

Luigi Cavallo

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/3064882/luigi-cavallo-publications-by-year.pdf>

Version: 2024-04-24

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

545
papers

27,270
citations

80
h-index

138
g-index

586
ext. papers

31,575
ext. citations

8.2
avg, IF

7.42
L-index

#	Paper	IF	Citations
545	Preferred Orientation of TiN Coatings Enables Stable Zinc Anodes. <i>ACS Energy Letters</i> , 2022 , 7, 197-203	20.1	13
544	IronCobalt-Based Materials: An Efficient Bimetallic Catalyst for Ammonia Synthesis at Low Temperatures. <i>ACS Catalysis</i> , 2022 , 12, 587-599	13.1	2
543	Mechanistic insights into photochemical nickel-catalyzed cross-couplings enabled by energy transfer.. <i>Nature Communications</i> , 2022 , 13, 2737	17.4	4
542	Nickel Mediated Enantioselective Photoredox Allylation of Aldehydes with Visible Light.. <i>Angewandte Chemie - International Edition</i> , 2021 ,	16.4	8
541	Gold N-Heterocyclic Carbene Catalysts for the Hydrofluorination of Alkynes Using Hydrofluoric Acid: Reaction Scope, Mechanistic Studies and the Tracking of Elusive Intermediates. <i>Chemistry - A European Journal</i> , 2021 ,	4.8	2
540	Selectivity descriptors for the direct hydrogenation of CO to hydrocarbons during zeolite-mediated bifunctional catalysis. <i>Nature Communications</i> , 2021 , 12, 5914	17.4	7
539	[Ag(1,2-BDT)]: How Square-Pyramidal Building Blocks Self-Assemble into the Smallest Silver Nanocluster. <i>Inorganic Chemistry</i> , 2021 , 60, 4306-4312	5.1	3
538	Tungsten Blue Oxide as a Reusable Electrocatalyst for Acidic Water Oxidation by Plasma-Induced Vacancy Engineering. <i>CCS Chemistry</i> , 2021 , 3, 1553-1561	7.2	8
537	Adsorptive Molecular Sieving of Styrene over Ethylbenzene by Trianglimine Crystals. <i>Journal of the American Chemical Society</i> , 2021 , 143, 4090-4094	16.4	16
536	A Multivariate Linear Regression Approach to Predict Ethene/1-Olefin Copolymerization Statistics Promoted by Group 4 Catalysts. <i>ACS Catalysis</i> , 2021 , 11, 4061-4070	13.1	7
535	Highly Active Heterogeneous Catalyst for Ethylene Dimerization Prepared by Selectively Doping Ni on the Surface of a Zeolitic Imidazolate Framework. <i>Journal of the American Chemical Society</i> , 2021 , 143, 7144-7153	16.4	15
534	Chemically Induced Mismatch of Rings and Stations in [3]Rotaxanes. <i>Journal of the American Chemical Society</i> , 2021 , 143, 8046-8055	16.4	4
533	D936Y and Other Mutations in the Fusion Core of the SARS-CoV-2 Spike Protein Heptad Repeat 1: Frequency, Geographical Distribution, and Structural Effect. <i>Molecules</i> , 2021 , 26,	4.8	11
532	Need for Rationally Designed SnWO4 Photo(electro)catalysts to Overcome the Performance Limitations for O2 and H2 Evolution Reactions. <i>Journal of Physical Chemistry C</i> , 2021 , 125, 8488-8496	3.8	4
531	Synthesis of Gold(I)-Trifluoromethyl Complexes and their Role in Generating Spectroscopic Evidence for a Gold(I)-Difluorocarbene Species. <i>Chemistry - A European Journal</i> , 2021 , 27, 8461-8467	4.8	2
530	Fluxional bis(phenoxy-imine) Zr and Ti catalysts for polymerization. <i>Theoretical Chemistry Accounts</i> , 2021 , 140, 1	1.9	
529	Operando Elucidation on the Working State of Immobilized Fluorinated Iron Porphyrin for Selective Aqueous Electroreduction of CO2 to CO. <i>ACS Catalysis</i> , 2021 , 11, 6499-6509	13.1	6

