2+ + H2 .fwdarw. Rh+ + CH4. The Journal of Physical Chemistry, 1993, 97, 4064-4075.	2.9	55
86	Mechanistic Details of Pd(II)-Catalyzed Câ€“H Iodination with Molecular I₂: Oxidative Addition vs Electrophilic Cleavage. Journal of the American Chemical Society, 2015, 137, 9022-9031.	6.6	53
87	Title is missing!. Topics in Catalysis, 1999, 7, 107-123.	1.3	52
88	Insights into Photoinduced Electron Transfer between [Ru(bpy)3]2+ and [S2O8]2â^' in Water: Computational and Experimental Studies. Journal of Physical Chemistry A, 2010, 114, 73-80.	1.1	51
89	Theoretical Studies of Oxidative Addition of Eâ^'E Bonds (E = S, Se, Te) to Palladium(0) and Platinum(0) Complexes. Organometallics, 2005, 24, 4908-4914.	1.1	50
90	Cu-based Polyoxometalate Catalyst for Efficient Catalytic Hydrogen Evolution. Inorganic Chemistry, 2016, 55, 6750-6758.	1.9	50

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91	Synthesis, Structures, and Photochemistry of Tricarbonyl Metal Polyoxoanion Complexes, [X₂W₂₀O₇₀{M(CO)₃}₂]^{12â€“} (X = Sb, Bi and M = Re, Mn). Inorganic Chemistry, 2013, 52, 671-678.	1.9	49
92	Iridium(iii)-bis(oxazolinyl)phenyl catalysts for enantioselective Câ€“H functionalization. Chemical Science, 2013, 4, 2590.	3.7	49
93	Adsorption of Multiple H2 Molecules on Pd3 and Pd4 Clusters. A Density Functional Study. Journal of Physical Chemistry A, 2000, 104, 11606-11614.	1.1	48
94	A Role for Pd(IV) in Catalytic Enantioselective Câ€“H Functionalization with Monoprotected Amino Acid Ligands under Mild Conditions. Journal of the American Chemical Society, 2017, 139, 9238-9245.	6.6	48
95	Site-Selective Carbene-Induced Câ€“H Functionalization Catalyzed by Dirhodium Tetrakis(triarylcyclopropanecarboxylate) Complexes. ACS Catalysis, 2018, 8, 678-682.	5.5	48
96	Calculation of Nuclear Quadrupole Parameters in Imidazole Derivatives and Extrapolation to Coenzyme B12. A Theoretical Study. Journal of Physical Chemistry B, 1999, 103, 8618-8627.	1.2	47
97	The Flexibility of Carboxylate Ligands in Methane Monooxygenase and Ribonucleotide Reductase:Â A Density Functional Study. Journal of Physical Chemistry B, 2001, 105, 322-327.	1.2	47
98	All-Inorganic Networks and Tetramer Based on Tin(II)-Containing Polyoxometalates: Tuning Structural and Spectral Properties with Lone-Pairs. Journal of the American Chemical Society, 2014, 136, 12085-12091.	6.6	47
99	Theoretical Studies of Biological Nitrogen Fixation. I. Density Functional Modeling of the Mo-Site of the FeMo-Cofactor. Inorganic Chemistry, 2001, 40, 766-775.	1.9	46
100	Real size of ligands, reactants and catalysts: Studies of structure, reactivity and selectivity by ONIOM and other hybrid computational approachesâ˜†. Journal of Molecular Catalysis A, 2010, 324, 104-119.	4.8	46
101	Metalâ€“Organic Framework- and Polyoxometalate-Based Sorbents for the Uptake and Destruction of Chemical Warfare Agents. ACS Applied Materials & Interfaces, 2020, 12, 14641-14661.	4.0	46
102	Mono-N-protected amino acid ligands stabilize dimeric palladium(<scp>ii</scp>) complexes of importance to Câ€“H functionalization. Chemical Science, 2017, 8, 5746-5756.	3.7	45
103	Structure, Stability, and Electronic and NMR Properties of Various Oxo- and Nitrido-Derivatives of [L(Salen)Mn(III)]+, Where L = None and Imidazole. A Density Functional Study. Inorganic Chemistry, 2003, 42, 2606-2621.	1.9	44
104	Câ€“C Cleavage Approach to Câ€“H Functionalization of Saturated Aza-Cycles. ACS Catalysis, 2020, 10, 2929-2941.	5.5	43
105	Rhodium-Stabilized Diarylcarbenes Behaving as Donor/Acceptor Carbenes. ACS Catalysis, 2020, 10, 6240-6247.	5.5	43
106	Electronic states of the triply charged molecular ionN23+and laser-induced Coulomb explosion. Physical Review A, 1999, 59, 4309-4315.	1.0	42
107	Theoretical Studies on the Mechanism of the Methane â†' Methanol Conversion Reaction Catalyzed by Methane Monooxygenase:Â O-Side vs N-Side Mechanisms. Journal of Physical Chemistry A, 2001, 105, 3615-3622.	1.1	42
108	The Role of the Central Atom in Structure and Reactivity of Polyoxometalates with Adjacent d-Electron Metal Sites. Computational and Experimental Studies of Î³-[(Xn+O4)RuIII2(OH)2(MFM)10O32](8-n)-for MFM= Mo and W, and X = AlIII, SiIV, PV, and SVI. Journal of Physical Chemistry B, 2006, 110, 170-173.	1.2	42

