Feliu Maseras

List of Publications by Year
in descending order

294 papers	16,867 citations	16437 64 h-index	20343 116 g-index
315 all docs	315 docs citations	315 times ranked	11674 citing authors

#	Article	IF	Citations
1	IMOMM: A new integratedab initio + molecular mechanics geometry optimization scheme of equilibrium structures and transition states. Journal of Computational Chemistry, 1995, 16, 1170-1179.	1.5	1,635
2	Proton Abstraction Mechanism for the Palladium-Catalyzed Intramolecular Arylation. Journal of the American Chemical Society, 2006, 128, 1066-1067.	6.6	698
3	Proton-Abstraction Mechanism in the Palladium-Catalyzed Intramolecular Arylation:Â Substituent Effects. Journal of the American Chemical Society, 2007, 129, 6880-6886.	6.6	509
4	Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform. Journal of Chemical Information and Modeling, 2015, 55, 95-103.	2.5	403
5	Direct Arylation of Arene Câ^'H Bonds by Cooperative Action of NHCarbeneâ^'Ruthenium(II) Catalyst and Carbonate via Proton Abstraction Mechanism. Journal of the American Chemical Society, 2008, 130, 1156-1157.	6.6	367
6	A DFT Study of the Full Catalytic Cycle of the Suzukiâ^'Miyaura Cross-Coupling on a Model System. Organometallics, 2006, 25, 3647-3658.	1.1	348
7	Transition Metal Polyhydrides:â€‰ From Qualitative Ideas to Reliable Computational Studies. Chemical Reviews, 2000, 100, 601-636.	23.0	341
8	Computational Characterization of the Role of the Base in the Suzukiâ^'Miyaura Cross-Coupling Reaction. Journal of the American Chemical Society, 2005, 127, 9298-9307.	6.6	317
9	Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634.	7.6	306
10	Merging Sustainability with Organocatalysis in the Formation of Organic Carbonates by Using CO₂ as a Feedstock. ChemSusChem, 2012, 5, 2032-2038.	3.6	283
11	Redox Non-innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts. Journal of the American Chemical Society, 2015, 137, 6758-6761.	6.6	266
12	[(NHC)AuI]-Catalyzed Formation of Conjugated Enones and Enals: An Experimental and Computational Study. Chemistry - A European Journal, 2007, 13, 6437-6451.	1.7	180
13	Câ^'C Reductive Elimination in Palladium Complexes, and the Role of Coupling Additives. A DFT Study Supported by Experiment. Journal of the American Chemical Society, 2009, 131, 3650-3657.	6.6	178
14	A General Mechanism for the Copper- and Silver-Catalyzed Olefin Aziridination Reactions: Concomitant Involvement of the Singlet and Triplet Pathways. Journal of the American Chemical Society, 2013, 135, 1338-1348.	6.6	160
15	A Valuable, Inexpensive CuI/N-Heterocyclic Carbene Catalyst for the Selective Diboration of Styrene. Chemistry - A European Journal, 2007, 13, 2614-2621.	1.7	156
16	Catecholborane Bound to Titanocene. Unusual Coordination of Ligand Ïƒ-Bonds. Journal of the American Chemical Society, 1996, 118, 10936-10937.	6.6	151
17	Experimental and Theoretical Investigations of New Dinuclear Palladium Complexes as Precatalysts for the Amination of Aryl Chlorides. Journal of the American Chemical Society, 2006, 128, 6376-6390.	6.6	148
18	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. ACS Catalysis, 2019, 9, 6803-6813.	5.5	145

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19	Application of the New â€œIntegrated MO + MMâ€•(IMOMM) Method to the Organometallic Reaction Pt(PR3)2+ H2(R = H, Me,t-Bu, and Ph). The Journal of Physical Chemistry, 1996, 100, 2573-2580.	2.9	142
20	Metalâ€“Arene Interactions in Dialkylbiarylphosphane Complexes of Copper, Silver, and Gold. Chemistry - A European Journal, 2010, 16, 5324-5332.	1.7	142