528	Electrolyte Chemistry in 3D Metal Oxide Nanorod Arrays Deciphers Lithium Dendrite-Free Plating/Stripping Behaviors for High-Performance Lithium Batteries. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 4857-4866	6.4	11
527	Simple Synthetic Routes to Carbene-M-Amido (M=Cu, Ag, Au) Complexes for Luminescence and Photocatalysis Applications. <i>Chemistry - A European Journal</i> , 2021 , 27, 11904-11911	4.8	15
526	Influence of the anionic ligands on properties and reactivity of Hoveyda-Grubbs catalysts. <i>Molecular Catalysis</i> , 2021 , 509, 111612	3.3	1
525	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. <i>Applied Organometallic Chemistry</i> , 2021 , 35, e6362	3.1	3
524	Active and stable Fe-based catalyst, mechanism, and key role of alkali promoters in ammonia synthesis. <i>Journal of Catalysis</i> , 2021 , 394, 353-365	7.3	2
523	Unraveling the New Role of an Ethylene Carbonate Solvation Shell in Rechargeable Metal Ion Batteries. <i>ACS Energy Letters</i> , 2021 , 6, 69-78	20.1	41
522	Ambiguities in solvation free energies from cluster-continuum quasichemical theory: lithium cation in protic and aprotic solvents. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 16077-16088	3.6	4
521	Replacing thymine with a strongly pairing fifth Base: A combined quantum mechanics and molecular dynamics study. <i>Computational and Structural Biotechnology Journal</i> , 2021 , 19, 1312-1324	6.8	2
520	Suzuki-Miyaura Cross-Coupling of Esters by Selective O-C(O) Cleavage Mediated by Air- and Moisture-Stable [Pd(NHC)(ECI)Cl] Precatalysts: Catalyst Evaluation and Mechanism. <i>Catalysis Science and Technology</i> , 2021 , 11, 3189-3197	5.5	8
519	Electrolyte-Mediated Stabilization of High-Capacity Micro-Sized Antimony Anodes for Potassium-Ion Batteries. <i>Advanced Materials</i> , 2021 , 33, e2005993	24	48
518	CO ₂ hydrogenation to methanol and hydrocarbons over bifunctional Zn-doped ZrO ₂ /zeolite catalysts. <i>Catalysis Science and Technology</i> , 2021 , 11, 1249-1268	5.5	8
517	Molecular recognition and adsorptive separation of -xylene by trianglimine crystals. <i>Chemical Communications</i> , 2021 , 57, 9124-9127	5.8	3
516	Superconductivity and High-Pressure Performance of 2D MoC Crystals. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 2219-2225	6.4	1
515	Structural Insights in Mammalian Sialyltransferases and Fucosyltransferases: We Have Come a Long Way, but It Is Still a Long Way Down. <i>Molecules</i> , 2021 , 26,	4.8	5
514	Molecular Engineering of Covalent Organic Framework Cathodes for Enhanced Zinc-Ion Batteries. <i>Advanced Materials</i> , 2021 , 33, e2103617	24	31
513	Spontaneous Production of Ultrastable Reactive Oxygen Species on Titanium Oxide Surfaces Modified with Organic Ligands. <i>Advanced Materials Interfaces</i> , 2021 , 8, 2100629	4.6	2
512	Au ⁺ -H-C Hydrogen Bonds as Design Principle in Gold(I) Catalysis. <i>Angewandte Chemie - International Edition</i> , 2021 , 60, 21014-21024	16.4	17
511	Au ⁺ -H π Hydrogen Bonds as Design Principle in Gold(I) Catalysis. <i>Angewandte Chemie</i> , 2021 , 133, 21182-21192	3.6	4

