Lionel Perrin

List of Publications by Year
in descending order

78 papers	2,786 citations	172457 29 h-index	189892 50 g-index
92 all docs	92 docs citations	92 times ranked	2880 citing authors

#	Article	IF	Citations
1	Design of selective divalent chain transfer agents for coordinative chain transfer polymerization of ethylene and its copolymerization with butadiene. Polymer Chemistry, 2022, 13, 1970-1977.	3.9	11
2	Salt-Enhanced Oxidative Addition of Iodobenzene to Pd: An Interplay Between Cation, Anion, and Pdâ€“Pd Cooperative Effects. Inorganic Chemistry, 2022, 61, 7935-7944.	4.0	6
3	Cationic Phenoxyimine Complexes of Yttrium: Synthesis, Characterization, and Living Polymerization of Isoprene. Organometallics, 2022, 41, 2106-2118.	2.3	3
4	Block copolymers based on ethylene and methacrylates using a combination of catalytic chain transfer polymerisation (CCTP) and radical polymerization. Angewandte Chemie, 2021, 133, 25560.	2.0	0
5	Block Copolymers Based on Ethylene and Methacrylates Using a Combination of Catalytic Chain Transfer Polymerisation (CCTP) and Radical Polymerisation. Angewandte Chemie - International Edition, 2021, 60, 25356-25364.	13.8	5
6	Monocationic Bis-Alkyl and Bis-Allyl Yttrium Complexes: Synthesis, ⁸⁹Y NMR Characterization, Ethylene or Isoprene Polymerization, and Modeling. Organometallics, 2021, 40, 218-230.	2.3	8
7	Ene/Diene Copolymerization Catalyzed by Cationic Sc and Gd d⁰ Metal Complexes: Speciation, Ion Pairing, and Selectivity from a Computational Perspective. ACS Catalysis, 2020, 10, 12359-12369.	11.2	6
8	Iodineâ€Transfer Polymerization (ITP) of Ethylene and Copolymerization with Vinyl Acetate. Angewandte Chemie - International Edition, 2020, 59, 19304-19310.	13.8	15
9	Iodineâ€Transfer Polymerization (ITP) of Ethylene and Copolymerization with Vinyl Acetate. Angewandte Chemie, 2020, 132, 19466-19472.	2.0	5
10	Relating circular dichroism to atomic structure by means of MD simulations and computed CD spectra with Î±-peptoids as an example. Physical Chemistry Chemical Physics, 2020, 22, 13192-13200.	2.8	2
11	A Career in Catalysis: Odile Eisenstein. ACS Catalysis, 2019, 9, 10375-10388.	11.2	2
12	Identification of a Transient but Key Motif in the Living Coordinative Chain Transfer Cyclocopolymerization of Ethylene with Butadiene. ACS Catalysis, 2019, 9, 9298-9309.	11.2	14
13	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. ACS Catalysis, 2019, 9, 6803-6813.	11.2	145
14	High Glassâ€Transition Temperature Polymer Networks Harnessing the Dynamic Ring Opening of Pinacol Boronates. Angewandte Chemie - International Edition, 2019, 58, 12216-12222.	13.8	24
15	Zirconocene-Mediated Selective Câ€“C Bond Cleavage of Strained Carbocycles: Scope and Mechanism. Journal of Organic Chemistry, 2018, 83, 3497-3515.	3.2	27
16	Coordinative chain transfer copolymerization of ethylene and styrene using an ansa-bis(fluorenyl) neodymium complex and dialkylmagnesium. Polymer Chemistry, 2018, 9, 3262-3271.	3.9	2
17	Dialkenylmagnesium Compounds in Coordinative Chain Transfer Polymerization of Ethylene. Reversible Chain Transfer Agents and Tools To Probe Catalyst Selectivities toward Ring Formation. Organometallics, 2018, 37, 1546-1554.	2.3	16
18	Exploring the Conformation of Mixed Cisâ€“Trans Î±,Î²-Oligopeptoids: AÂJoint Experimental and Computational Study. Journal of Organic Chemistry, 2018, 83, 6382-6396.	3.2	13

