Luigi Cavallo

List of Publications by Year
in descending order

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549	35,792	3149 92	6454 157
papers	citations	h-index	g-index

587	587	587	25101
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Selectivity in Propene Polymerization with Metallocene Catalysts. Chemical Reviews, 2000, 100, 1253-1346.	23.0	1,313
2	SambVca: A Web Application for the Calculation of the Buried Volume of Nâ€Heterocyclic Carbene Ligands. European Journal of Inorganic Chemistry, 2009, 2009, 1759-1766.	1.0	717
3	Towards the online computer-aided design of catalytic pockets. Nature Chemistry, 2019, 11, 872-879.	6.6	710
4	SambVca 2. A Web Tool for Analyzing Catalytic Pockets with Topographic Steric Maps. Organometallics, 2016, 35, 2286-2293.	1.1	658
5	Understanding the M(NHC) (NHC=N-heterocyclic carbene) bond. Coordination Chemistry Reviews, 2009, 253, 687-703.	9.5	651
6	Steric and Electronic Properties of N-Heterocyclic Carbenes (NHC):Â A Detailed Study on Their Interaction with Ni(CO)4. Journal of the American Chemical Society, 2005, 127, 2485-2495.	6.6	591
7	Determination of N-Heterocyclic Carbene (NHC) Steric and Electronic Parameters using the [(NHC)Ir(CO)₂Cl] System. Organometallics, 2008, 27, 202-210.	1.1	541
8	Steric and electronic effects in the bonding of N-heterocyclic ligands to transition metals. Journal of Organometallic Chemistry, 2005, 690, 5407-5413.	0.8	431
9	A Highly Selective Copperâ€“Indium Bimetallic Electrocatalyst for the Electrochemical Reduction of Aqueous CO₂ to CO. Angewandte Chemie - International Edition, 2015, 54, 2146-2150.	7.2	403
10	Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method [DLPNO-CCSD(T)]. Journal of Chemical Physics, 2018, 148, 011101.	1.2	402
11	A Combined Experimental and Theoretical Study Examining the Binding of N-Heterocyclic Carbenes (NHC) to the Cp*RuCl (Cp* = Î·5-C5Me5) Moiety:â€‰ Insight into Stereoelectronic Differences between Unsaturated and Saturated NHC Ligands. Organometallics, 2003, 22, 4322-4326.	1.1	400
12	High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. Nature Catalysis, 2020, 3, 985-992.	16.1	390
13	Cuâ€“Sn Bimetallic Catalyst for Selective Aqueous Electroreduction of CO₂ to CO. ACS Catalysis, 2016, 6, 2842-2851.	5.5	380
14	2D Nanomaterials for Photocatalytic Hydrogen Production. ACS Energy Letters, 2019, 4, 1687-1709.	8.8	375
15	Aqueous Zinc-Ion Storage in MoS₂ by Tuning the Intercalation Energy. Nano Letters, 2019, 19, 3199-3206.	4.5	362
16	(NHC)Copper(I)-Catalyzed [3+2] Cycloaddition of Azides and Mono- or Disubstituted Alkynes. Chemistry - A European Journal, 2006, 12, 7558-7564.	1.7	343
17	The Role of Bulky Substituents in Brookhart-Type Ni(II) Diimine Catalyzed Olefin Polymerization:Â A Combined Density Functional Theory and Molecular Mechanics Study. Journal of the American Chemical Society, 1997, 119, 6177-6186.	6.6	334
18	Synthetic and Structural Studies of (NHC)Pd(allyl)Cl Complexes (NHC =N-heterocyclic carbene). Organometallics, 2004, 23, 1629-1635.	1.1	296

#	Article	IF	Citations
19	Interaction of a BulkyN-Heterocyclic Carbene Ligand with Rh(I) and Ir(I). Double Câ^'H Activation and Isolation of Bare 14-Electron Rh(III) and Ir(III) Complexes. Journal of the American Chemical Society, 2005, 127, 3516-3526.	6.6	285
20	Golden Carousel in Catalysis: The Cationic Gold/Propargylic Ester Cycle. Angewandte Chemie - International Edition, 2008, 47, 718-721.	7.2	265
21	MoS₂ Polymorphic Engineering Enhances Selectivity in the Electrochemical Reduction of Nitrogen to Ammonia. ACS Energy Letters, 2019, 4, 430-435.	8.8	261