510	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021 , 89, 1800-1823	4.2	17
509	Interfacial Model Deciphering High-Voltage Electrolytes for High Energy Density, High Safety, and Fast-Charging Lithium-Ion Batteries. <i>Advanced Materials</i> , 2021 , 33, e2102964	24	33
508	Illuminating the Intrinsic Effect of Water Co-feeding on Methane Dehydroaromatization: A Comprehensive Study. <i>ACS Catalysis</i> , 2021 , 11, 11671-11684	13.1	4
507	Adsorption of industrial dyes on functionalized and nonfunctionalized asphaltene: A combined molecular dynamics and quantum mechanics study. <i>Journal of Molecular Liquids</i> , 2021 , 337, 116433	6	6
506	Design, scope and mechanism of highly active and selective chiral NHC-iridium catalysts for the intramolecular hydroamination of a variety of unactivated aminoalkenes. <i>Chemical Science</i> , 2021 , 12, 3751-3767	9.4	3
505	Conversion of Pd(I) off-cycle species into highly efficient cross-coupling catalysts. <i>Dalton Transactions</i> , 2021 , 50, 5420-5427	4.3	3
504	Occurrence and stability of lone pair- and OH-interactions between water and nucleobases in functional RNAs. <i>Nucleic Acids Research</i> , 2020 , 48, 5825-5838	20.1	10
503	Precision Molecular Threading/Dethreading. <i>Angewandte Chemie</i> , 2020 , 132, 14935-14944	3.6	3
502	Precision Molecular Threading/Dethreading. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 14825-14834	14.3	20
501	3D Crumpled Ultrathin 1T MoS ₂ for Inkjet Printing of Mg-Ion Asymmetric Micro-supercapacitors. <i>ACS Nano</i> , 2020 , 14, 7308-7318	16.7	55
500	Catalysis of silica-based anode (de-)lithiation: compositional design within a hollow structure for accelerated conversion reaction kinetics. <i>Journal of Materials Chemistry A</i> , 2020 , 8, 12306-12313	13	27
499	Phenanthroline Covalent Organic Framework Electrodes for High-Performance Zinc-Ion Supercapattery. <i>ACS Energy Letters</i> , 2020 , 5, 2256-2264	20.1	74
498	Tricyclic Sulfoxide-Alkene Hybrid Ligands for Chiral Rh(I) Complexes: The Matched Diastereomer Catalyzes Asymmetric C-C Bond Formations. <i>Organometallics</i> , 2020 , 39, 1348-1359	3.8	3
497	Conversion of racemic alcohols to optically pure amine precursors enabled by catalyst dynamic kinetic resolution: experiment and computation. <i>Chemical Communications</i> , 2020 , 56, 9094-9097	5.8	3
496	Using sodium acetate for the synthesis of [Au(NHC)X] complexes. <i>Dalton Transactions</i> , 2020 , 49, 9694-9700	10	14
495	Evidence for Silica Surface Three- and Five-Membered Metallacycle Intermediates in the Catalytic Cycle of Hydroaminoalkylation of Olefins Using Single-Ti-Metal Catalysts. <i>Organometallics</i> , 2020 , 39, 2438-2445	3.8	1
494	Significant Impact of Exposed Facets on the BiVO ₄ Material Performance for Photocatalytic Water Splitting Reactions. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5497-5503	6.4	24
493	Barium-Catalysed Dehydrocoupling of Hydrosilanes and Borinic Acids: A Mechanistic Insight. <i>Chemistry - A European Journal</i> , 2020 , 26, 3445	4.8	1

