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	Understanding the Binding Properties of Nâ€heterocyclic Carbenes through BDE Matrix App. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	5
2	Mechanism and selectivity of photocatalyzed CO₂reduction by a function-integrated Ru catalyst. Dalton Transactions, 2022, 51, 3747-3759.	1.6	4
3	Seeking the Optimal Descriptor for S_N2 Reactions through Statistical Analysis of Density Functional Theory Results. Journal of Organic Chemistry, 2022, 87, 363-372.	1.7	3
4	Mechanistic Studies on the Synthesis of Pyrrolidines and Piperidines via Copper-Catalyzed Intramolecular Câ€“H Amination. Organometallics, 2022, 41, 1099-1105.	1.1	4
5	Introducing the Catalytic Amination of Silanes via Nitrene Insertion. Journal of the American Chemical Society, 2022, 144, 10608-10614.	6.6	6
6	Two Copper-Carbenes from One Diazo Compound. Journal of the American Chemical Society, 2021, 143, 4837-4843.	6.6	20
7	Redefining the Mechanistic Scenario of Carbonâ^'Sulfur Nucleophilic Coupling via Highâ€Valent Cp*Co^{IV} Species. Angewandte Chemie - International Edition, 2021, 60, 11217-11221.	7.2	14
8	Redefining the Mechanistic Scenario of Carbonâ^'Sulfur Nucleophilic Coupling via Highâ€Valent Cp*Co IV Species. Angewandte Chemie, 2021, 133, 11317-11321.	1.6	1
9	The Effect of Added Ligands on the Reactions of [Ni(COD)(dppf)] with Alkyl Halides: Halide Abstraction May Be Reversible. Organometallics, 2021, 40, 1997-2007.	1.1	12
10	Understanding Ball Milling Mechanochemical Processes with DFT Calculations and Microkinetic Modeling. ChemSusChem, 2021, 14, 2763-2768.	3.6	17
11	An Expanded SET Model Associated with the Functional Hindrance Dominates the Amide-Directed Distal sp³ Câ€“H Functionalization. Journal of the American Chemical Society, 2021, 143, 19406-19416.	6.6	11
12	Computational insights into metal-catalyzed asymmetric hydrogenation. Advances in Catalysis, 2021, 68, 385-426.	0.1	1
13	Photolytic Activation of Late-Transition-Metalâ€“Carbon Bonds and Their Reactivity toward Oxygen. Organometallics, 2021, 40, 4077-4091.	1.1	8
14	A Quantitative Model for Alkane Nucleophilicity Based on Câ^'H Bond Structural/Topological Descriptors. Angewandte Chemie, 2020, 132, 3136-3140.	1.6	4
15	A Quantitative Model for Alkane Nucleophilicity Based on Câ^'H Bond Structural/Topological Descriptors. Angewandte Chemie - International Edition, 2020, 59, 3112-3116.	7.2	18
16	Water oxidation electrocatalysis using ruthenium coordination oligomers adsorbed on multiwalled carbon nanotubes. Nature Chemistry, 2020, 12, 1060-1066.	6.6	54
17	Photosynthesis of a Dihydroimidazopyridine Chelate Shines Light on the Reactions of a Photoactivated Iron(III) Complex with O₂. Inorganic Chemistry, 2020, 59, 16281-16290.	1.9	5
18	Computational Modeling of Selected Photoactivated Processes. Topics in Organometallic Chemistry, 2020, , 131-152.	0.7	0

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19	Unexpected Nickel Complex Speciation Unlocks Alternative Pathways for the Reactions of Alkyl Halides with dppf-Nickel(0). ACS Catalysis, 2020, 10, 10717-10725.	5.5	18
20	Excellence versus Diversity? Not an Either/Or Choice. ACS Catalysis, 2020, 10, 7310-7311.	5.5	4
21	Intermolecular Allene Functionalization by Silver-Nitrene Catalysis. Journal of the American Chemical Society, 2020, 142, 13062-13071.	6.6	25
22	The Challenge of Reproducing with Calculations Raw Experimental Kinetic Data for an Organic Reaction. Organic Letters, 2020, 22, 2873-2877.	2.4	25
23	2 Mechanistic Aspects of Carbonâ€“Boron Bond Formation. , 2020, , .		0
