David Balcells

List of Publications by Year in descending order

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79 papers	4,876 citations	126907 33 h-index	91884 69 g-index
88 all docs	88 docs citations	88 times ranked	5161 citing authors

#	Article	IF	Citations
1	Câ€”H Bond Activation in Transition Metal Species from a Computational Perspective. Chemical Reviews, 2010, 110, 749-823.	47.7	959
2	Highly Active and Robust Cp* Iridium Complexes for Catalytic Water Oxidation. Journal of the American Chemical Society, 2009, 131, 8730-8731.	13.7	561
3	Half-Sandwich Iridium Complexes for Homogeneous Water-Oxidation Catalysis. Journal of the American Chemical Society, 2010, 132, 16017-16029.	13.7	507
4	Mechanism of Homogeneous Iridium-Catalyzed Alkylation of Amines with Alcohols from a DFT Study. Organometallics, 2008, 27, 2529-2535.	2.3	149
5	Design of a Versatile and Improved Precatalyst Scaffold for Palladium-Catalyzed Cross-Coupling: (Î·³-1-^tBu-indenyl)₂(Î¼-Cl)₂Pd₂. ACS Catalysis, 2015, 5, 3680-3688.	11.2	133
6	Mechanistic Study of an Improved Ni Precatalyst for Suzukiâ€“Miyaura Reactions of Aryl Sulfamates: Understanding the Role of Ni(I) Species. Journal of the American Chemical Society, 2017, 139, 922-936.	13.7	130
7	Insight into the Efficiency of Cinnamyl-Supported Precatalysts for the Suzukiâ€“Miyaura Reaction: Observation of Pd(I) Dimers with Bridging Allyl Ligands During Catalysis. Journal of the American Chemical Society, 2014, 136, 7300-7316.	13.7	115
8	Computational approaches to asymmetric synthesis. New Journal of Chemistry, 2007, 31, 333.	2.8	108
9	An Experimentalâˆ’Theoretical Study of the Factors That Affect the Switch between Ruthenium-Catalyzed Dehydrogenative Amide Formation versus Amine Alkylation. Organometallics, 2010, 29, 6548-6558.	2.3	103
10	Manganese Catalysts for Câˆ’H Activation: An Experimental/Theoretical Study Identifies the Stereoelectronic Factor That Controls the Switch between Hydroxylation and Desaturation Pathways. Journal of the American Chemical Society, 2010, 132, 7605-7616.	13.7	100
11	Machine learning dihydrogen activation in the chemical space surrounding Vaska's complex. Chemical Science, 2020, 11, 4584-4601.	7.4	93
12	Introducing Copper as Catalyst for Oxidative Alkane Dehydrogenation. Journal of the American Chemical Society, 2013, 135, 3887-3896.	13.7	89
13	Understanding Precatalyst Activation in Cross-Coupling Reactions: Alcohol Facilitated Reduction from Pd(II) to Pd(0) in Precatalysts of the Type (Î·3-allyl)Pd(L)(Cl) and (Î·3-indenyl)Pd(L)(Cl). ACS Catalysis, 2015, 5, 5596-5606.	11.2	89
14	A Rational Basis for the Axial Ligand Effect in Câˆ’H Oxidation by [MnO(porphyrin)(X)]+ (X = H2O, OHâˆ’,) Tj ETQq0 0 0 rgBT /Overlock 1	4.0	87
15	Cp* Iridium Precatalysts for Selective Câ€“H Oxidation via Direct Oxygen Insertion: A Joint Experimental/Computational Study. ACS Catalysis, 2012, 2, 208-218.	11.2	82
16	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.	13.7	73
17	Designing Pd and Ni Catalysts for Cross-Coupling Reactions by Minimizing Off-Cycle Species. ACS Catalysis, 2018, 8, 3499-3515.	11.2	72
18	The rebound mechanism in catalytic Câ€“H oxidation by MnO(tpp)Cl from DFT studies: electronic nature of the active species. Chemical Communications, 2008, , 744-746.	4.1	68