22	COCOMAPS: a web application to analyze and visualize contacts at the interface of biomolecular complexes. Bioinformatics, 2011, 27, 2915-2916.	1.8	253
23	Mechanism of Ruthenium-Catalyzed Olefin Metathesis Reactions from a Theoretical Perspective. Journal of the American Chemical Society, 2002, 124, 8965-8973.	6.6	250
24	What can NMR spectroscopy of selenoureas and phosphinidenes teach us about the Ï€-accepting abilities of N-heterocyclic carbenes?. Chemical Science, 2015, 6, 1895-1904.	3.7	244
25	Do New Century Catalysts Unravel the Mechanism of Stereocontrol of Old Zieglerâ^'Natta Catalysts?. Accounts of Chemical Research, 2004, 37, 231-241.	7.6	232
26	Recognizing the Mechanism of Sulfurized Polyacrylonitrile Cathode Materials for Liâ€“S Batteries and beyond in Alâ€“S Batteries. ACS Energy Letters, 2018, 3, 2899-2907.	8.8	224
27	The structure and binding mode of citrate in the stabilization of gold nanoparticles. Nature Chemistry, 2017, 9, 890-895.	6.6	222
28	New Insights on Graphite Anode Stability in Rechargeable Batteries: Li Ion Coordination Structures Prevail over Solid Electrolyte Interphases. ACS Energy Letters, 2018, 3, 335-340.	8.8	217
29	Thermodynamics of N-Heterocyclic Carbene Dimerization: The Balance of Sterics and Electronics. Organometallics, 2008, 27, 2679-2681.	1.1	213
30	POPS: a fast algorithm for solvent accessible surface areas at atomic and residue level. Nucleic Acids Research, 2003, 31, 3364-3366.	6.5	212
31	Rational Electrodeâ€“Electrolyte Design for Efficient Ammonia Electrosynthesis under Ambient Conditions. ACS Energy Letters, 2018, 3, 1219-1224.	8.8	204
32	The Comparison between Single Atom Catalysis and Surface Organometallic Catalysis. Chemical Reviews, 2020, 120, 734-813.	23.0	201
33	Lewis pair polymerization by classical and frustrated Lewis pairs: acid, base and monomer scope and polymerization mechanism. Dalton Transactions, 2012, 41, 9119.	1.6	191
34	Ï€-Acidity and Ï€-basicity of N-heterocyclic carbene ligands. A computational assessment. Journal of Organometallic Chemistry, 2006, 691, 4350-4358.	0.8	184
35	Comparing the Enantioselective Power of Steric and Electrostatic Effects in Transitionâ€Metalâ€Catalyzed Asymmetric Synthesis. Chemistry - A European Journal, 2010, 16, 14348-14353.	1.7	182
36	Electronic Properties of N-Heterocyclic Carbene (NHC) Ligands:â€‰ Synthetic, Structural, and Spectroscopic Studies of (NHC)Platinum(II) Complexes. Organometallics, 2007, 26, 5880-5889.	1.1	181

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37	Solution processable metalâ€“organic frameworks for mixed matrix membranes using porous liquids. Nature Materials, 2020, 19, 1346-1353.	13.3	181
38	Phenanthroline Covalent Organic Framework Electrodes for High-Performance Zinc-Ion Supercapattery. ACS Energy Letters, 2020, 5, 2256-2264.	8.8	175
39	Shape and Volume of Cavities in Thermoplastic Molecular Sieves Based on Syndiotactic Polystyrene. Chemistry of Materials, 2001, 13, 1506-1511.	3.2	174
40	Feasibility of N₂ Binding and Reduction to Ammonia on Feâ€Deposited MoS₂ 2D Sheets: A DFT Study. Chemistry - A European Journal, 2017, 23, 8275-8279.	1.7	173
41	[Pd(IPr*)(cinnamyl)Cl]: An Efficient Preâ€catalyst for the Preparation of Tetraâ€orthoâ€substituted Biaryls by Suzukiâ€“Miyaura Crossâ€Coupling. Chemistry - A European Journal, 2012, 18, 4517-4521.	1.7	164
42	Flexibility of N-Heterocyclic Carbene Ligands in Ruthenium Complexes Relevant to Olefin Metathesis and Their Impact in the First Coordination Sphere of the Metal. Journal of the American Chemical Society, 2010, 132, 4249-4258.	6.6	162