24	Enantioselective Synthesis of 3â€Heterosubstitutedâ€2â€aminoâ€1â€ols by Sequential Metalâ€Free Diene Aziridination/Kinetic Resolution. Chemistry - A European Journal, 2019, 25, 12628-12635.	1.7	4
25	A Career in Catalysis: Odile Eisenstein. ACS Catalysis, 2019, 9, 10375-10388.	5.5	2
26	Caesium fluoride-mediated hydrocarboxylation of alkenes and allenes: scope and mechanistic insights. Chemical Science, 2019, 10, 10072-10078.	3.7	9
27	Four Oxidation States in a Single Photoredox Nickelâ€Based Catalytic Cycle: A Computational Study. Angewandte Chemie - International Edition, 2019, 58, 3898-3902.	7.2	27
28	Four Oxidation States in a Single Photoredox Nickelâ€Based Catalytic Cycle: A Computational Study. Angewandte Chemie, 2019, 131, 3938-3942.	1.6	3
29	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. ACS Catalysis, 2019, 9, 6803-6813.	5.5	145
30	Mechanistic Study on the Asymmetric Synthesis of the Wielandâ€Miescher Ketone and Analogs. ChemCatChem, 2019, 11, 4064-4071.	1.8	5
31	Diastereodivergent Enantioselective [8 + 2] Annulation of Tropones and Enals Catalyzed by N-Heterocyclic Carbenes. Organic Letters, 2019, 21, 3187-3192.	2.4	42
32	Copperâ€Catalyzed Nâ€“F Bond Activation for Uniform Intramolecular Câ€“H Amination Yielding Pyrrolidines and Piperidines. Angewandte Chemie - International Edition, 2019, 58, 8912-8916.	7.2	71
33	Eine Kupferâ€katalysierte Nâ€Fâ€Bindungsaktivierung fÃ¼r die einheitliche intramolekulare Câ€Hâ€Aminierung zu Pyrrolidinen und Piperidinen. Angewandte Chemie, 2019, 131, 9004-9009.	1.6	13
34	The Role of Electronâ€Donor Substituents in the Family of OPBANâ€Cu Water Oxidation Catalysts: Effect on the Degradation Pathways and Efficiency. European Journal of Inorganic Chemistry, 2019, 2019, 2109-2114.	1.0	10
35	Computational Characterization of Single-Electron Transfer Steps in Water Oxidation. Inorganics, 2019, 7, 32.	1.2	13
36	DFT characterization of the mechanism for Staudinger/aza-Wittig tandem organocatalysis. Tetrahedron, 2019, 75, 1852-1859.	1.0	10

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37	The diverse mechanisms for the oxidative addition of Câ€“Br bonds to Pd(PR₃) and Pd(PR₃)₂ complexes. Dalton Transactions, 2019, 48, 16242-16248.	1.6	21
38	On the Use of Thermodynamic Cycles for the Calculation of Standard Potentials for the Oxidation of Solid Metals in Solution. ChemPhysChem, 2019, 20, 159-162.	1.0	0
39	GARLEEK: Adding an extra flavor to ONIOM. Journal of Computational Chemistry, 2019, 40, 381-386.	1.5	6
40	Exploring the Role of Coinage Metalates in Trifluoromethylation: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2019, 25, 9390-9394.	1.7	21
41	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
42	Copper-Catalyzed Borylative Ring Closing Câ€“C Coupling toward Spiro- and Dispiroheterocycles. ACS Catalysis, 2018, 8, 2833-2838.	5.5	40
43	Computational Description of a Huisgen Cycloaddition Inside a Selfâ€Assembled Nanocapsule. European Journal of Organic Chemistry, 2018, 2018, 2103-2109.	1.2	14
44	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
45	Enantioselective Synthesis of Aminodiols by Sequential Rhodiumâ€Catalysed Oxyamination/Kinetic Resolution: Expanding the Substrate Scope of Amidineâ€Based Catalysis. Chemistry - A European Journal, 2018, 24, 4635-4642.	1.7	15
46	Oxidative Coupling Mechanisms: Current State of Understanding. ACS Catalysis, 2018, 8, 1161-1172.	5.5	83
47	Calculation of Reaction Free Energies in Solution: A Comparison of Current Approaches. Journal of Physical Chemistry A, 2018, 122, 1392-1399.	1.1	101
