Jorge J CarbÃ³

List of Publications by Year
in descending order

106 papers	4,643 citations	81839 39 h-index	110317 64 g-index
113 all docs	113 docs citations	113 times ranked	4698 citing authors

#	Article	IF	Citations
1	Structure, properties and reactivity of polyoxometalates: a theoretical perspective. Chemical Society Reviews, 2012, 41, 7537.	18.7	392
2	Polyoxometalate electrocatalysts based on earth-abundant metals for efficient water oxidation in acidic media. Nature Chemistry, 2018, 10, 24-30.	6.6	375
3	Trivalent boron nucleophile as a new tool in organic synthesis: reactivity and asymmetric induction. Chemical Society Reviews, 2012, 41, 3558.	18.7	220
4	Mechanistic Insights into Alkene Epoxidation with H₂O₂by Ti- and other TM-Containing Polyoxometalates: Role of the Metal Nature and Coordination Environment. Journal of the American Chemical Society, 2010, 132, 7488-7497.	6.6	148
5	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
6	Cobalt Polyoxometalates as Heterogeneous Water Oxidation Catalysts. Inorganic Chemistry, 2013, 52, 4753-4755.	1.9	118
7	ZrIV-Monosubstituted Keggin-Type Dimeric Polyoxometalates:â€‰ Synthesis, Characterization, Catalysis of H2O2-Based Oxidations, and Theoretical Study. Inorganic Chemistry, 2006, 45, 7224-7234.	1.9	113
8	On the Origin of Alternating Bond Distortions and the Emergence of Chirality in Polyoxometalate Anions. Journal of the American Chemical Society, 2008, 130, 8223-8233.	6.6	107
9	First X-ray Characterization and Theoretical Study of Ï€-Alkyne, Alkynyl-Hydride, and Vinylidene Isomers for the Same Transition Metal Fragment [Cp*Ru(PEt3)2]+. Journal of the American Chemical Society, 2003, 125, 3311-3321.	6.6	90
10	Polyoxopalladates Encapsulating Yttrium and Lanthanide Ions, [X^{III}Pd^{II}₁₂(AsPh)₈O₃₂]^{5â^'} (X=Y, Pr, Nd, Sm, Eu, Gd, Tb, Dy, Ho, Er, Tm, Yb, Lu). Chemistry - A European Journal, 2010, 16, 9076-9085.	1.7	81
11	¹H NMR Investigation of Paramagnetic Chromium(III) Olefin Polymerization Catalysts:â€‰ Experimental Results, Shift Assignment and Prediction by Quantum Chemical Calculations. Organometallics, 2007, 26, 4402-4412.	1.1	80
12	Aerobic Carbonâ€“Carbon Bond Cleavage of Alkenes to Aldehydes Catalyzed by First-Row Transition-Metal-Substituted Polyoxometalates in the Presence of Nitrogen Dioxide. Journal of the American Chemical Society, 2014, 136, 10941-10948.	6.6	77
13	Mixed diboration of alkenes in a metal-free context. Chemical Communications, 2015, 51, 1693-1696.	2.2	77
14	The Rateâ€Determining Step in the Rhodiumâ€“Xantphosâ€Catalysed Hydroformylation of 1â€Octene. Chemistry - A European Journal, 2008, 14, 1843-1853.	1.7	75
15	Current trends in the computational modelling of polyoxometalates. Theoretical Chemistry Accounts, 2011, 128, 393-404.	0.5	69
16	Disclosing the Structure/Activity Correlation in Trivalent Boronâ€Containing Compounds: A Tendency Map. Chemistry - A European Journal, 2012, 18, 12794-12802.	1.7	69
17	Real-time molecular scale observation of crystal formation. Nature Chemistry, 2017, 9, 369-373.	6.6	69
18	Unsymmetrical 1,1-diborated multisubstituted sp³-carbons formed via a metal-free concerted-asynchronous mechanism. Organic and Biomolecular Chemistry, 2015, 13, 9659-9664.	1.5	66

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19	Palladiumâ€“NHC complexes do catalyse the diboration of alkenes: mechanistic insights. Chemical Communications, 2007, , 3380.	2.2	59
20	Alkaline Earth Guests in Polyoxopalladate Chemistry: From Nanocube to Nanostar via an Openâ€Shell Structure. Angewandte Chemie - International Edition, 2014, 53, 11974-11978.	7.2	59