21	Stereoselective and Versatile Preparation of Tri- and Tetrasubstituted Allylic Amine Scaffolds under Mild Conditions. Journal of the American Chemical Society, 2016, 138, 11970-11978.	6.6	142
22	Unraveling the Origin of Regioselectivity in Rhodium Diphosphine Catalyzed Hydroformylation. A DFT QM/MM Study. Journal of the American Chemical Society, 2001, 123, 7630-7637.	6.6	141
23	Computational study of the transmetalation process in the Suzukiâ€“Miyaura cross-coupling of aryls. Journal of Organometallic Chemistry, 2006, 691, 4459-4466.	0.8	140
24	Catalytic Mechanism of Galactose Oxidase:Â A Theoretical Study. Journal of the American Chemical Society, 2000, 122, 8031-8036.	6.6	134
25	Bidentate phosphines as ligands in the palladium-catalyzed intramolecular arylation: the intermolecular base-assisted proton abstraction mechanism. Tetrahedron, 2008, 64, 6021-6029.	1.0	123
26	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
27	Computational Evidence of the Importance of Substituent Bulk on Agostic Interactions in Ir(H)2(PtBu2Ph)2+. Journal of the American Chemical Society, 1998, 120, 361-365.	6.6	121
28	Selective Homogeneous and Heterogeneous Gold Catalysis with Alkynes and Alkenes: Similar Behavior, Different Origin. ChemPhysChem, 2008, 9, 1624-1629.	1.0	119
29	Gold(I)-Catalyzed Intermolecular Hydroalkoxylation of Allenes: A DFT study. Organic Letters, 2009, 11, 2237-2240.	2.4	118
30	A Domino Process toward Functionally Dense Quaternary Carbons through Pd-Catalyzed Decarboxylative C(sp³)â€“C(sp³) Bond Formation. Journal of the American Chemical Society, 2018, 140, 3981-3987.	6.6	113
31	Computational approaches to asymmetric synthesis. New Journal of Chemistry, 2007, 31, 333.	1.4	108
32	Computational and Experimental Test of Steric Influence on Agostic Interactions:Â A Homologous Series for Ir(III). Journal of the American Chemical Society, 1999, 121, 97-106.	6.6	105
33	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. Journal of Physical Chemistry A, 2018, 122, 1392-1399.	1.1	101
34	A Critical Analysis of the Cyclic and Open Alternatives of the Transmetalation Step in the Stille Cross-Coupling Reaction. Journal of the American Chemical Society, 2006, 128, 14571-14578.	6.6	100
35	Protonation of transition-metal hydrides: a not so simple process. Chemical Society Reviews, 2009, 38, 957.	18.7	99
36	Theoretical Study on the Origin of Enantioselectivity in the Bis(dihydroquinidine)-3,6-pyridazineÂ·Osmium Tetroxide-Catalyzed Dihydroxylation of Styrene. Journal of the American Chemical Society, 1999, 121, 1317-1323.	6.6	94

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37	Transition metal catalysis by density functional theory and density functional theory/molecular mechanics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 375-385.	6.2	91
38	Inertness of the Arylâ˜F Bond toward Oxidative Addition to Osmium and Rhodium Complexes:â€‰ Thermodynamic or Kinetic Origin?. Journal of the American Chemical Society, 1998, 120, 12634-12640.	6.6	90
39	Bond energy, Mâ€“C/Hâ€“C correlations: dual theoretical and experimental approach to the sensitivity of Mâ€“C bond strength to substituentsElectronic supplementary information (ESI) available: methods of calculation; Fig. S1: Comparison of calculated and experimental Câ€“H bond dissociation energies for organic molecules; Table S1, comparison of calculated and experimental CO-stretching frequencies; Table S2, total energies, BDE for Reâ€“C and Hâ€“C; Table S3, NPA charges q(C) and q(aryl) for the organic fragments C6H6â€•. Chemical Communications, 2003, , 490-491.	2.2	89