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19	Nickel(I) Monomers and Dimers with Cyclopentadienyl and Indenyl Ligands. Chemistry - A European Journal, 2014, 20, 5327-5337.	3.3	65
20	Generation and Structural Characterization of a Gold(III) Alkene Complex. Angewandte Chemie - International Edition, 2013, 52, 1660-1663.	13.8	58
21	Density Functional Study on the Mechanism of the Vanadium-Catalyzed Oxidation of Sulfides by Hydrogen Peroxide. Journal of Organic Chemistry, 2003, 68, 4265-4274.	3.2	57
22	The Key Role of the Hemiaminal Intermediate in the Iron-Catalyzed Deaminative Hydrogenation of Amides. ACS Catalysis, 2018, 8, 8751-8762.	11.2	53
23	Câ€“H oxidation by hydroxo manganese(v) porphyrins: a DFT study. Chemical Communications, 2009, , 1772.	4.1	45
24	Basic ancillary ligands promote Oâ€“O bond formation in iridium-catalyzed water oxidation: A DFT study. Dalton Transactions, 2011, 40, 11241.	3.3	45
25	Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. Journal of the American Chemical Society, 2017, 139, 9672-9683.	13.7	45
26	tmQM Datasetâ€”Quantum Geometries and Properties of 86k Transition Metal Complexes. Journal of Chemical Information and Modeling, 2020, 60, 6135-6146.	5.4	45
27	Experimental and computational studies of borohydride catalyzed hydrosilylation of a variety of C€O and C€N functionalities including esters, amides and heteroarenes. New Journal of Chemistry, 2014, 38, 1694-1700.	2.8	42
28	A Carbeneâ€Rich but Carbonylâ€Poor [Ir₆(IMe)₈(CO)₂H₁₄]²⁺ Polyhydride Cluster as a Deactivation Product from Catalytic Glycerol Dehydrogenation. Angewandte Chemie - International Edition, 2014, 53, 12808-12811.	13.8	42
29	High Oxidation State Iridium Mono-Î¼-oxo Dimers Related to Water Oxidation Catalysis. Journal of the American Chemical Society, 2016, 138, 15917-15926.	13.7	41
30	Mechanism of the Base-Assisted Displacement of Chloride by Alcohol in Sulfinyl Derivatives. Journal of Organic Chemistry, 2006, 71, 6388-6396.	3.2	39
31	Effect of 2-Substituents on Allyl-Supported Precatalysts for the Suzukiâ€“Miyaura Reaction: Relating Catalytic Efficiency to the Stability of Palladium(I) Bridging Allyl Dimers. Organometallics, 2015, 34, 381-394.	2.3	38
32	Atom economic synthesis of amides via transition metal catalyzed rearrangement of oxaziridines. Green Chemistry, 2007, 9, 976.	9.0	36
33	trans-Mutation at Gold(III): A Mechanistic Study of a Catalytic Acetylene Functionalization via a Double Insertion Pathway. ACS Catalysis, 2017, 7, 5023-5034.	11.2	35
34	Polyene Cyclization by a Double Intramolecular Heck Reaction. A DFT Study. Organometallics, 2004, 23, 2784-2796.	2.3	33
35	Dinitrogen-Facilitated Reversible Formation of a Siâ€“H Bond in a Pincer-Supported Ni Complex. Organometallics, 2016, 35, 3154-3162.	2.3	33
36	Understanding the Solution and Solid-State Structures of Pd and Pt PSiP Pincer-Supported Hydrides. Inorganic Chemistry, 2015, 54, 11411-11422.	4.0	31