48	A DFT-based mechanistic proposal for the light-driven insertion of dioxygen into Pt(ii)â€“C bonds. Chemical Science, 2018, 9, 5039-5046.	3.7	18
49	Computationally Guided Design of a Readily Assembled Phosphiteâ€“Thioether Ligand for a Broad Range of Pd-Catalyzed Asymmetric Allylic Substitutions. ACS Catalysis, 2018, 8, 3587-3601.	5.5	27
50	Computational Characterization of the Mechanism for the Oxidative Coupling of Benzoic Acid and Alkynes by Rhodium/Copper and Rhodium/Silver Systems. Chemistry - A European Journal, 2018, 24, 12383-12388.	1.7	28
51	Titelbild: Measuring the Relative Reactivity of the Carbonâ€“Hydrogen Bonds of Alkanes as Nucleophiles (Angew. Chem. 42/2018). Angewandte Chemie, 2018, 130, 13885-13885.	1.6	0
52	Searching for Hidden Descriptors in the Metalâ€“Ligand Bond through Statistical Analysis of Density Functional Theory (DFT) Results. Inorganic Chemistry, 2018, 57, 14660-14670.	1.9	21
53	Measuring the Relative Reactivity of the Carbonâ€“Hydrogen Bonds of Alkanes as Nucleophiles. Angewandte Chemie, 2018, 130, 14044-14048.	1.6	12
54	The role of computational results databases in accelerating the discovery of catalysts. Nature Catalysis, 2018, 1, 809-810.	16.1	52

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55	Photoinduced O₂-Dependent Stepwise Oxidative Deglycination of a Nonheme Iron(III) Complex. Journal of the American Chemical Society, 2018, 140, 14150-14160.	6.6	11
56	Copper-mediated reduction of azides under seemingly oxidising conditions: catalytic and computational studies. Catalysis Science and Technology, 2018, 8, 5763-5773.	2.1	19
57	Steric effects determine the mechanisms of reactions between bis(N-heterocyclic carbene)-nickel(0) complexes and aryl halides. Chemical Communications, 2018, 54, 10646-10649.	2.2	23
58	New Vistas in Transmetalation with Discrete â€œAgCF 3 â€•Species: Implications in Pdâ€Mediated Trifluoromethylation Reactions. Chemistry - A European Journal, 2018, 24, 11895-11898.	1.7	21
59	Microkinetic modeling in homogeneous catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1372.	6.2	85
60	Palladium-Catalyzed Aerobic Homocoupling of Alkynes: Full Mechanistic Characterization of a More Complex Oxidase-Type Behavior. ACS Catalysis, 2018, 8, 7495-7506.	5.5	30
61	Accelerated Ruâ€“Cu Trinuclear Cooperative Câ€“H Bond Functionalization of Carbazoles: A Kinetic and Computational Investigation. Chemistry - A European Journal, 2018, 24, 15178-15184.	1.7	14
62	The Acetate Proton Shuttle between Mutually Trans Ligands. Organometallics, 2018, 37, 2645-2651.	1.1	9
63	Measuring the Relative Reactivity of the Carbonâ€“Hydrogen Bonds of Alkanes as Nucleophiles. Angewandte Chemie - International Edition, 2018, 57, 13848-13852.	7.2	40
64	Expanding the Range of Force Fields Available for ONIOM Calculations: The SICTWO Interface. Journal of Chemical Information and Modeling, 2018, 58, 1828-1835.	2.5	18
65	Single Electron Transfer Steps in Water Oxidation Catalysis. Redefining the Mechanistic Scenario. ACS Catalysis, 2017, 7, 1712-1719.	5.5	66
66	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
67	Lightâ€Driven Enantioselective Organocatalytic Î²â€Benzylation of Enals. Angewandte Chemie - International Edition, 2017, 56, 3304-3308.	7.2	55
68	Lightâ€Driven Enantioselective Organocatalytic Î²â€Benzylation of Enals. Angewandte Chemie, 2017, 129, 3352-3356.	1.6	19
69	Computational study on the mechanism of the reaction of carbon dioxide with siloxy silanes. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	3