40	Chemo-, Regio-, and Stereoselective Silver-Catalyzed Aziridination of Dienes: Scope, Mechanistic Studies, and Ring-Opening Reactions. Journal of the American Chemical Society, 2014, 136, 5342-5350.	6.6	89
41	Reactions of a Hexahydrideâ˜Osmium Complex with Aromatic Ketones:Â Câ˜H Activation versus Câ˜F ActivationÂ§. Organometallics, 2001, 20, 442-452.	1.1	88
42	Mechanism of the gold-catalyzed cyclopropanation of alkenes with 1,6-enynes. Chemical Science, 2011, 2, 141-149.	3.7	87
43	Microkinetic modeling in homogeneous catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1372.	6.2	85
44	Mechanism of Alkane Câ˜H Bond Activation by Copper and Silver Homoscorpionate Complexes. Organometallics, 2006, 25, 5292-5300.	1.1	84
45	Application of the natural population analysis to transition-metal complexes. Should the empty metal p orbitals be included in the valence space?. Chemical Physics Letters, 1992, 195, 500-504.	1.2	83
46	Oxidative Coupling Mechanisms: Current State of Understanding. ACS Catalysis, 2018, 8, 1161-1172.	5.5	83
47	Practical Implications of Boronâ€toâ€Zinc Transmetalation for the Catalytic Asymmetric Arylation of Aldehydes. Angewandte Chemie - International Edition, 2008, 47, 1098-1101.	7.2	82
48	Oxidative Additions of Aryl Halides to Palladium Proceed through the Monoligated Complex. ChemCatChem, 2013, 5, 3604-3609.	1.8	79
49	RuX(CO)(NO)L2and Ru(CO)(NO)L2+:Â Ru(0) or Ru(II) or In Between?. Journal of the American Chemical Society, 1997, 119, 8642-8651.	6.6	77
50	QM/MM methods in inorganic chemistry. Dalton Transactions, 2008, , 2911.	1.6	77
51	Palladium Round Trip in the Negishi Coupling of transâ€[PdMeCl(PMePh₂)₂] with ZnMeCl: An Experimental and DFT Study of the Transmetalation Step. Chemistry - A European Journal, 2010, 16, 8596-8599.	1.7	76
52	A Density Functional Study on the Effect of the Trans Axial Ligand of Cobalamin on the Homolytic Cleavage of the Coâ˜C Bond. Journal of Physical Chemistry B, 2001, 105, 7564-7571.	1.2	74
53	Influence of Media and Homoconjugate Pairing on Transition Metal Hydride Protonation. An IR and DFT Study on Proton Transfer to CpRuH(CO)(PCy3). Journal of the American Chemical Society, 2003, 125, 7715-7725.	6.6	74
54	The IMOMM method opens the way for the accurate calculation of â€œrealâ€•transition metal complexes. Chemical Communications, 2000, , 1821-1827.	2.2	73

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55	Computational Rationalization of the Dependence of the Enantioselectivity on the Nature of the Catalyst in the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. Journal of the American Chemical Society, 2005, 127, 3624-3634.	6.6	73
56	Synthesis of PCPâ€Supported Nickel Complexes and their Reactivity with Carbon Dioxide. Chemistry - A European Journal, 2012, 18, 6915-6927.	1.7	73
57	BrÃ¸nsted Acid Catalyzed Moritaâ€“Baylisâ€“Hillman Reaction: A New Mechanistic View for Thioureas Revealed by ESIâ€MS(/MS) Monitoring and DFT Calculations. Chemistry - A European Journal, 2009, 15, 12460-12469.	1.7	72
58	Copperâ€Catalyzed Nâˆ’F Bond Activation for Uniform Intramolecular Câˆ’H Amination Yielding Pyrrolidines and Piperidines. Angewandte Chemie - International Edition, 2019, 58, 8912-8916.	7.2	71
59	A Quantum Mechanics/Molecular Mechanics Study of the Highly Enantioselective Addition of Diethylzinc to Benzaldehyde Promoted by (R)-2-Piperidino-1,1,2-triphenylethanol. Journal of Organic Chemistry, 2000, 65, 7303-7309.	1.7	70