21	A Clearâ€Cut Example of Selective Bpinï£¿Bdan Activation and Precise Bdan Transfer on Boron Conjugate Addition. Chemistry - A European Journal, 2014, 20, 3616-3620.	1.7	59
22	Tetracobalt-polyoxometalate catalysts for water oxidation: Key mechanistic details. Journal of Catalysis, 2017, 350, 56-63.	3.1	59
23	Polynuclear Pd(II) Encapsulating 8-Coordinated Metal Ions: [MO₈Pd^{II}₁₂L₈]^{nâ^'} (M =) Tj ETQq1 1 0.784314 rgBT /Overlock 13214-13228.	1.9	58
24	Photoreduction Mechanism of CO₂ to CO Catalyzed by a Rhenium(I)â€“Polyoxometalate Hybrid Compound. ACS Catalysis, 2016, 6, 6422-6428.	5.5	58
25	Quantifying the Donorâ^'Acceptor Properties of Phosphine and N-Heterocyclic Carbene Ligands in Grubbsâ€™ Catalysts Using a Modified EDA Procedure Based on Orbital Deletion. Organometallics, 2009, 28, 4283-4287.	1.1	57
26	Two- and Four-Electron Alkyne Ligands in Osmiumâ^'Cyclopentadienyl Chemistry:Â Consequences of the Ï€âŠ¥â†'M Interaction. Organometallics, 2002, 21, 305-314.	1.1	54
27	Catalytic Nonâ€Conventional transâ€Hydroboration: A Theoretical and Experimental Perspective. Chemistry - A European Journal, 2012, 18, 1512-1521.	1.7	54
28	Relevance of Protons in Heterolytic Activation of H₂O₂ over Nb(V): Insights from Model Studies on Nb-Substituted Polyoxometalates. ACS Catalysis, 2018, 8, 9722-9737.	5.5	52
29	Probing Polyoxometalateâ€“Protein Interactions Using Molecular Dynamics Simulations. Chemistry - A European Journal, 2016, 22, 15280-15289.	1.7	50
30	Palladium Complexes of a Phosphorus Ylide with Two Stabilizing Groups:Â Synthesis, Structure, and DFT Study of the Bonding Modesâ€. Inorganic Chemistry, 2006, 45, 6803-6815.	1.9	49
31	New Quantum Mechanics-Based Three-Dimensional Molecular Descriptors for Use in QSSR Approaches:â€‰ Application to Asymmetric Catalysis. Journal of Chemical Information and Modeling, 2007, 47, 2228-2234.	2.5	48
32	Alkene oxidation by Ti-containing polyoxometalates. Unambiguous characterization of the role of the protonation state. Chemical Communications, 2012, 48, 9266.	2.2	48
33	Theoretical Studies of Asymmetric Hydroformylation Using the Rhï£¿(R,S)â€BINAPHOS Catalystâ€”Origin of Coordination Preferences and Stereoinduction. Chemistry - A European Journal, 2012, 18, 995-1005.	1.7	45
34	Catalyst Design for Alkene Epoxidation by Molecular Analogues of Heterogeneous Titanium-Silicalite Catalysts. ACS Catalysis, 2020, 10, 4737-4750.	5.5	45
35	Understanding Î±,Î²-Unsaturated Imine Formation from Amine Additions to Î±,Î²-Unsaturated Aldehydes and Ketones: An Analytical and Theoretical Investigation. Journal of Organic Chemistry, 2014, 79, 5163-5172.	1.7	43
36	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

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37	Epoxidation of Alkenes with H₂O₂ Catalyzed by Dititaniumâ€Containing 19â€Tungstodiarsenate(III): Experimental and Theoretical Studies. European Journal of Inorganic Chemistry, 2010, 2010, 5312-5317.	1.0	42
38	Alkene Epoxidation Catalyzed by Ti-Containing Polyoxometalates: Unprecedented Î²-Oxygen Transfer Mechanism. Inorganic Chemistry, 2016, 55, 6080-6084.	1.9	40
39	Copper-Catalyzed Borylative Ring Closing Câ€“C Coupling toward Spiro- and Dispiroheterocycles. ACS Catalysis, 2018, 8, 2833-2838.	5.5	40
40	Ammonia Activation by Î¼₃-Alkylidyne Fragments Supported on a Titanium Molecular Oxide Model. Inorganic Chemistry, 2011, 50, 6269-6279.	1.9	39
41	Predicting the Enantioselectivity of the Copperâ€Catalysed Cyclopropanation of Alkenes by Using Quantitative Quadrantâ€Diagram Representations of the Catalysts. Chemistry - A European Journal, 2012, 18, 14026-14036.	1.7	39