70	Frontispiece: Catalytic Nitrene Transfer To Alkynes: A Novel and Versatile Route for the Synthesis of Sulfinamides and Isothiazoles. Angewandte Chemie - International Edition, 2017, 56, .	7.2	0
71	Frontispiz: Catalytic Nitrene Transfer To Alkynes: A Novel and Versatile Route for the Synthesis of Sulfinamides and Isothiazoles. Angewandte Chemie, 2017, 129, .	1.6	0
72	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

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73	Computational characterization of the mechanism for the light-driven catalytic trichloromethylation of acylpyridines. Organic and Biomolecular Chemistry, 2017, 15, 8641-8647.	1.5	22
74	Catalytic Nitrene Transfer To Alkynes: A Novel and Versatile Route for the Synthesis of Sulfinamides and Isothiazoles. Angewandte Chemie, 2017, 129, 13022-13027.	1.6	10
75	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
76	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
77	ONIOM(QM:AMOEBA09) Study on Binding Energies and Binding Preference of OH, HCO, and CH₃ Radicals on Hexagonal Water Ice (I_h). Journal of Physical Chemistry C, 2017, 121, 15223-15232.	1.5	19
78	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
79	DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes. Chemistry - A European Journal, 2016, 22, 7545-7553.	1.7	32
80	Cooperative Reductive Elimination: The Missing Piece in the Oxidativeâ€Coupling Mechanistic Puzzle. Angewandte Chemie - International Edition, 2016, 55, 2764-2767.	7.2	45
81	Computational Characterization of the Origin of Selectivity in Cycloaddition Reactions Catalyzed by Phosphoric Acid Derivatives. Chemistry - an Asian Journal, 2016, 11, 411-416.	1.7	25
82	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
83	Mechanistic Investigation of Iridium-Catalyzed Câ€“H Borylation of Methyl Benzoate: Ligand Effects in Regioselectivity and Activity. Organometallics, 2016, 35, 3221-3226.	1.1	23
84	Cooperative Reductive Elimination: The Missing Piece in the Oxidativeâ€Coupling Mechanistic Puzzle. Angewandte Chemie, 2016, 128, 2814-2817.	1.6	13
85	QM/MM Calculations on Selectivity in Homogeneous Catalysis. Structure and Bonding, 2015, , 59-79.	1.0	7
86	Functionalization of C_nH_{2n+2} Alkanes: Supercritical Carbon Dioxide Enhances the Reactivity towards Primary Carbonâ€“Hydrogen Bonds. ChemCatChem, 2015, 7, 3254-3260.	1.8	23
87	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
88	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
89	Computational Study with DFT and Kinetic Models on the Mechanism of Photoinitiated Aromatic Perfluoroalkylations. Organic Letters, 2015, 17, 2676-2679.	2.4	63
90	Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform. Journal of Chemical Information and Modeling, 2015, 55, 95-103.	2.5	403

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91	A computational view on the reactions of hydrocarbons with coinage metal complexes. Journal of Organometallic Chemistry, 2015, 784, 2-12.	0.8	39
92	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
93	Î²-H Abstraction/1,3-CH Bond Addition as a Mechanism for the Activation of CH Bonds at Early Transition Metal Centers. Organometallics, 2014, 33, 7270-7278.	1.1	16
94	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
95	Rationale for the sluggish oxidative addition of aryl halides to Au(<scp>i</scp>). Chemical Communications, 2014, 50, 1533-1536.	2.2	64
96	Toward a mechanistic understanding of oxidative homocoupling: the Glaserâ€“Hay reaction. Catalysis Science and Technology, 2014, 4, 4200-4209.	2.1	57