43	A Siteâ€Selective Doping Strategy of Carbon Anodes with Remarkable Kâ€Ion Storage Capacity. Angewandte Chemie - International Edition, 2020, 59, 4448-4455.	7.2	162
44	New Insight on the Role of Electrolyte Additives in Rechargeable Lithium Ion Batteries. ACS Energy Letters, 2019, 4, 2613-2622.	8.8	160
45	Ascorbic Acid as a Bifunctional Hydrogen Bond Donor for the Synthesis of Cyclic Carbonates from CO₂ under Ambient Conditions. ACS Sustainable Chemistry and Engineering, 2017, 5, 6392-6397.	3.2	156
46	A possible model for the stereospecificity in the syndiospecific polymerization of propene with group 4a metallocenes. Macromolecules, 1991, 24, 1784-1790.	2.2	154
47	Ligand-Controlled Chemoselective C(acyl)â€“O Bond vs C(aryl)â€“C Bond Activation of Aromatic Esters in Nickel Catalyzed C(sp²)â€“C(sp³) Cross-Couplings. Journal of the American Chemical Society, 2018, 140, 3724-3735.	6.6	154
48	Molecular Engineering of Covalent Organic Framework Cathodes for Enhanced Zincâ€Ion Batteries. Advanced Materials, 2021, 33, e2103617.	11.1	151
49	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	1.5	148
50	Hydrogenation of CO₂â€Derived Carbonates and Polycarbonates to Methanol and Diols by Metalâ€“Ligand Cooperative Manganese Catalysis. Angewandte Chemie - International Edition, 2018, 57, 13439-13443.	7.2	147
51	Implementation of the IMOMM methodology for performing combined QM/MM molecular dynamics simulations and frequency calculations. Theoretical Chemistry Accounts, 1998, 100, 307-313.	0.5	145
52	Key Elements in the Structure and Function Relationship of the MgCl₂/TiCl₄/Lewis Base Zieglerâ^'Natta Catalytic System. Macromolecules, 2007, 40, 9181-9189.	2.2	145
53	Selective Reduction of CO₂ to CH₄ by Tandem Hydrosilylation with Mixed Al/B Catalysts. Journal of the American Chemical Society, 2016, 138, 5321-5333.	6.6	140
54	Energyâ€Efficient Nitrogen Reduction to Ammonia at Low Overpotential in Aqueous Electrolyte under Ambient Conditions. ChemSusChem, 2018, 11, 3416-3422.	3.6	140

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55	Mechanistic Features of Isomerizing Alkoxycarbonylation of Methyl Oleate. Journal of the American Chemical Society, 2012, 134, 17696-17703.	6.6	137
56	Electrolyte Engineering Enables High Stability and Capacity Alloying Anodes for Sodium and Potassium Ion Batteries. ACS Energy Letters, 2020, 5, 766-776.	8.8	134
57	The Quest for Converting Biorenewable Bifunctional Î±-Methylene-Î³-butyrolactone into Degradable and Recyclable Polyester: Controlling Vinyl-Addition/Ring-Opening/Cross-Linking Pathways. Journal of the American Chemical Society, 2016, 138, 14326-14337.	6.6	132
58	Nickel-catalyzed Câ€“N bond activation: activated primary amines as alkylating reagents in reductive cross-coupling. Chemical Science, 2019, 10, 4430-4435.	3.7	131
59	The Elusive Mechanism of Olefin Metathesis Promoted by (NHC)Ru-Based Catalysts:Â A Trade between Steric, Electronic, and Solvent Effects. Journal of the American Chemical Society, 2006, 128, 13352-13353.	6.6	129
60	Goldâ€•and Platinumâ€Catalyzed Cycloisomerization of Enynyl Esters versus Allenenyl Esters: An Experimental and Theoretical Study. Chemistry - A European Journal, 2009, 15, 3243-3260.	1.7	129
61	Geometry and Stability of Titanium Chloride Species Adsorbed on the (100) and (110) Cuts of the MgCl2Support of the Heterogeneous Zieglerâ^'Natta Catalysts. Macromolecules, 2000, 33, 8953-8962.	2.2	127