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19	Preparation of monopodal and bipodal aluminum surface species by selective protonolysis of highly reactive [AlH3(NMe2Et)] on silica. Dalton Transactions, 2017, 46, 11547-11551.	3.3	3
20	Experimental and DFT Computational Study of Î²-Me and Î²-H Elimination Coupled with Proton Transfer: From Amides to Enamides in Cp*₂MX (M = La, Ce). Organometallics, 2017, 36, 97-108.	2.3	11
21	Development of a Modified Julia Olefination of Imides for the Synthesis of Alkaloids. European Journal of Organic Chemistry, 2016, 2016, 2944-2953.	2.4	15
22	Preparation and Reactivity of Acyclic Chiral Allylzinc Species by a Zincâ€Brook Rearrangement. Angewandte Chemie - International Edition, 2016, 55, 6057-6061.	13.8	24
23	Deciphering Selectivity in Organic Reactions: A Multifaceted Problem. Accounts of Chemical Research, 2016, 49, 1070-1078.	15.6	31
24	Ethyleneâ€“Butadiene Copolymerization by Neodymocene Complexes: A Ligand Structure/Activity/Polymer Microstructure Relationship Based on DFT Calculations. ACS Catalysis, 2016, 6, 1028-1036.	11.2	37
25	Weak backbone CHâ‹¯Oî€€ and side chain tBuâ‹¯tBu London interactions help promote helix folding of achiral NtBu peptoids. Chemical Communications, 2016, 52, 4573-4576.	4.1	31
26	The role of H₂O in the electron transfer-activation of substrates using SmI₂: insights from DFT. Dalton Transactions, 2016, 45, 3706-3710.	3.3	15
27	Water-soluble, heterometallic chalcogenide oligomers as building blocks for functional films. Inorganic Chemistry Frontiers, 2016, 3, 689-701.	6.0	3
28	New perspectives in organolanthanide chemistry from redox to bond metathesis: insights from theory. Chemical Society Reviews, 2016, 45, 2516-2543.	38.1	44
29	Deciphering the Mechanism of Coordinative Chain Transfer Polymerization of Ethylene Using Neodymocene Catalysts and Dialkylmagnesium. ACS Catalysis, 2016, 6, 851-860.	11.2	50
30	Straightforward Synthesis of 5â€Bromopentaâ€2,4â€diynenitrile and Its Reactivity Towards Terminal Alkynes: A Direct Access to Diene and Benzofulvene Scaffolds. Chemistry - A European Journal, 2015, 21, 6042-6047.	3.3	21
31	Can a pentamethylcyclopentadienyl ligand act as a proton-relay in f-element chemistry? Insights from a joint experimental/theoretical study. Dalton Transactions, 2015, 44, 2575-2587.	3.3	25
32	Remote functionalization of hydrocarbons with reversibility enhanced stereocontrol. Chemical Science, 2015, 6, 2770-2776.	7.4	65
33	Modelling and Rationalizing Organometallic Chemistry with Computation: Where Are We?. Structure and Bonding, 2015, , 1-37.	1.0	13
34	Theoretical treatment of one electron redox transformation of a small molecule using f-element complexes. Dalton Transactions, 2014, 43, 12124-12134.	3.3	19
35	Computational insights into carbonâ€“carbon homocoupling reactions mediated by organolanthanide(iii) complexes. Dalton Transactions, 2014, 43, 4520.	3.3	10
36	Synthesis and biological evaluation of tetrahydro[1,4]diazepino[1,2-a]indol-1-ones as cyclin-dependent kinase inhibitors. European Journal of Medicinal Chemistry, 2014, 83, 617-629.	5.5	14