97	On the Feasibility of Nickel-Catalyzed Trifluoromethylation of Aryl Halides. Organometallics, 2014, 33, 6531-6543.	1.1	43
98	Catalytic Copper-Mediated Ring Opening and Functionalization of Benzoxazoles. ACS Catalysis, 2014, 4, 4215-4222.	5.5	16
99	Chiral transition-metal complexes as BrÃ¸nsted-acid catalysts for the asymmetric Friedelâ€“Crafts hydroxyalkylation of indoles. Dalton Transactions, 2014, 43, 11260-11268.	1.6	23
100	Pdâ€Catalysed Monoâ€•and Dicarbonylation of Aryl Iodides: Insights into the Mechanism and the Selectivity. Chemistry - A European Journal, 2014, 20, 10982-10989.	1.7	26
101	The Transmetalation Process in Suzukiâ€“Miyaura Reactions: Calculations Indicate Lower Barrier via Boronate Intermediate. ChemCatChem, 2014, 6, 3132-3138.	1.8	68
102	Computational Characterization of the Mechanism for Coinage-Metal-Catalyzed Carboxylation of Terminal Alkynes. Journal of Organic Chemistry, 2014, 79, 11981-11987.	1.7	35
103	Silverâ€Catalyzed Functionalization of Esters by Carbene Transfer: The Role of Ylide Zwitterionic Intermediates. ChemCatChem, 2014, 6, 2206-2210.	1.8	22
104	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
105	Computational Perspective on Pd-Catalyzed Câ€“C Cross-Coupling Reaction Mechanisms. Accounts of Chemical Research, 2013, 46, 2626-2634.	7.6	306
106	Catalytic cross-coupling of diazo compounds with coinage metal-based catalysts: an experimental and theoretical study. Dalton Transactions, 2013, 42, 4132.	1.6	57
107	Computational characterization of a mechanism for the copper-catalyzed aerobic oxidative trifluoromethylation of terminal alkynes. Chemical Communications, 2013, 49, 10486.	2.2	37
108	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

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109	Oxidative Additions of Aryl Halides to Palladium Proceed through the Monoligated Complex. ChemCatChem, 2013, 5, 3604-3609.	1.8	79
110	A computational study on the intriguing mechanisms of the gas-phase thermal activation of methane by bare [Ni(H)(OH)]+. Physical Chemistry Chemical Physics, 2012, 14, 9306.	1.3	10
111	Mild, Reversible Reaction of Iridium(III) Amido Complexes with Carbon Dioxide. Inorganic Chemistry, 2012, 51, 9683-9693.	1.9	20
112	Substitution Reactions in Dinuclear Ru-Hbpp Complexes: an Evaluation of Through-Space Interactions. Inorganic Chemistry, 2012, 51, 1889-1901.	1.9	21
113	Merging Sustainability with Organocatalysis in the Formation of Organic Carbonates by Using CO₂ as a Feedstock. ChemSusChem, 2012, 5, 2032-2038.	3.6	283
114	Homogeneous Computational Catalysis: The Mechanism for Cross-Coupling and Other C-C Bond Formation Processes. NATO Science for Peace and Security Series B: Physics and Biophysics, 2012, , 185-206.	0.2	1
115	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
116	Synthesis of PCPâ€Supported Nickel Complexes and their Reactivity with Carbon Dioxide. Chemistry - A European Journal, 2012, 18, 6915-6927.	1.7	73
117	The role of cyclobutenes in gold(i)-catalysed skeletal rearrangement of 1,6-enynes. Organic and Biomolecular Chemistry, 2012, 10, 6105.	1.5	60
118	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
119	Mechanism of the gold-catalyzed cyclopropanation of alkenes with 1,6-enynes. Chemical Science, 2011, 2, 141-149.	3.7	87
120	Quantum mechanics/molecular mechanics methods can be more accurate than full quantum mechanics in systems involving dispersion correlations. Physical Chemistry Chemical Physics, 2011, 13, 10520.	1.3	18
121	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