62	Cooperative Effect of Monopodal Silica-Supported Niobium Complex Pairs Enhancing Catalytic Cyclic Carbonate Production. Journal of the American Chemical Society, 2015, 137, 7728-7739.	6.6	123
63	A multicomponent synthesis of stereodefined olefins via nickel catalysis and single electron/triplet energy transfer. Nature Catalysis, 2019, 2, 678-687.	16.1	123
64	Interfacial Model Deciphering Highâ€Voltage Electrolytes for High Energy Density, High Safety, and Fastâ€Charging Lithiumâ€Ion Batteries. Advanced Materials, 2021, 33, e2102964.	11.1	122
65	Synthesis of 3â€Fluoroâ€3â€aryl Oxindoles: Direct Enantioselective Î±â€…Arylation of Amides. Angewandte Chemie - International Edition, 2012, 51, 2870-2873.	7.2	121
66	Computational modeling of heterogeneous Ziegler-Natta catalysts for olefins polymerization. Progress in Polymer Science, 2018, 84, 89-114.	11.8	120
67	Molecular-Scale Interfacial Model for Predicting Electrode Performance in Rechargeable Batteries. ACS Energy Letters, 2019, 4, 1584-1593.	8.8	117
68	Thermoplastic Molecular Sieves. Chemistry of Materials, 2000, 12, 363-368.	3.2	116
69	Origin of Enantioselectivity in the Asymmetric Ru-Catalyzed Metathesis of Olefins. Journal of the American Chemical Society, 2004, 126, 9592-9600.	6.6	116
70	Selectivity Switch in the Synthesis of Vinylgold(I) Intermediates. Organometallics, 2011, 30, 6328-6337.	1.1	116
71	Bifunctional (Cyclopentadienone)Ironâ€“Tricarbonyl Complexes: Synthesis, Computational Studies and Application in Reductive Amination. Chemistry - A European Journal, 2013, 19, 17881-17890.	1.7	115
72	A Comprehensive Mechanistic Picture of the Isomerizing Alkoxycarbonylation of Plant Oils. Journal of the American Chemical Society, 2014, 136, 16871-16881.	6.6	114

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73	[{Au(IPr)}₂(Î¼â€OH)]X Complexes: Synthetic, Structural and Catalytic Studies. Chemistry - A European Journal, 2011, 17, 1238-1246.	1.7	111
74	Mechanisms of Propagation and Termination Reactions in Classical Heterogeneous Zieglerâ^'Natta Catalytic Systems:Â A Nonlocal Density Functional Study. Journal of the American Chemical Society, 1998, 120, 2428-2436.	6.6	109
75	Identification and Characterization of a New Family of Catalytically Highly Active Imidazolin-2-ylidenes. Journal of the American Chemical Society, 2008, 130, 6848-6858.	6.6	105
76	Enhancing Charge Carrier Lifetime in Metal Oxide Photoelectrodes through Mild Hydrogen Treatment. Advanced Energy Materials, 2017, 7, 1701536.	10.2	104
77	Enantioselectivity in the Regioirregular Placements and Regiospecificity in the Isospecific Polymerization of Propene with Homogeneous Ziegler-Natta Catalysts. Journal of the American Chemical Society, 1994, 116, 2988-2995.	6.6	103
78	[OSSO]-Type Iron(III) Complexes for the Low-Pressure Reaction of Carbon Dioxide with Epoxides: Catalytic Activity, Reaction Kinetics, and Computational Study. ACS Catalysis, 2018, 8, 6882-6893.	5.5	103
79	Oxidative Addition to Palladium(0) Made Easy through Photoexcitedâ€State Metal Catalysis: Experiment and Computation. Angewandte Chemie - International Edition, 2019, 58, 3412-3416.	7.2	103
80	Relationship between Regiospecificity and Type of Stereospecificity in Propene Polymerization with Zirconocene-Based Catalysts1. Journal of the American Chemical Society, 1997, 119, 4394-4403.	6.6	102
81	Substrate Lattice-Guided Seed Formation Controls the Orientation of 2D Transition-Metal Dichalcogenides. ACS Nano, 2017, 11, 9215-9222.	7.3	102