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37	Stereoselective Synthesis of Enantiopure Cycloalkylglycines by 1,3â€Dipolar Cycloaddition of a Chiral Nitrone to Cycloalkenes. European Journal of Organic Chemistry, 2014, 2014, 6017-6024.	2.4	11
38	Two [1,2,4-(Me₃C)₃C₅H₂]₂CeH Molecules are Involved in Hydrogenation of Pyridine to Piperidine as Shown by Experiments and Computations. Inorganic Chemistry, 2014, 53, 6361-6373.	4.0	19
39	Qualitative Estimation of the Single-Electron Transfer Step Energetics Mediated by Samarium(II) Complexes: A â€œSOMOâ€“LUMO Gapâ€•Approach. Inorganic Chemistry, 2014, 53, 3427-3433.	4.0	24
40	Preliminary Theoretical Insights into SmI2-Mediated Reactions: Activation of Ketones in THF. European Journal of Inorganic Chemistry, 2013, 2013, 4042-4049.	2.0	19
41	Structural Role of Counterions Adsorbed on Self-Assembled Peptide Nanotubes. Journal of the American Chemical Society, 2012, 134, 723-733.	13.7	41
42	Mechanistic insights into Î²-oxygen atom transfer in olefinepoxidation mediated by W(vi) complexes and H2O2. Dalton Transactions, 2012, 41, 1131-1133.	3.3	13
43	Reversible 1,4â€Insertion of Pyridine Into a Highly Polar Metalâ€“Carbon Bond: Effect of the Second Metal. Chemistry - A European Journal, 2012, 18, 6448-6452.	3.3	14
44	Metabolism of Nâ€methylâ€amide by cytochrome P450s. FEBS Journal, 2011, 278, 2167-2178.	4.7	9
45	Isoselective Styrene Polymerization Catalyzed by ansa-Bis(indenyl) Allyl Rare Earth Complexes. Stereochemical and Mechanistic Aspects. Macromolecules, 2011, 44, 3312-3322.	4.8	40
46	Theoretical and Experimental Studies on the Carbonâ€Nanotube Surface Oxidation by Nitric Acid: Interplay between Functionalization and Vacancy Enlargement. Chemistry - A European Journal, 2011, 17, 11467-11477.	3.3	93
47	Control of peptide nanotube diameter by chemical modifications of an aromatic residue involved in a single close contact. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 7679-7684.	7.1	81
48	A Joint Experimental/Theoretical Investigation of the Statistical Olefin/Conjugated Diene Copolymerization Catalyzed by a Hemiâ€Lanthanidocene [(Cp*)(BH₄)LnR]. Chemistry - A European Journal, 2010, 16, 11376-11385.	3.3	34
49	Olefin Epoxidation by H₂O₂/MeCN Catalysed by Cyclopentadienyloxidotungsten(VI) and Molybdenum(VI) Complexes: Experiments and Computations. Chemistry - A European Journal, 2010, 16, 9572-9584.	3.3	71
50	Facile Interconversion of [Cp₂(Cl)Hf(SnH₃)] and [Cp₂(Cl)Hf(Î¼â€H)SnH₂]: DFT Investigations of Hafnocene Stannyl Complexes as Masked Stannylenes. Angewandte Chemie - International Edition, 2010, 49, 1816-1819.	13.8	14
51	Insertion of Pyridine into the Calcium Allyl Bond: Regioselective 1,4â€Dihydropyridine Formation and Cï£¿H Bond Activation. Angewandte Chemie - International Edition, 2010, 49, 7795-7798.	13.8	46
52	Probing the stereoâ€electronic properties of cationic rhodium complexes bearing chiral diphosphine ligands by ¹⁰³Rh NMR. Magnetic Resonance in Chemistry, 2010, 48, 848-856.	1.9	16
53	Elucidation of the Self-Assembly Pathway of Lanreotide Octapeptide into Î²-Sheet Nanotubes: Role of Two Stable Intermediates. Journal of the American Chemical Society, 2010, 132, 4230-4241.	13.7	75
54	DFT Investigation of the Tacticity Control during Styrene Polymerization Catalyzed by Single-Component Allyl ansa-Lanthanidocenes		