492	Amino acid ionic liquids as potential candidates for CO ₂ capture: Combined density functional theory and molecular dynamics simulations. <i>Chemical Physics Letters</i> , 2020 , 745, 137239	2.5	38
491	Electrolyte Engineering Enables High Stability and Capacity Alloying Anodes for Sodium and Potassium Ion Batteries. <i>ACS Energy Letters</i> , 2020 , 5, 766-776	20.1	91
490	Hydration-Effect-Promoting Ni-Fe Oxyhydroxide Catalysts for Neutral Water Oxidation. <i>Advanced Materials</i> , 2020 , 32, e1906806	24	33
489	A Site-Selective Doping Strategy of Carbon Anodes with Remarkable K-Ion Storage Capacity. <i>Angewandte Chemie</i> , 2020 , 132, 4478-4485	3.6	26
488	Biodegradable Polyhydroxyalkanoates by Stereoselective Copolymerization of Racemic Diolides: Stereocontrol and Polyolefin-Like Properties. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 7881-7890	16.4	19
487	Bio-inspired heteroatom-doped hollow auricle-like structured carbon for high-performance sodium-ion batteries and supercapacitors. <i>Journal of Power Sources</i> , 2020 , 461, 228128	8.9	16
486	Engineering Sodium-Ion Solvation Structure to Stabilize Sodium Anodes: Universal Strategy for Fast-Charging and Safer Sodium-Ion Batteries. <i>Nano Letters</i> , 2020 , 20, 3247-3254	11.5	41
485	Gas-Phase Thermochemistry of MX and MX ₂ (M = Sc, Y; X = F, Cl, Br, I) from a Composite Reaction-Based Approach: Homolytic versus Heterolytic Cleavage. <i>Inorganic Chemistry</i> , 2020 , 59, 17084-17095	5.1	1
484	Regio, stereo and chemoselectivity of 2nd generation Grubbs ruthenium-catalyzed olefin metathesis. <i>Catalysis Today</i> , 2020 , 388-389, 394-394	5.3	6
483	Nature of Nitrogen Incorporation in BiVO ₄ Photoanodes through Chemical and Physical Methods. <i>Solar Rrl</i> , 2020 , 4, 1900290	7.1	14
482	Phenoxylation of Alkynes through Mono- and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. <i>European Journal of Inorganic Chemistry</i> , 2020 , 2020, 1123-1134	2.3	4
481	A Site-Selective Doping Strategy of Carbon Anodes with Remarkable K-Ion Storage Capacity. <i>Angewandte Chemie - International Edition</i> , 2020 , 59, 4448-4455	16.4	86
480	Buchwald-Hartwig cross-coupling of amides (transamidation) by selective N-O cleavage mediated by air- and moisture-stable [Pd(NHC)(allyl)Cl] precatalysts: catalyst evaluation and mechanism. <i>Catalysis Science and Technology</i> , 2020 , 10, 710-716	5.5	35
479	Barium-Catalysed Dehydrocoupling of Hydrosilanes and Borinic Acids: A Mechanistic Insight. <i>Chemistry - A European Journal</i> , 2020 , 26, 3535-3544	4.8	4
478	The CASP13-CAPRI targets as case studies to illustrate a novel scoring pipeline integrating CONSRANK with clustering and interface analyses. <i>BMC Bioinformatics</i> , 2020 , 21, 262	3.6	1
477	High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. <i>Nature Catalysis</i> , 2020 , 3, 985-992	36.5	149
476	Methane dry reforming on supported cobalt nanoparticles promoted by boron. <i>Journal of Catalysis</i> , 2020 , 392, 126-134	7.3	11
475	Role of Oxidized Mo Species on the Active Surface of NiMo Electro catalysts for Hydrogen Evolution under Alkaline Conditions. <i>ACS Catalysis</i> , 2020 , 10, 12858-12866	13.1	24