122	Theoretical Evaluation of Phosphine Effects in Cross-Coupling Reactions. Catalysis By Metal Complexes, 2011, , 57-84.	0.6	12
123	Aromatic versus Benzylic CH Bond Activation of Alkylaromatics by a Transient Î·²-Cyclopropene Complex. Organometallics, 2011, 30, 3999-4007.	1.1	17
124	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
125	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
126	A Computational Study on the Role of Chiral Nâ€Oxides in Enantioselective Pausonâ€"Khand Reactions. Chemistry - A European Journal, 2011, 17, 10050-10057.	1.7	15

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127	Highly Modular Pï£¿OP Ligands for Asymmetric Hydrogenation: Synthesis, Catalytic Activity, and Mechanism. Chemistry - A European Journal, 2010, 16, 6495-6508.	1.7	67
128	Metalâ€“Arene Interactions in Dialkylbiarylphosphane Complexes of Copper, Silver, and Gold. Chemistry - A European Journal, 2010, 16, 5324-5332.	1.7	142
129	Throughâ€Space Ligand Interactions in Enantiomeric Dinuclear Ru Complexes. Chemistry - A European Journal, 2010, 16, 7965-7968.	1.7	20
130	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
131	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
132	Origin of enantioselectivity in asymmetric Pausonâ€“Khand reactions catalyzed by [(BINAP)Co2(CO)6]â¯†. Journal of Molecular Catalysis A, 2010, 324, 127-132.	4.8	10
133	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
134	Copper(I)â¯Olefin Complexes: The Effect of the Trispyrazolylborate Ancillary Ligand in Structure and Reactivity. Organometallics, 2010, 29, 3481-3489.	1.1	32
135	Mechanism for Hydride-Assisted Rearrangement from Ethylidene to Ethylene in Iridium Cationic Complexes. Organometallics, 2010, 29, 2040-2045.	1.1	28
136	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
137	Mechanistic Study of Amine to Imine Oxidation in a Dinuclear Cu(II) Complex Containing an Octaaza Dinucleating Ligand. Inorganic Chemistry, 2010, 49, 5977-5985.	1.9	29
138	Structural Analysis of Zincocenes with Substituted Cyclopentadienyl Rings. Chemistry - A European Journal, 2009, 15, 924-935.	1.7	18
139	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
140	The role of amide ligands in the stabilization of Pd(II) tricoordinated complexes: is the Pdâ€“NR2 bond order single or higher?. Theoretical Chemistry Accounts, 2009, 123, 75-84.	0.5	10
141	Agostic interactions in alkyl derivatives of sterically hindered tris(pyrazolyl)borate complexes of niobium. Coordination Chemistry Reviews, 2009, 253, 635-646.	9.5	45
142	Protonation of transition-metal hydrides: a not so simple process. Chemical Society Reviews, 2009, 38, 957.	18.7	99
143	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
144	Câ¯C Coupling Constants, JCC, Are Reliable Probes for Î±-Câ¯C Agostic Structures. Organometallics, 2009, 28, 940-943.	1.1	26

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145	The Nature of Mâ˜B Versus Mâ•B Bonds in Cationic Terminal Borylene Complexes: Structure and Energy Analysis in the Borylene Complexes [(Î·5-C5H5)(CO)2M{B(Î·5-C5Me5)}]+, [(Î·5-C5H5)(CO)2M(BMes)]+, and [(Î·5-C5H5)(CO)2M(BNMe2)]+ (M = Fe, Ru, Os). Organometallics, 2009, 28, 6442-6449.	1.1	21
146	Vinyl Acetate Synthesis on Homogeneous and Heterogeneous Pd-Based Catalysts: A Theoretical Analysis on the Reaction Mechanisms. Journal of Physical Chemistry A, 2009, 113, 11758-11762.	1.1	13
147	The Mechanism of the Catalytic Functionalization of Haloalkanes by Carbene Insertion: An Experimental and Theoretical Study. Organometallics, 2009, 28, 5968-5981.	1.1	49
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