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37	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. Accounts of Chemical Research, 2016, 49, 1070-1078.	15.6	31
38	A competing, dual mechanism for catalytic direct benzene hydroxylation from combined experimental-DFT studies. Chemical Science, 2017, 8, 8373-8383.	7.4	30
39	Molecular recognition in Mn-catalyzed Câ€“H oxidation. Reaction mechanism and origin of selectivity from a DFT perspective. Dalton Transactions, 2009, , 5989.	3.3	27
40	Some critical issues in the application of quantum mechanics/molecular mechanics methods to the study of transition metal complexes. Faraday Discussions, 2003, 124, 429-441.	3.2	26
41	Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,Oâ€Đonor Organic Ligand. Angewandte Chemie - International Edition, 2017, 56, 13047-13051.	13.8	24
42	Influence of a â€œDanglingâ€•Co(II) Ion Bound to a [MnCo₃O₄] Oxo Cubane. Journal of the American Chemical Society, 2018, 140, 9030-9033.	13.7	22
43	Isolation and Study of Rutheniumâ€“Cobalt Oxo Cubanes Bearing a High-Valent, Terminal Ru^Vâ€“Oxo with Significant Oxyl Radical Character. Journal of the American Chemical Society, 2019, 141, 19859-19869.	13.7	21
44	Bis(dialkylphosphino)ferrocene-Ligated Nickel(II) Precatalysts for Suzukiâ€“Miyaura Reactions of Aryl Carbonates. Organometallics, 2019, 38, 3377-3387.	2.3	21
45	Gel-assisted crystallization of [Ir₄(IMe)₇(CO)H₁₀]²⁺ and [Ir₄(IMe)₈H₉]³⁺ clusters derived from catalytic glycerol dehydrogenation. Dalton Transactions, 2015, 44, 18403-18410.	3.3	20
46	Synthetic and Computational Studies on the Rhodium-Catalyzed Hydroamination of Aminoalkenes. ACS Catalysis, 2016, 6, 5651-5665.	11.2	20
47	Coordination and insertion of alkenes and alkynes in Au^{III}complexes: nature of the intermediates from a computational perspective. Dalton Transactions, 2016, 45, 5504-5513.	3.3	20
48	An oscillating C22? unit inside a copper rectangleElectronic supplementary information (ESI) available: NMR spectra and computational details. See http://www.rsc.org/suppdata/cc/b3/b301842c/. Chemical Communications, 2003, , 1260.	4.1	19
49	Base-Catalyzed Inversion of Chiral Sulfur Centers. A Computational Study. Organic Letters, 2004, 6, 2197-2200.	4.6	18
50	How does the Achiral Base Decide the Stereochemical Outcome in the Dynamic Kinetic Resolution of Sulfinyl Chlorides? A Computational Study. Advanced Synthesis and Catalysis, 2007, 349, 2103-2110.	4.3	18
51	Does the metal protect the ancillary ligands? Câ€“H strengthening and deactivation in amines and phosphines upon metal-binding. Chemical Communications, 2014, 50, 614-616.	4.1	17
52	A Dinuclear Iridium(V,V) Oxo-Bridged Complex Characterized Using a Bulk Electrolysis Technique for Crystallizing Highly Oxidizing Compounds. Inorganic Chemistry, 2018, 57, 5684-5691.	4.0	17
53	Small-molecule activation at Au(iii): metallacycle construction from ethylene, water, and acetonitrile. Dalton Transactions, 2016, 45, 14719-14724.	3.3	15
54	DFT Investigation of Suzukiâ€“Miyaura Reactions with Aryl Sulfamates Using a Dialkylbiarylphosphine-Ligated Palladium Catalyst. Organometallics, 2017, 36, 3664-3675.	2.3	15