42	Influence of polyoxometalate ligands on the nature of high-valent transition metal nitrido species. A theoretical analysis of experimentally known and unprecedented compounds. Dalton Transactions, 2008, , 5166.	1.6	38
43	Effective Storage of Electrons in Water by the Formation of Highly Reduced Polyoxometalate Clusters. Journal of the American Chemical Society, 2022, 144, 8951-8960.	6.6	37
44	Origin of Stereoinduction by Chiral Aminophosphane Phosphinite Ligands in Enantioselective Catalysis: Asymmetric Hydroformylation. Chemistry - A European Journal, 2006, 12, 1457-1467.	1.7	36
45	Why Does Nb(V) Show Higher Heterolytic Pathway Selectivity Than Ti(IV) in Epoxidation with H₂O₂? Answers from Model Studies on Nb- and Ti-Substituted Lindqvist Tungstates. ACS Catalysis, 2019, 9, 6262-6275.	5.5	36
46	3D-QSPR models for predicting the enantioselectivity and the activity for asymmetric hydroformylation of styrene catalyzed by Rhâ€“diphosphane. Catalysis Science and Technology, 2012, 2, 1694.	2.1	35
47	Facile Synthesis of Alkynylâˆ’ and Vinylideneâˆ’Niobocene Complexes. Unexpected Î·1-Vinylideneâˆ’Î·2-Alkyne Isomerization. Organometallics, 2000, 19, 1749-1765.	1.1	32
48	Strong 1,4-Pâˆ’O Intramolecular Interactions as a Source of Conformational Preferences in Î±-Stabilized Phosphorus Ylides. Inorganic Chemistry, 2001, 40, 4913-4917.	1.9	32
49	Arene C(sp²)-H Metalation at Ni^{II} Modeled with a Reactive PONC_{Ph} Ligand. Inorganic Chemistry, 2016, 55, 8041-8047.	1.9	32
50	Mixed Pâˆ’N and Asâˆ’N Bis-Ylide Palladium Complexes:Â Cooperative Intramolecular Interactions, Conformational Preferences, and Câˆ’H Bond Activationsâ€. Organometallics, 2006, 25, 4653-4664.	1.1	31
51	Discrete Silver(I)â€Palladium(II)â€Oxo Nanoclusters, {Ag₄Pd₁₃} and {Ag₅Pd₁₅}, and the Role of Metalâ€“Metal Bonding Induced by Cation Confinement. Angewandte Chemie - International Edition, 2016, 55, 15766-15770.	7.2	31
52	Structureâ€“Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins. Chemistry - A European Journal, 2020, 26, 5799-5809.	1.7	31
53	Electronic Ligand Effects on the Regioselectivity of the Rhodiumâˆ’Diphosphine-Catalyzed Hydroformylation of Propene. Organometallics, 2007, 26, 2234-2242.	1.1	30
54	A theoretical study of the activity in Rh-catalysed hydroformylation: the origin of the enhanced activity of the Ï€-acceptor phosphinine ligand. Catalysis Science and Technology, 2014, 4, 979-987.	2.1	30

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55	Self-assembly study of nanometric spheres from polyoxometalate-phenylalanine hybrids, an experimental and theoretical approach. Dalton Transactions, 2018, 47, 6304-6313.	1.6	30
56	Mechanism of Thioether Oxidation over Diâ€•and Tetrameric Ti Centres: Kinetic and DFT Studies Based on Model Tiâ€Containing Polyoxometalates. Chemistry - A European Journal, 2015, 21, 14496-14506.	1.7	27
57	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
58	Modeling the Oxygen Vacancy at a Molecular Vanadium(III) Silica-Supported Catalyst. Journal of the American Chemical Society, 2018, 140, 14903-14914.	6.6	26
59	Activation of H₂O₂ over Zr(IV). Insights from Model Studies on Zr-Monosubstituted Lindqvist Tungstates. ACS Catalysis, 2021, 11, 10589-10603.	5.5	25
60	Understanding the Regioselectivity of Aromatic Hydroxylation over Divanadium-Substituted Î³-Keggin Polyoxotungstate. ACS Catalysis, 2017, 7, 8514-8523.	5.5	23
61	9-Cobalt(II)-Containing 27-Tungsto-3-germanate(IV): Synthesis, Structure, Computational Modeling, and Heterogeneous Water Oxidation Catalysis. Inorganic Chemistry, 2019, 58, 11308-11316.	1.9	23