82	Mechanistic Insights on Acrylate Insertion Polymerization. Journal of the American Chemical Society, 2010, 132, 4418-4426.	6.6	101
83	High-performance pan-tactic polythioesters with intrinsic crystallinity and chemical recyclability. Science Advances, 2020, 6, eabc0495.	4.7	101
84	Efficient and simultaneous capture of iodine and methyl iodide achieved by a covalent organic framework. Nature Communications, 2022, 13, .	5.8	101
85	3D Crumpled Ultrathin 1T MoS₂ for Inkjet Printing of Mg-Ion Asymmetric Micro-supercapacitors. ACS Nano, 2020, 14, 7308-7318.	7.3	100
86	Generation of Cuâ€“In alloy surfaces from CuInO₂as selective catalytic sites for CO₂electroreduction. Journal of Materials Chemistry A, 2015, 3, 19085-19092.	5.2	99
87	Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	1.5	99
88	Unraveling the New Role of an Ethylene Carbonate Solvation Shell in Rechargeable Metal Ion Batteries. ACS Energy Letters, 2021, 6, 69-78.	8.8	99
89	A Possible Mechanism for Enantioselectivity in the Chiral Epoxidation of Olefins with [Mn(salen)] Catalysts. Chemistry - A European Journal, 2001, 7, 800-807.	1.7	98
90	Doping-Induced Anisotropic Self-Assembly of Silver Icosahedra in [Pt₂Ag₂₃Cl₇(PPh₃)₁₀] Nanoclusters. Journal of the American Chemical Society, 2017, 139, 1053-1056.	6.6	98

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91	Site Chirality as a Messenger in Chain-End Stereocontrolled Propene Polymerization. Journal of the American Chemical Society, 2002, 124, 13368-13369.	6.6	96
92	The Isolation of [Pd{OC(O)H}(H)(NHC)(PR₃)] (NHC = N-Heterocyclic Carbene) and Its Role in Alkene and Alkyne Reductions Using Formic Acid. Journal of the American Chemical Society, 2013, 135, 4588-4591.	6.6	96
93	The Activation Mechanism of Ruâ€“Indenylidene Complexes in Olefin Metathesis. Journal of the American Chemical Society, 2013, 135, 7073-7079.	6.6	96
94	Toward a Unified Model Explaining Heterogeneous Zieglerâ€“Natta Catalysis. ACS Catalysis, 2015, 5, 5431-5435.	5.5	96
95	Electrolyteâ€Mediated Stabilization of Highâ€Capacity Microâ€Sized Antimony Anodes for Potassiumâ€Ion Batteries. Advanced Materials, 2021, 33, e2005993.	11.1	96
96	Blue-Emitting Dinuclear N-heterocyclic Dicarbene Gold(I) Complex Featuring a Nearly Unit Quantum Yield. Inorganic Chemistry, 2012, 51, 1778-1784.	1.9	95
97	Preferred Orientation of TiN Coatings Enables Stable Zinc Anodes. ACS Energy Letters, 2022, 7, 197-203.	8.8	95
98	Parameter optimized surfaces (POPS): analysis of key interactions and conformational changes in the ribosome. Nucleic Acids Research, 2002, 30, 2950-2960.	6.5	94
99	Magnesiumâ€Catalyzed Hydroboration of Terminal and Internal Alkynes. Angewandte Chemie - International Edition, 2019, 58, 7025-7029.	7.2	94
100	Back-Skip of the Growing Chain at Model Complexes for the Metallocene Polymerization Catalysis. Macromolecules, 1996, 29, 4834-4845.	2.2	91
101	Moving up and down the Titanium Oxidation State in Zieglerâ^'Natta Catalysis. Macromolecules, 2011, 44, 778-783.	2.2	91
102	Organocatalytic Conjugate-Addition Polymerization of Linear and Cyclic Acrylic Monomers by N-Heterocyclic Carbenes: Mechanisms of Chain Initiation, Propagation, and Termination. Journal of the American Chemical Society, 2013, 135, 17925-17942.	6.6	91
103	Enantioselective Polymerization of Epoxides Using Biaryl-Linked Bimetallic Cobalt Catalysts: A Mechanistic Study. Journal of the American Chemical Society, 2013, 135, 18901-18911.	6.6	91
104	Assessing the pK_aâ€Dependent Activity of Hydroxyl Hydrogen Bond Donors in the Organocatalyzed Cycloaddition of Carbon Dioxide to Epoxides: Experimental and Theoretical Study. Advanced Synthesis and Catalysis, 2019, 361, 366-373.	2.1	91