60	Towards Configurationally Stable [4]Helicenes: Enantioselective Synthesis of 12â€Substituted 7,8â€Dihydro[4]helicene Quinones. Chemistry - A European Journal, 2008, 14, 603-620.	1.7	70
61	Experimental and Theoretical Studies of Bonding and Oxidative Addition of Germanes and Silanes, EH4-nPhn(E = Si, Ge;n= 0âˆ’3), to Mo(CO)(diphosphine)2. The First Structurally Characterized Germane Ïƒ Complex. Organometallics, 2003, 22, 5307-5323.	1.1	68
62	The Transmetalation Process in Suzukiâ€“Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. ChemCatChem, 2014, 6, 3132-3138.	1.8	68
63	Highly Modular Pï£¿OP Ligands for Asymmetric Hydrogenation: Synthesis, Catalytic Activity, and Mechanism. Chemistry - A European Journal, 2010, 16, 6495-6508.	1.7	67
64	The importance of conformational search: a test case on the catalytic cycle of the Suzukiâ€“Miyaura cross-coupling. Theoretical Chemistry Accounts, 2011, 128, 639-646.	0.5	67
65	Mechanistic insights into the transmetalation step of a Suzukiâ€“Miyaura reaction of 2(4)-bromopyridines: characterization of an intermediate. Tetrahedron, 2008, 64, 7437-7443.	1.0	66
66	Single Electron Transfer Steps in Water Oxidation Catalysis. Redefining the Mechanistic Scenario. ACS Catalysis, 2017, 7, 1712-1719.	5.5	66
67	Competitive and Selective Csp³ï£¿Br versus Csp²ï£¿Br Bond Activation in Palladiumâ€Catalysed Suzuki Crossâ€Coupling: An Experimental and Theoretical Study of the Role of Phosphine Ligands. Chemistry - A European Journal, 2010, 16, 13390-13397.	1.7	65
68	Rationale for the sluggish oxidative addition of aryl halides to Au(<scp>i</scp>). Chemical Communications, 2014, 50, 1533-1536.	2.2	64
69	Computational Study with DFT and Kinetic Models on the Mechanism of Photoinitiated Aromatic Perfluoroalkylations. Organic Letters, 2015, 17, 2676-2679.	2.4	63
70	Cyclobutene vs 1,3-Diene Formation in the Gold-Catalyzed Reaction of Alkynes with Alkenes: The Complete Mechanistic Picture. Journal of the American Chemical Society, 2017, 139, 10302-10311.	6.6	63
71	Functional-Group-Tolerant, Silver-Catalyzed Nâ€“N Bond Formation by Nitrene Transfer to Amines. Journal of the American Chemical Society, 2017, 139, 2216-2223.	6.6	62
72	Theoretical Study of the Hydrogen Exchange Coupling in the Metallocene Trihydride Complexes [(C5H5)2MH3]n+(M = Mo, W,n= 1; M = Nb, Ta,n= 0). Journal of the American Chemical Society, 1996, 118, 4617-4621.	6.6	60

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73	The role of cyclobutenes in gold(i)-catalysed skeletal rearrangement of 1,6-enynes. Organic and Biomolecular Chemistry, 2012, 10, 6105.	1.5	60
74	Computational Study on the Mechanism of the Acceleration of 1,3-Dipolar Cycloaddition inside Cucurbit[6]uril. ACS Catalysis, 2015, 5, 2445-2451.	5.5	60
75	Amine conformational change and spin conversion induced by metal-assisted ligand oxidation: from the seven-coordinate iron(II)â€“TPAA complex to the two oxidized iron(II)â€“(py)3tren isomers. Characterization, crystal structures, and density functional study. Inorganica Chimica Acta, 2000, 297, 338-350.	1.2	59
76	Equilibria between Î±- and Î²-Agostic Stabilized Rotamers of Secondary Alkyl Niobium Complexes. Journal of the American Chemical Society, 2001, 123, 6000-6013.	6.6	59
77	Experimental and Computational Studies of Hydrogen Bonding and Proton Transfer to [Cp*Fe(dppe)H]. Chemistry - A European Journal, 2005, 11, 873-888.	1.7	58
78	Hydride Exchange Processes in the Coordination Sphere of Transition Metal Complexes:â€‰ The OsH3(BH4)(PR3)2 System. Journal of the American Chemical Society, 1996, 118, 8388-8394.	6.6	57