62	Influence of the Nature of the Ligand on Dirhodium(II) Carbene Species: A Theoretical Analysis. Organometallics, 2008, 27, 2873-2876.	1.1	22
63	Nature of Zr-Monosubstituted Monomeric and Dimeric Polyoxometalates in Water Solution at Different pH Conditions: Static Density Functional Theory Calculations and Dynamic Simulations. Inorganic Chemistry, 2014, 53, 778-786.	1.9	22
64	Transition-Metal-Free Allylic Borylation of 1,3-Dienes. Organic Letters, 2019, 21, 2251-2255.	2.4	21
65	Addition of Terminal Alkynes to a Molecular Titaniumâ€“Zinc Nitride. Angewandte Chemie - International Edition, 2007, 46, 3095-3098.	7.2	20
66	Construction of Titanasiloxanes by Incorporation of Silanols to the Metal Oxide Model [{Ti(Î·⁵â€C₅Me₅)(Î¼â€O)}₃(Î¼₃â€CR)]: DFT Elucidation of the Reaction Mechanism. Chemistry - A European Journal, 2008, 14, 7930-7938.	3.7	20
67	A fast metalâ€“metal bonded water oxidation catalyst. Journal of Catalysis, 2014, 315, 25-32.	3.1	20
68	Size and charge effect of guest cations in the formation of polyoxopalladates: a theoretical and experimental study. Chemical Science, 2017, 8, 7862-7872.	3.7	20
69	Alkoxide activation of tetra-alkoxy diboron reagents in Câ€“B bond formation: a decade of unpredictable reactivity. Chemical Communications, 2021, 57, 11935-11947.	2.2	20
70	Transitionâ€Metalâ€Free Stereoselective Borylation of Allenamides. Chemistry - A European Journal, 2018, 24, 14059-14063.	1.7	18
71	How Does the Redox State of Polyoxovanadates Influence the Collective Behavior in Solution? A Case Study with [I@V18O42]qâ¯ (q = 3, 5, 7, 11, and 13). Inorganic Chemistry, 2019, 58, 3881-3894.	1.9	18
72	Experimental and Computational Study of the Bonding Properties of Mixed Bisâ¯Ylides of Phosphorus and Sulfur. Inorganic Chemistry, 2009, 48, 6823-6834.	1.9	16

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73	Strong 1,4 Pâ€“O intramolecular interactions as a source of conformational preferences in Î±-stabilised phosphorus ylides. Part 2: metallic complexes. Inorganica Chimica Acta, 2004, 357, 1444-1456.	1.2	15
74	Synthesis and Characterization of PdIIComplexes with Bis-Pyridinium and Isoquinolinium N-Ylides:Â Moderate CHÂ·Â·Â·OC Intramolecular Hydrogen Bonds as Source of Conformational Preferences. Inorganic Chemistry, 2004, 43, 7622-7635.	1.9	15
75	Quantitative Structureâ€“Activity Relationships for the Nucleophilicity of Trivalent Boron Compounds. Chemistry - A European Journal, 2017, 23, 5066-5075.	1.7	15
76	Assembly Mechanism of Zr-Containing and Other TM-Containing Polyoxometalates. Inorganic Chemistry, 2017, 56, 4148-4156.	1.9	15
77	Intermetallic Cooperation in Câ€“H Activation Involving Transient Titanium-Alkylidene Species: A Synthetic and Mechanistic Study. Organometallics, 2017, 36, 3076-3083.	1.1	14
78	Lewis Base Behavior of Bridging Nitrido Ligands of Titanium Polynuclear Complexes. Chemistry - A European Journal, 2009, 15, 11619-11631.	1.7	13
79	Hydron-Transfer Processes Involving an Organotitanium Oxide and Alcohols. European Journal of Inorganic Chemistry, 2009, 2009, 643-653.	1.0	13
80	Understanding the mechanism of transition metal-free anti addition to alkynes: the selenoboration case. Catalysis Science and Technology, 2018, 8, 3617-3628.	2.1	13
81	Origin of Selectivity in Protein Hydrolysis by Zr(IV)-Containing Metal Oxides as Artificial Proteases. ACS Catalysis, 2020, 10, 13455-13467.	5.5	13
82	Reaction Pathway Discrimination in Alkene Oxidation Reactions by Designed Tiâ€“Siloxyâ€“Polyoxometalates. ChemCatChem, 2021, 13, 1220-1229.	1.8	13