474	Enzymatic Formation of an Artificial Base Pair Using a Modified Purine Nucleoside Triphosphate. <i>ACS Chemical Biology</i> , 2020 , 15, 2872-2884	4.9	10
473	In silico design of novel NRR electrocatalysts: cobalt-molybdenum alloys. <i>Chemical Communications</i> , 2020 , 56, 13343-13346	5.8	6
472	The role of noncovalent interactions in olefin polymerization catalysis: a further look to the fluorinated ligand effect. <i>Molecular Catalysis</i> , 2020 , 494, 111118	3.3	2
471	Regiodivergent Hydroborative Ring Opening of Epoxides via Selective C-O Bond Activation. <i>Journal of the American Chemical Society</i> , 2020 , 142, 14286-14294	16.4	19
470	Plasticity of NHCs on the Ruthenium Phosphine and Ruthenium Ylidene Bonds in Olefin Metathesis Catalysts. <i>Organometallics</i> , 2020 , 39, 3972-3982	3.8	4
469	Optically Pure β -Symmetric Cyclic(alkyl)(amino)carbene Ruthenium Complexes for Asymmetric Olefin Metathesis. <i>Journal of the American Chemical Society</i> , 2020 , 142, 19895-19901	16.4	12
468	Solution processable metal-organic frameworks for mixed matrix membranes using porous liquids. <i>Nature Materials</i> , 2020 , 19, 1346-1353	27	78
467	Model-Based Design of Graphite-Compatible Electrolytes in Potassium-Ion Batteries. <i>ACS Energy Letters</i> , 2020 , 5, 2651-2661	20.1	49
466	Remarkable Influence of β - SnWO_4 Exposed Facets on Their Photocatalytic Performance for H_2 and O_2 Evolution Reactions. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 18684-18689	3.8	6
465	From Capsule to Helix: Guest-Induced Superstructures of Chiral Macrocyclic Crystals. <i>Journal of the American Chemical Society</i> , 2020 , 142, 15823-15829	16.4	13
464	[Pd(NHC)(ECI)Cl]: Versatile and Highly Reactive Complexes for Cross-Coupling Reactions that Avoid Formation of Inactive Pd(I) Off-Cycle Products. <i>IScience</i> , 2020 , 23, 101377	6.1	24
463	Thermochemistry of 5,10,15,20-tetraphenylporphyrin. <i>Journal of Chemical Thermodynamics</i> , 2020 , 151, 106244	2.9	3
462	Model-Based Design of Stable Electrolytes for Potassium Ion Batteries. <i>ACS Energy Letters</i> , 2020 , 5, 3124-3131	23.1	32
461	The anticancer activity of an air-stable Pd(II)-NHC (NHC = N-heterocyclic carbene) dimer. <i>Chemical Communications</i> , 2020 , 56, 12238-12241	5.8	14
460	Metathesis of Classical and Functionalized Olefins Catalyzed by Silica-Supported Single-Site Well-Defined W and Mo Pre-catalysts. <i>ChemCatChem</i> , 2020 , 12, 6067-6075	5.2	4
459	Additives Engineered Nonflammable Electrolyte for Safer Potassium Ion Batteries. <i>Advanced Functional Materials</i> , 2020 , 30, 2001934	15.6	37
458	Mechanistic Insight into the Photoredox-Nickel-HAT Triple Catalyzed Arylation and Alkylation of β -Amino C-H Bonds. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16942-16952	16.4	27
457	Extension of Surface Organometallic Chemistry to Metal-Organic Frameworks: Development of a Well-Defined Single Site [(η -Zr-O)-W(η -O)(CHBu)] Olefin Metathesis Catalyst. <i>Journal of the American Chemical Society</i> , 2020 , 142, 16690-16703	16.4	19

456	High-performance pan-tactic polythioesters with intrinsic crystallinity and chemical recyclability. <i>Science Advances</i> , 2020 , 6, eabc0495	14.3	31
455	The Comparison between Single Atom Catalysis and Surface Organometallic Catalysis. <i>Chemical Reviews</i> , 2020 , 120, 734-813	68.1	120
454	Iridium-Catalyzed Enantioselective Hydroarylation of Alkenes through C-H bond Activation: Experiment and Computation. <i>Chemistry - A European Journal</i> , 2020 , 26, 8308-8313	4.8	17
453	Designing an active TaN photocatalyst for H and O evolution reactions by specific exposed facet engineering: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 10295-10304	3.6	5
452	A Novel [OSSO]-Type Chromium(III) Complex as a Versatile Catalyst for Copolymerization of Carbon Dioxide with Epoxides. <i>Chemistry - A European Journal</i> , 2020 , 26, 5347-5353	4.8	7
451	A Mechanistically and Operationally Simple Route to Metal-N-Heterocyclic Carbene (NHC) Complexes. <i>Chemistry - A European Journal</i> , 2020 , 26, 4515-4519	4.8	31
450	Towards the online computer-aided design of catalytic pockets. <i>Nature Chemistry</i> , 2019 , 11, 872-879	17.6	350
449	Ligand Effects in Pd-Catalyzed Intermolecular Alkyne Hydroarylations. <i>Organometallics</i> , 2019 , 38, 3730-3739	3.6	1
448	Electrochemical Conversion of CO ₂ to 2-Bromoethanol in a Membraneless Cell. <i>ACS Energy Letters</i> , 2019 , 4, 600-605	20.1	6
447	Titelbild: Oxidative Addition to Palladium(0) Made Easy through Photoexcited-State Metal Catalysis: Experiment and Computation (Angew. Chem. 11/2019). <i>Angewandte Chemie</i> , 2019 , 131, 3263-3263	3.6	36
446	Turning a Methanation Co Catalyst into an In Situ Methanol Producer. <i>ACS Catalysis</i> , 2019 , 9, 6910-6918	13.1	54
445	Quantifying electronic similarities between NHC-gold(i) complexes and their isolobal imidazolium precursors. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 15615-15622	3.6	7
444	Gas Phase Silver Thermochemistry from First Principles. <i>Inorganic Chemistry</i> , 2019 , 58, 7873-7885	5.1	5
443	Molecular-Scale Interfacial Model for Predicting Electrode Performance in Rechargeable Batteries. <i>ACS Energy Letters</i> , 2019 , 4, 1584-1593	20.1	61
442	2D Nanomaterials for Photocatalytic Hydrogen Production. <i>ACS Energy Letters</i> , 2019 , 4, 1687-1709	20.1	212
441	Closed-Loop Polymer Upcycling by Installing Property-Enhancing Comonomer Sequences and Recyclability. <i>Macromolecules</i> , 2019 , 52, 4570-4578	5.5	24
440	Regression analysis of properties of [Au(IPr)(CHR)] complexes. <i>Dalton Transactions</i> , 2019 , 48, 7693-7703	4.3	4
439	Synthesis and reactivity of [Au(NHC)(Bpin)] complexes. <i>Chemical Communications</i> , 2019 , 55, 6799-6802	5.8	17