79	Synthesis and Spectroscopic Properties of Dihydrogen Isocyanide Niobocene [Nb(Î·5-C5H4SiMe3)2(Î·2-H2)(CNR)]+Complexes. Experimental and Theoretical Study of the Blocked Rotation of a Coordinated Dihydrogen. Journal of the American Chemical Society, 1997, 119, 6107-6114.	6.6	57
80	Density Functional Study on the Mechanism of the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. Journal of Organic Chemistry, 2003, 68, 4265-4274.	1.7	57
81	A DFT Study of the Effect of the Ligands in the Reductive Elimination from Palladium Bis(allyl) Complexes. Organometallics, 2010, 29, 4983-4991.	1.1	57
82	Catalytic cross-coupling of diazo compounds with coinage metal-based catalysts: an experimental and theoretical study. Dalton Transactions, 2013, 42, 4132.	1.6	57
83	Toward a mechanistic understanding of oxidative homocoupling: the Glaserâ€“Hay reaction. Catalysis Science and Technology, 2014, 4, 4200-4209.	2.1	57
84	Dynamic Behavior in Solution of the Transâ€Hydridodihydrogen Complex [OsHCl(n²â€H₂)(CO)(PiPr₃)₂]: Ab Initio and NMR Studies. Chemistry - A European Journal, 1996, 2, 815-825.	1.7	56
85	Bonding in Elongated Dihydrogen Complexes. Theoretical Analysis of the Electron Density in [MLn(HÂ·Â·Â·H)] Species. Organometallics, 1996, 15, 2947-2953.	1.1	55
86	Lightâ€Driven Enantioselective Organocatalytic Î²â€Benzylation of Enals. Angewandte Chemie - International Edition, 2017, 56, 3304-3308.	7.2	55
87	A theoretical analysis of a classic example of supramolecular catalysis. Chemical Communications, 2007, , 748-750.	2.2	54
88	On the Origin of Î±- and Î²-Agostic Distortions in Early-Transition-Metal Alkyl Complexes. Organometallics, 2008, 27, 1128-1134.	1.1	54
89	Why Is the Suzukiâ^'Miyaura Cross-Coupling of sp³Carbons in Î±-Bromo Sulfoxide Systems Fast and Stereoselective? A DFT Study on the Mechanism. Journal of Organic Chemistry, 2009, 74, 4049-4054.	1.7	54
90	Water oxidation electrocatalysis using ruthenium coordination oligomers adsorbed on multiwalled carbon nanotubes. Nature Chemistry, 2020, 12, 1060-1066.	6.6	54

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91	Elucidating the Mechanism of Aryl Aminations Mediated by NHC-Supported Nickel Complexes: Evidence for a Nonradical Ni(0)/Ni(II) Pathway. ACS Catalysis, 2018, 8, 3733-3742.	5.5	53
92	Oxidative Addition of Group 14 Element Hydrido Compounds to OsH2(Î·2-CH2CHEt)(CO)(PiPr3)2:Â Synthesis and Characterization of the First Trihydridoâ˜Silyl, Trihydridoâ˜Germyl, and Trihydridoâ˜Stannyl Derivatives of Osmium(IV). Inorganic Chemistry, 1996, 35, 1250-1256.	1.9	52
93	Critical Role of the Correlation Functional in DFT Descriptions of an Agostic Niobium Complex. Journal of Chemical Theory and Computation, 2007, 3, 1329-1336.	2.3	52
94	Mechanistic Studies on Gold-Catalyzed Direct Arene Câ€“H Bond Functionalization by Carbene Insertion: The Coinage-Metal Effect. Organometallics, 2017, 36, 172-179.	1.1	52
95	The role of computational results databases in accelerating the discovery of catalysts. Nature Catalysis, 2018, 1, 809-810.	16.1	52
96	Molecular hydrogen complexes with a hydride ligand. An ab initio study on the iron hydride, [Fe(PR3)4H(H2)]+, system. Journal of the American Chemical Society, 1991, 113, 2879-2884.	6.6	51
97	Competition between Steric and Electronic Control of Structure in Ru(CO)2L2Lâ€˜ Complexes. Organometallics, 1997, 16, 1979-1993.	1.1	51