105	Electronic Effects in (salen)Mn-Based Epoxidation Catalysts. Journal of Organic Chemistry, 2003, 68, 6202-6207.	1.7	90
106	Mixed Phosphite/N-Heterocyclic Carbene Complexes: Synthesis, Characterization and Catalytic Studies. Organometallics, 2010, 29, 1443-1450.	1.1	90
107	Roomâ€Temperature Synthesis of Tetraâ€orthoâ€Substituted Biaryls by NHCâ€Catalyzed Suzukiâ€“Miyaura Couplings. Chemistry - A European Journal, 2011, 17, 12886-12890.	1.7	90
108	Theoretical Investigation of Active Sites at the Corners of MgCl₂ Crystallites in Supported Zieglerâ€“Natta Catalysts. Macromolecules, 2012, 45, 3695-3701.	2.2	90

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109	Highly Chemo- and Stereoselective Transfer Semihydrogenation of Alkynes Catalyzed by a Stable, Well-Defined Manganese(II) Complex. ACS Catalysis, 2018, 8, 4103-4109.	5.5	90
110	In-operando elucidation of bimetallic CoNi nanoparticles during high-temperature CH4/CO2 reaction. Applied Catalysis B: Environmental, 2017, 213, 177-189.	10.8	88
111	Turning a Methanation Co Catalyst into an Inâ€“Co Methanol Producer. ACS Catalysis, 2019, 9, 6910-6918.	5.5	88
112	Model-Based Design of Graphite-Compatible Electrolytes in Potassium-Ion Batteries. ACS Energy Letters, 2020, 5, 2651-2661.	8.8	88
113	Chain Propagation and Termination Mechanisms for Polymerization of Conjugated Polar Alkenes by [Al]-Based Frustrated Lewis Pairs. Macromolecules, 2014, 47, 7765-7774.	2.2	87
114	Tuning the properties of visible-light-responsive tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first-principles viewpoint. Physical Chemistry Chemical Physics, 2014, 16, 20548-20560.	1.3	86
115	Radical Intermediates in the Jacobsen - Katsuki Epoxidation. Angewandte Chemie - International Edition, 2000, 39, 589-592.	7.2	85
116	â€œLivingâ€•Propene Polymerization with Bis(phenoxyimine) Group 4 Metal Catalysts:Â New Strategies and Old Concepts. Organometallics, 2004, 23, 5989-5993.	1.1	85
117	Accuracy of DLPNOâ€“CCSD(T) Method for Noncovalent Bond Dissociation Enthalpies from Coinage Metal Cation Complexes. Journal of Chemical Theory and Computation, 2015, 11, 4664-4676.	2.3	85
118	Origin of the Regiochemistry of Propene Insertion at Octahedral Column 4 Polymerization Catalysts:Â Design or Serendipity?. Journal of the American Chemical Society, 2003, 125, 7172-7173.	6.6	83
119	Influence of 1,3-Diethers on the Stereospecificity of Propene Polymerization by Supported Zieglerâ^'Natta Catalysts. A Theoretical Investigation on Their Adsorption on (110) and (100) Lateral Cuts of MgCl2Platelets. Macromolecules, 2000, 33, 1134-1140.	2.2	82
120	[Pd(NHC)(allyl)Cl] Complexes: Synthesis and Determination of the NHC Percent Buried Volume (%V_{bur}) Steric Parameter. European Journal of Inorganic Chemistry, 2009, 2009, 1767-1773.	1.0	82
121	Model catalytic sites for olefin polymerization and diastereoselectivity in the cyclopolymerization of 1,5-hexadiene. Macromolecules, 1993, 26, 260-267.	2.2	81
122	Control of Chain Walking by Weak Neighboring Group Interactions in Unsymmetrical Catalysts. Journal of the American Chemical Society, 2018, 140, 1305-1312.	6.6	80
123	Accurate energies of hydrogen bonded nucleic acid base pairs and triplets in tRNA tertiary interactions. Nucleic Acids Research, 2006, 34, 865-879.	6.5	79
124	Mg²⁺ binding and archaeosine modification stabilize the G15â€“C48 Levitt base pair in tRNAs. Rna, 2007, 13, 1427-1436.	1.6	79