83	Transborylation of alkenylboranes with diboranes. Chemical Communications, 2021, 57, 13361-13364.	2.2	13
84	Carbonâ€“Nitrogen Bond Construction and Carbonâ€“Oxygen Double Bond Cleavage on a Molecular Titanium Oxonitride: A Combined Experimental and Computational Study. Inorganic Chemistry, 2015, 54, 9401-9412.	1.9	12
85	Core-substituted naphthalenediimides anchored on BiVO₄ for visible light-driven water splitting. Green Chemistry, 2017, 19, 2448-2462.	4.6	11
86	Consecutive borylcupration/Câ€“C coupling of Î³-alkenyl aldehydes towards diastereoselective 2-(borylmethyl)cycloalkanols. Chemical Communications, 2020, 56, 5973-5976.	2.2	11
87	Carbonylative Cycloaddition of Allyl Halides and Acetylenes Promoted by Ni(CO)4. A DFT Study on the Reaction Mechanism. Organometallics, 2000, 19, 3516-3526.	1.1	10
88	Mapping the Electronic Structure and the Reactivity Trends for Stabilized Î±â€“Boryl Carbanions. Chemistry - A European Journal, 2021, 27, 12352-12361.	1.7	10
89	Discovering the chemical reactivity of the molecular oxonitride [{Ti(Î·5-C5Me5)(Î¼-O)}3(Î¼3-N)]. Journal of Organometallic Chemistry, 2011, 696, 4011-4017.	0.8	9
90	Regioselectivity Control in Pd-Catalyzed Telomerization of Isoprene Enabled by Solvent and Ligand Selection. ACS Catalysis, 2020, 10, 11458-11465.	5.5	9

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91	Computational Modelling of the Interactions Between Polyoxometalates and Biological Systems. Frontiers in Chemistry, 2022, 10, 876630.	1.8	9
92	Theoretical characterization of a Ru N-Heterocyclic Carbene derivative of a polyoxometalate. Enhanced Ï€-interaction in oxide supported TM-organic linkages. Dalton Transactions, 2011, 40, 2975.	1.6	8
93	Redox-Active Behavior of the [{Ti(Î·⁵-C₅Me₅)(Î¼-NH)}₃(Î¼₃-N)] Metalloligand. Inorganic Chemistry, 2013, 52, 6103-6109.	1.9	8
94	Diskrete Silber(I)â€Palladium(II)â€Oxoâ€Nanocluster, {Ag₄Pd₁₃} und {Ag₅Pd₁₅}, sowie die Rolle der Metallâ€Metallâ€Bindung induziert durch Kationenâ€Einschluss. Angewandte Chemie, 2016, 128, 15998-16002.	1.6	7
95	Synthesis, molecular structure and computational study of a ruthenium bis(thietane) complex. Inorganica Chimica Acta, 2001, 316, 13-18.	1.2	5
96	Self-Consistency versus â€œBest-Fitâ€•Approaches in Understanding the Structure of Metal Nitrosyl Complexes. Organometallics, 2004, 23, 6008-6014.	1.1	5
97	Peptide Hydrolysis by Metal (Oxa)cyclen Complexes: Revisiting the Mechanism and Assessing Ligand Effects. Inorganic Chemistry, 2021, 60, 807-815.	1.9	5
98	Nâ•N Bond Cleavage by Tantalum Hydride Complexes: Mechanistic Insights and Reactivity. Inorganic Chemistry, 2022, 61, 474-485.	1.9	5
99	A Bridging bis-Allyl Titanium Complex: Mechanistic Insights into the Electronic Structure and Reactivity. Inorganic Chemistry, 2019, 58, 12157-12166.	1.9	4
100	Selective Carbonâ€“Carbon Bond Activation of Oxirane by a Bisphosphine Pt(0) Complexâ€”A Theoretical Study. Organometallics, 2015, 34, 3764-3773.	1.1	3
101	Rhodium Diphosphine Hydroformylation. Catalysis By Metal Complexes, 2002, , 161-187.	0.6	2
102	Structure and Reactivity of Polyoxometalates. , 2013, , 887-906.		2
103	[Co9(H2O)6(OH)3(HPO4)2(PW9O34)3]16â˜. Advances in Inorganic Chemistry, 2017, , 155-179.	0.4	2
104	Rhodium Diphosphine Hydroformylation. ChemInform, 2003, 34, no.	0.1	0
105	Frontispiece: Structureâ€“Activity Relationships for the Affinity of Chaotropic Polyoxometalate Anions towards Proteins. Chemistry - A European Journal, 2020, 26, .	1.7	0
106	2 Mechanistic Aspects of Carbonâ€“Boron Bond Formation. , 2020, , .		0