98	Crucial Role of Anions on the Deprotonation of the Cationic Dihydrogen Complex trans-[FeH(Î·2-H2)(dppe)2]+. Journal of the American Chemical Society, 2007, 129, 6608-6618.	6.6	51
99	An unprecedented Î±-Câ€“C agostic interaction in a cyclopropyl tris(pyrazolyl)boratoniobium complexElectronic supplementary information (ESI) available: experimental section. See http://www.rsc.org/suppdata/cc/b3/b300324h/. Chemical Communications, 2003, , 876-877.	2.2	50
100	Phosphine and solvent effects on oxidative addition of CH3Br to Pd(PR3) and Pd(PR3)2 complexes. Dalton Transactions, 2011, 40, 11089.	1.6	50
101	Câ€“H and Câ€“C agostic interactions in cycloalkyl tris(pyrazolyl)boratoniobium complexes. Dalton Transactions, 2003, , 4057-4064.	1.6	49
102	The Mechanism of the Catalytic Functionalization of Haloalkanes by Carbene Insertion: An Experimental and Theoretical Study. Organometallics, 2009, 28, 5968-5981.	1.1	49
103	Density Functional Study on the Effect of the trans Axial Ligand ofB12Cofactors on the Heterolytic Cleavage of the Coâ˜C Bond. Journal of Physical Chemistry B, 2003, 107, 306-315.	1.2	48
104	Intramolecular atom exchange between molecular hydrogen and hydride ligands in cis-[Fe(PR3)4H(H2)]+ complexes. An ab initio theoretical study. Journal of the American Chemical Society, 1992, 114, 2922-2928.	6.6	47
105	Stabilization of the adenosyl radical in coenzyme B12 â€“ a theoretical study. Chemical Physics Letters, 2004, 386, 174-178.	1.2	47
106	Computational study on the difference between the Coâ€“C bond dissociation energy in methylcobalamin and adenosylcobalamin. Journal of Biological Inorganic Chemistry, 2005, 10, 509-517.	1.1	47
107	Mechanism of Side Reactions in Alkane Cï¿¿H Bond Functionalization by Diazo Compounds Catalyzed by Ag and Cu Homoscorpionate Complexesâ€”A DFT Study. ChemCatChem, 2011, 3, 1646-1652.	1.8	47
108	Preparation and Characterization of Osmiumâ˜Stannyl Polyhydrides:Â d4â˜d2Oxidative Addition of Neutral Molecules in a Late Transition Metal. Organometallics, 2003, 22, 2087-2096.	1.1	46

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109	Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with [Ni(PMe_nPh_(3â^'n))₄]. Chemistry - A European Journal, 2017, 23, 16728-16733.	1.7	46
110	Agostic interactions in alkyl derivatives of sterically hindered tris(pyrazolyl)borate complexes of niobium. Coordination Chemistry Reviews, 2009, 253, 635-646.	9.5	45
111	Reaction of Alkynes and Azides: Not Triazoles Through Copperâ€"Acetylides but Oxazoles Through Copperâ€"Nitrene Intermediates. Chemistry - A European Journal, 2014, 20, 3463-3474.	1.7	45
112	Cooperative Reductive Elimination: The Missing Piece in the Oxidativeâ€Coupling Mechanistic Puzzle. Angewandte Chemie - International Edition, 2016, 55, 2764-2767.	7.2	45
113	Ab Initio MO and MM Study on the Nature of [Ru(P-P)2"H3"]+ (P-P = dppb, diop, dpmb, dppe) Complexes. Organometallics, 1994, 13, 4008-4016.	1.1	44
114	On the Feasibility of Nickel-Catalyzed Trifluoromethylation of Aryl Halides. Organometallics, 2014, 33, 6531-6543.	1.1	43
115	The reaction of the unsaturated rhenium fragment {Re(Î·5-C5Me5)(CO)2} with 1,4-difluorobenzene. Thermal intramolecular conversion of a rhenium (difluorophenyl)(hydride) to Re(Î·2-C6H4F2) and a [1,4]-metallotropic shift. Dalton Transactions RSC, 2001, , 1452-1461.	2.3	42
116	Mechanism of the [(NHC)AuI]-Catalyzed Rearrangement of Allylic Acetates. A DFT Study. Organic Letters, 2009, 11, 81-84.	2.4	42
117	Diastereodivergent Enantioselective [8 + 2] Annulation of Tropones and Enals Catalyzed by N-Heterocyclic Carbenes. Organic Letters, 2019, 21, 3187-3192.	2.4	42