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55	Concerted Protonâ€“Electron Transfer Reactivity at a Multimetallic Co4O4 Cubane Cluster. Inorganic Chemistry, 2020, 59, 15553-15560.	4.0	14
56	Rational selection of co-catalysts for the deaminative hydrogenation of amides. Chemical Science, 2020, 11, 2225-2230.	7.4	13
57	Concerted Cycloaddition Mechanism in the CuAAC Reaction Catalyzed by 1,8-Naphthyridine Dicopper Complexes. ACS Catalysis, 2022, 12, 4744-4753.	11.2	13
58	First-Principles Calculation of ¹H NMR Chemical Shifts of Complex Metal Polyhydrides: The Essential Inclusion of Relativity and Dynamics. Inorganic Chemistry, 2020, 59, 17509-17518.	4.0	12
59	Synthesis and Characterization of Iridium(V) Coordination Complexes With an N,Oâ€Donor Organic Ligand. Angewandte Chemie, 2017, 129, 13227-13231.	2.0	11
60	Automated Construction and Optimization Combined with Machine Learning to Generate Pt(II) Methane Câ€“H Activation Transition States. Topics in Catalysis, 2022, 65, 312-324.	2.8	11
61	A Carbeneâ€Rich but Carbonylâ€Poor [Ir₆(IMe)₈(CO)₂H₁₄]²⁺ Polyhydride Cluster as a Deactivation Product from Catalytic Glycerol Dehydrogenation. Angewandte Chemie, 2014, 126, 13022-13025.	2.0	9
62	Rhodium Complexes Promoting Câˆ’O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. Chemistry - A European Journal, 2017, 23, 5232-5243.	3.3	9
63	Quantum chemical modeling of the reaction path of chorismate mutase based on the experimental substrate/product complex. FEBS Open Bio, 2017, 7, 789-797.	2.3	9
64	The neutron diffraction structure of [Ir4(IMe)8H10]2+ polyhydride cluster: Testing the computational hydride positional assignments. Journal of Organometallic Chemistry, 2017, 849-850, 17-21.	1.8	8
65	Unmasking the constitution and bonding of the proposed lithium nickelate â€œLi₃NiPh₃(solv)₃â€• revealing the hidden C₆H₄ligand. Chemical Science, 2022, 13, 5268-5276.	7.4	8
66	Synthesis and Characterization of Stable Gold(III) PNP Pincer Complexes. European Journal of Inorganic Chemistry, 2018, 2018, 3113-3117.	2.0	7
67	Cyclometalated ruthenium complexes with carboxylated ligands from a combined experimental/computational perspective. Dalton Transactions, 2018, 47, 2589-2601.	3.3	6
68	Câ€“H Activation by RuCo₃O₄ Oxo Cubanes: Effects of Oxyl Radical Character and Metalâ€“Metal Cooperativity. Journal of the American Chemical Society, 2021, 143, 12108-12119.	13.7	6
69	Self-Consistency versus â€œBest-Fitâ€•Approaches in Understanding the Structure of Metal Nitrosyl Complexes. Organometallics, 2004, 23, 6008-6014.	2.3	5
70	Synthesis, Characterization, and Reactivity of Cyclometalated Gold(III) Dihalide Complexes in Aqua Regia. European Journal of Inorganic Chemistry, 2020, 2020, 3249-3258.	2.0	5
71	Computational Studies on the Mechanisms for Deaminative Amide Hydrogenation by Homogeneous Bifunctional Catalysts. Topics in Catalysis, 2022, 65, 82-95.	2.8	5
72	A DFT Perspective on Diels-Alder Organocatalysts Based on Substituted Phosphoramides. European Journal of Organic Chemistry, 2019, 2019, 442-450.	2.4	4

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73	Synthesis of Triarylmethanes via Palladium-Catalyzed Suzukiâ€“Miyaura Reactions of Diarylmethyl Esters. Organometallics, 2021, 40, 2332-2344.	2.3	4
74	Unsymmetrical Naphthyridine-Based Dicopper(I) Complexes: Synthesis, Stability, and Carbonâ€“Hydrogen Bond Activations. Organometallics, 2021, 40, 1866-1873.	2.3	3
75	Conformational complexity of morphine and morphinum in the gas phase and in water. A DFT and MP2 study. RSC Advances, 2014, 4, 24729-24735.	3.6	2
76	Distortional Effects of Noncovalent Interactions in the Crystal Lattice of a Cp*Ir(III) Acylhydroxamic Acid Complex: A Joint Experimentalâ€“Computational Study. Organometallics, 2014, 33, 4417-4424.	2.3	2
77	A Career in Catalysis: Odile Eisenstein. ACS Catalysis, 2019, 9, 10375-10388.	11.2	2
78	Computational Studies on Asymmetric Reactions with Sulfur Reagents. , 0, , 399-416.		1
79	Frontispiece: Rhodium Complexes Promoting Câ^'O Bond Formation in Reactions with Oxygen: The Role of Superoxo Species. Chemistry - A European Journal, 2017, 23, .	3.3	0