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55	A DFT study of conjugated dienes polymerisation catalyzed by [Cp*ScR]+: insights into the propensity for cis-1,4 insertion. Chemical Communications, 2010, 46, 2965.	4.1	17
56	On the Initiation Mechanism of Syndiospecific Styrene Polymerization Catalyzed by Singleâ€Component ansaâ€Lanthanidocenes. Chemistry - A European Journal, 2009, 15, 3773-3783.	3.3	42
57	Bis(allyl)calcium. Angewandte Chemie - International Edition, 2009, 48, 5715-5719.	13.8	81
58	Bond Activations of PhSiH₃ by Cp₂SmH: A Mechanistic Investigation by the DFT Method. Organometallics, 2009, 28, 3767-3775.	2.3	32
59	Intramolecular hydrogen bonding as a determinant of the inhibitory potency of N-unsubstituted imidazole derivatives towards mammalian hemoproteins. Metallomics, 2009, 1, 148-156.	2.4	4
60	The Effect of Ketoconazole on the Pharmacokinetics and Pharmacodynamics of Ixabepilone: A First in Class Epothilone B Analogue in Late-Phase Clinical Development. Clinical Cancer Research, 2008, 14, 2701-2709.	7.0	27
61	Metabolism of Phenylahistin Enantiomers by Cytochromes P450: A Possible Explanation for Their Different Cytotoxicity. Drug Metabolism and Disposition, 2008, 36, 2381-2392.	3.3	8
62	Chemoselectivity in Ïƒ bond activation by lanthanocene complexes from a DFT perspective: reactions of Cp2LnR (R = CH3, H, SiH3) with SiH4and CH3â€“SiH3. New Journal of Chemistry, 2007, 31, 549-555.	2.8	37
63	An electrochemical and DFT study on selected Î²-diketiminato metal complexes. Dalton Transactions, 2006, , 2591-2596.	3.3	18
64	A DFT Study of Stannane Dehydrocoupling Catalyzed by Cp2LaH. Organometallics, 2006, 25, 3143-3151.	2.3	15
65	CYTOCHROME P450-MEDIATED OXIDATION OF GLUCURONIDE DERIVATIVES: EXAMPLE OF ESTRADIOL-17Î²-GLUCURONIDE OXIDATION TO 2-HYDROXY-ESTRADIOL-17Î²-GLUCURONIDE BY CYP 2C8. Drug Metabolism and Disposition, 2005, 33, 466-473.	3.3	43
66	Hydrogen for Fluorine Exchange in C6F6and C6F5H by Monomeric [1,3,4-(Me3C)3C5H2]2CeH:Â Experimental and Computational Studies. Journal of the American Chemical Society, 2005, 127, 279-292.	13.7	190
67	Hydrogen for Fluorine Exchange in CH4-xFxby Monomeric [1,2,4-(Me3C)3C5H2]2CeH:Â Experimental and Computational Studies. Journal of the American Chemical Society, 2005, 127, 7781-7795.	13.7	91
68	Modelling Me5C5for reactivity studies in (Î·5-C5Me5)2Lnâ€“R: full DFT and QM/MM approaches. New Journal of Chemistry, 2004, 28, 1255-1259.	2.8	24
69	Lanthanide Complexes: Electronic Structure and Hâ€”H, Câ€”H, and Siâ€”H Bond Activation from a DFT Perspective. ACS Symposium Series, 2004, , 116-133.	0.5	16
70	Some structural and electronic properties of MX3(Mâ€‰=â€‰Ln, Sc, Y, Ti+, Zr+, Hf+; Xâ€‰=â€‰H, Me, Hal, NH2) from DFT calculations. Faraday Discussions, 2003, 124, 25-39.	3.2	59
71	Bonding of H2, N2, Ethylene, and Acetylene to Bivalent Lanthanide Metallocenes:Â Trends from DFT Calculations on Cp2M and Cp*2M (M = Sm, Eu, Yb) and Experiments with Cp*2Yb. Organometallics, 2003, 22, 5447-5453.	2.3	28
72	Mono-, Di-, and Trianionic Î²-Diketiminato Ligands:Â A Computational Study and the Synthesis and Structure of [(YbL)3(THF)], L = [{N(SiMe3)C(Ph)}2CH]. Journal of the American Chemical Society, 2003, 125, 10790-10791.	13.7	71

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73	CF4defluorination by Cp2Lnâ€“H: a DFT study. Dalton Transactions, 2003, , 4313-4318.	3.3	28
74	Î³ Agostic Câ€“H or Î² agostic Siâ€“C bonds in La{CH(SiMe3)2}3? A DFT study of the role of the ligand. New Journal of Chemistry, 2003, 27, 121-127.	2.8	88
75	A DFT Study of SiH4 Activation by Cp2LnH. Inorganic Chemistry, 2002, 41, 4355-4362.	4.0	75
76	Are the Carbon Monoxide Complexes of Cp2M (M = Ca, Eu, or Yb) Carbon or Oxygen Bonded? An Answer from DFT Calculations. Journal of the American Chemical Society, 2002, 124, 5614-5615.	13.7	43
77	DFT study of CH4 activation by d0 Cl2LnZ (Z = H, CH3) complexes. Dalton Transactions RSC, 2002, , 534-539.	2.3	74
78	Computed Ligand Electronic Parameters from Quantum Chemistry and Their Relation to Tolman Parameters, Lever Parameters, and Hammett Constants. Inorganic Chemistry, 2001, 40, 5806-5811.	4.0	233