118	Hybrid quantum-mechanical and molecular mechanics study of Cu atoms deposition on SiO2 surface defects. Chemical Physics Letters, 1998, 294, 611-618.	1.2	41
119	Applications of Hybrid DFT/Molecular Mechanics to Homogeneous Catalysis. Structure and Bonding, 2004, , 117-150.	1.0	41
120	Copper-Catalyzed Borylative Ring Closing Câ€"C Coupling toward Spiro- and Dispiroheterocycles. ACS Catalysis, 2018, 8, 2833-2838.	5.5	40
121	Measuring the Relative Reactivity of the Carbonâ€"Hydrogen Bonds of Alkanes as Nucleophiles. Angewandte Chemie - International Edition, 2018, 57, 13848-13852.	7.2	40
122	Theoretical modeling of the heme group with a hybrid QM/MM method. Journal of Computational Chemistry, 2000, 21, 282-294.	1.5	39
123	The Effect of the â€œInertâ€•Counteranions in the Deprotonation of the Dihydrogen Complextrans-[FeH(Î·2-H2)(dppe)2]+:Â Kinetic and Theoretical Studies. Journal of the American Chemical Society, 2004, 126, 2320-2321.	6.6	39
124	Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. Journal of Organic Chemistry, 2006, 71, 6388-6396.	1.7	39
125	Câ^'H Bond Activation of Benzene by Unsaturated Î·²-Cyclopropene and Î·²-Benzyne Complexes of Niobium. Journal of the American Chemical Society, 2010, 132, 14239-14250.	6.6	39
126	A computational view on the reactions of hydrocarbons with coinage metal complexes. Journal of Organometallic Chemistry, 2015, 784, 2-12.	0.8	39

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127	Thermally Activated Site Exchange and Quantum Exchange Coupling Processes in Unsymmetrical Trihydride Osmium Compounds. Inorganic Chemistry, 1999, 38, 1814-1824.	1.9	38
128	Computational characterization of a mechanism for the copper-catalyzed aerobic oxidative trifluoromethylation of terminal alkynes. Chemical Communications, 2013, 49, 10486.	2.2	37
129	An Unusual Example of Hypervalent Silicon: A Fiveâ€Coordinate Silyl Group Bridging Two Palladium or Nickel Centers through a Nonsymmetrical Fourâ€Center Twoâ€Electron Bond. Angewandte Chemie - International Edition, 2014, 53, 1103-1108.	7.2	37
130	Mechanistic and Computational Studies of the Atom Transfer Radical Addition of CCl₄ to Styrene Catalyzed by Copper Homoscorpionate Complexes. Inorganic Chemistry, 2011, 50, 2458-2467.	1.9	36
131	Catalytic Nitrene Transfer To Alkynes: A Novel and Versatile Route for the Synthesis of Sulfinamides and Isothiazoles. Angewandte Chemie - International Edition, 2017, 56, 12842-12847.	7.2	36
132	Computational Characterization of the Mechanism for Coinage-Metal-Catalyzed Carboxylation of Terminal Alkynes. Journal of Organic Chemistry, 2014, 79, 11981-11987.	1.7	35
133	Site Preference Energetics, Fluxionality, and Intramolecular Mâ^'HÂ·Â·Â·Hâ^'N Hydrogen Bonding in a Dodecahedral Transition Metal Polyhydrideâ€. Inorganic Chemistry, 1997, 36, 5505-5511.	1.9	34
134	Different van der Waals radii for organic and inorganic halogen atoms: a significant improvement in IMOMM performance. Theoretical Chemistry Accounts, 1997, 96, 146-150.	0.5	34
135	Opposing steric and electronic contributions in OsCl2H2(PPr3i)2. A theoretical study of an unusual structure. New Journal of Chemistry, 1998, 22, 5-9.	1.4	34
136	Polyene Cyclization by a Double Intramolecular Heck Reaction. A DFT Study. Organometallics, 2004, 23, 2784-2796.	1.1	33
137	Hybrid Quantum Mechanics/Molecular Mechanics Methods in Transition Metal Chemistry. Topics in Organometallic Chemistry, 1999, , 165-191.	0.7	33
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