125	The Doping Effect of Fluorinated Aromatic Solvents on the Rate of Rutheniumâ€Catalysed Olefin Metathesis. Chemistry - A European Journal, 2011, 17, 12981-12993.	1.7	79
126	A Density Functional and Molecular Mechanics Study Of Î²-Hydrogen Transfer in Homogeneous Zieglerâ^'Natta Catalysis. Macromolecules, 1996, 29, 2729-2737.	2.2	78

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127	Mechanistic Study of Suzukiâ€“Miyaura Crossâ€Coupling Reactions of Amides Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. ChemCatChem, 2018, 10, 3096-3106.	1.8	78
128	Engineering Sodium-Ion Solvation Structure to Stabilize Sodium Anodes: Universal Strategy for Fast-Charging and Safer Sodium-Ion Batteries. Nano Letters, 2020, 20, 3247-3254.	4.5	78
129	Breaking the regioselectivity rule for acrylate insertion in the Mizorokiâ€“Heck reaction. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 8955-8959.	3.3	77
130	The Right Computational Recipe for Olefin Metathesis with Ru-Based Catalysts: The Whole Mechanism of Ring-Closing Olefin Metathesis. Journal of Chemical Theory and Computation, 2014, 10, 4442-4448.	2.3	77
131	Additives Engineered Nonflammable Electrolyte for Safer Potassium Ion Batteries. Advanced Functional Materials, 2020, 30, 2001934.	7.8	77
132	Modeling the structureâ€property relationships of nanoneedles: A journey toward nanomedicine. Journal of Computational Chemistry, 2009, 30, 275-284.	1.5	76
133	Supramolecular Water Oxidation with Ruâ€“bdaâ€Based Catalysts. Chemistry - A European Journal, 2014, 20, 17282-17286.	1.7	76
134	Tailoring the Crystal Structure of Nanoclusters Unveiled High Photoluminescence via Ion Pairing. Chemistry of Materials, 2018, 30, 2719-2725.	3.2	76
135	Amino acid ionic liquids as potential candidates for CO2 capture: Combined density functional theory and molecular dynamics simulations. Chemical Physics Letters, 2020, 745, 137239.	1.2	76
136	Gold(i)-catalyzed synthesis of furans and pyrroles via alkyne hydration. Catalysis Science and Technology, 2011, 1, 58.	2.1	75
137	How does the addition of steric hindrance to a typical N-heterocyclic carbene ligand affect catalytic activity in olefin metathesis?. Dalton Transactions, 2013, 42, 7433.	1.6	75
138	Role of Oxidized Mo Species on the Active Surface of Niâ€“Mo Electrocatalysts for Hydrogen Evolution under Alkaline Conditions. ACS Catalysis, 2020, 10, 12858-12866.	5.5	75
139	Coordinatively Unsaturated Ruthenium Complexes As Efficient Alkyneâ€“Azide Cycloaddition Catalysts. Organometallics, 2012, 31, 756-767.	1.1	74
140	Coupling of Carbon Dioxide with Epoxides Efficiently Catalyzed by Thioetherâ€Triphenolate Bimetallic Iron(III) Complexes: Catalyst Structureâ€“Reactivity Relationship and Mechanistic DFT Study. Advanced Synthesis and Catalysis, 2016, 358, 3231-3243.	2.1	74
141	Prediction of protein assemblies, the next frontier: The <scp>CASP14â€CAPRI</scp> experiment. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1800-1823.	1.5	73
142	Propene Polymerization with the Isospecific, Highly Regioselectiverac-Me2C(3-t-Bu-1-Ind)2ZrCl2/MAO Catalyst. 2. Combined DFT/MM Analysis of Chain Propagation and Chain Release Reactions. Organometallics, 2001, 20, 1918-1931.	1.1	72
143	Model-Based Design of Stable Electrolytes for Potassium Ion Batteries. ACS Energy Letters, 2020, 5, 3124-3131.	8.8	71
144	Mechanistic Insights into the cisâ€“trans Isomerization of Ruthenium Complexes Relevant to Catalysis of Olefin Metathesis. Chemistry - A European Journal, 2010, 16, 14354-14364.	1.7	70

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