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109	Tailored quinones support high-turnover Pd catalysts for oxidative Câ€“H arylation with O ₂. Science, 2020, 370, 1454-1460.	6.0	42
110	Why Does the Reaction of the Dihydrogen Molecule with [P2N2]Zr(Î¼-Î·2-N2)Zr[P2N2] Produce [P2N2]Zr(Î¼-Î·2-N2H)Zr[P2N2](Î¼-H) but Not the Thermodynamically More Favorable [P2N2]Zr(Î¼-NH)2Zr[P2N2]? A Theoretical Study. Journal of the American Chemical Society, 1999, 121, 5754-5761.	6.6	41
111	Ab Initio Molecular Orbital Study of Electronic and Geometrical Structures of MCH₂⁺ Complex and its Reactivity with H₂, Where M = Co, Rh, and Ir. Israel Journal of Chemistry, 1993, 33, 307-316.	1.0	39
112	Does Reaction of Three-Coordinate Molybdenum(III) with N2O Proceed via the Same Mechanism as with N2? A Theoretical Study. Organometallics, 1999, 18, 5653-5660.	1.1	39
113	Is the Protein Surrounding the Active Site Critical for Hydrogen Peroxide Reduction by Selenoprotein Glutathione Peroxidase? An ONIOM Study. Journal of Physical Chemistry B, 2006, 110, 13608-13613.	1.2	39
114	Computational Studies of the Geometry and Electronic Structure of an All-Inorganic and Homogeneous Tetra-Ru-Polyoxotungstate Catalyst for Water Oxidation and Its Four Subsequent One-Electron Oxidized Forms. Journal of Physical Chemistry A, 2010, 114, 535-542.	1.1	39
115	Theoretical Study of the Mechanism of Alkane Hydroxylation and Ethylene Epoxidation Reactions Catalyzed by Diiron Bis-oxo Complexes. The Effect of Substrate Molecules. Journal of the American Chemical Society, 2002, 124, 4135-4148.	6.6	38
116	Insights into the Structure and Reactivity of Acylperoxo Complexes in the Kochiâ˜'Jacobsenâ˜'Katsuki Catalytic System. A Density Functional Study. Journal of the American Chemical Society, 2003, 125, 13879-13889.	6.6	38
117	The mechanism of directed Ni(<scp>ii</scp>)-catalyzed Câ€“H iodination with molecular iodine. Chemical Science, 2018, 9, 1144-1154.	3.7	38
118	Asymmetric Catalysis Special Feature Part II: Epoxidation of unfunctionalized olefins by Mn(salen) catalyst using organic peracids as oxygen source: A theoretical study. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 5743-5748.	3.3	37
119	Polyoxometalates in the Design of Effective and Tunable Water Oxidation Catalysts. Israel Journal of Chemistry, 2011, 51, 238-246.	1.0	37
120	Spectroscopic Studies of Light-driven Water Oxidation Catalyzed by Polyoxometalates. Industrial & Engineering Chemistry Research, 2012, 51, 11850-11859.	1.8	37
121	Enantioselectivity Model for Pd-Catalyzed Câ€“H Functionalization Mediated by the Mono-N-protected Amino Acid (MPAA) Family of Ligands. ACS Catalysis, 2017, 7, 4344-4354.	5.5	37
122	Buffer-Induced Acceleration and Inhibition in Polyoxometalate-Catalyzed Organophosphorus Ester Hydrolysis. ACS Catalysis, 2018, 8, 7068-7076.	5.5	37
123	An ab initio molecular orbital study of the unimolecular dissociation reactions of diâ€•and trichloroethylene. Journal of Chemical Physics, 1994, 101, 5942-5956.	1.2	36
124	Diminishing Ï€-Stabilization of an Unsaturated Metal Center:â€‰ Hydrogen Bonding to OsHCl(CO)(PtBu2Me)2. Journal of the American Chemical Society, 1998, 120, 12553-12563.	6.6	36
125	Extending Metalâ€toâ€Polyoxometalate Charge Transfer Lifetimes: The Effect of Heterometal Location. Chemistry - A European Journal, 2014, 20, 4297-4307.	1.7	36
126	Does Dinitrogen Hydrogenation Follow Different Mechanisms for [(Î·5-C5Me4H)2Zr]2(Î¼2,Î·2,Î·2-N2) and {[PhP(CH2SiMe2NSiMe2CH2)PPh]Zr}2(Î¼2,Î·2,Î·2-N2) Complexes? A Computational Study. Journal of the American Chemical Society, 2006, 128, 11391-11403.	6.6	35

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127	Enhancing photo-reduction quantum efficiency using quasi-type II core/shell quantum dots. Chemical Science, 2016, 7, 4125-4133.	3.7	35
128	Understanding Regiodivergence in a Pd(II)-Mediated Site-Selective Câ€“H Alkynylation. ACS Catalysis, 2018, 8, 4516-4527.	5.5	35
129	Density Functional Study of Ethylene Polymerization Catalyzed by a Zirconium Non-Cyclopentadienyl Complex, L2ZrCH3+. Effects of Ligands and Bulky Substituents. Organometallics, 2001, 20, 309-323.	1.1	34
130	Can Steric Effects Induce the Mechanism Switch in the Rhodium-Catalyzed Imine Boration Reaction? A Density Functional and ONIOM Study. Organometallics, 2005, 24, 1938-1946.	1.1	34
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