438	Tandem Conversion of CO ₂ to Valuable Hydrocarbons in Highly Concentrated Potassium Iron Catalysts. <i>ChemCatChem</i> , 2019 , 11, 2879-2886	5.2	37
437	Nickel-catalyzed Suzuki-Miyaura cross-couplings of aldehydes. <i>Nature Communications</i> , 2019 , 10, 1957	17.4	38
436	Unravelling the reaction mechanism for the Claisen–Ishchenko condensation catalysed by Mn(I)-PNN complexes: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2019 , 138, 1	1.9	5
435	Structural and Energetic Impact of Non-natural 7-Deaza-8-azaguanine, 7-Deaza-8-azaisoguanine, and Their 7-Substituted Derivatives on Hydrogen-Bond Pairing with Cytosine and Isocytosine. <i>ChemBioChem</i> , 2019 , 20, 2262-2270	3.8	3
434	Aqueous Zinc-Ion Storage in MoS ₂ by Tuning the Intercalation Energy. <i>Nano Letters</i> , 2019 , 19, 3199-3206	11.5	223
433	Lithium dendrite-free plating/stripping: a new synergistic lithium ion solvation structure effect for reliable lithium-sulfur full batteries. <i>Chemical Communications</i> , 2019 , 55, 5713-5716	5.8	20
432	Nickel-catalyzed C-N bond activation: activated primary amines as alkylating reagents in reductive cross-coupling. <i>Chemical Science</i> , 2019 , 10, 4430-4435	9.4	81
431	Unprecedented Diastereoselective Arylogous Michael Addition of Unactivated Phthalides. <i>Chemistry - A European Journal</i> , 2019 , 25, 7043-7043	4.8	
430	Magnesium-Catalyzed Hydroboration of Terminal and Internal Alkynes. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 7025-7029	16.4	56
429	Unprecedented Diastereoselective Arylogous Michael Addition of Unactivated Phthalides. <i>Chemistry - A European Journal</i> , 2019 , 25, 7131-7141	4.8	5
428	Evaluation of experimental alkali metal ion-ligand noncovalent bond strengths with DLPNO-CCSD(T) method. <i>Journal of Chemical Physics</i> , 2019 , 151, 014301	3.9	5
427	Mechanistic Study of Hydroamination of Alkyne through Tantalum-Based Silica-Supported Surface Species. <i>ACS Catalysis</i> , 2019 , 9, 8719-8725	13.1	8
426	A multicomponent synthesis of stereodefined olefins via nickel catalysis and single electron/triplet energy transfer. <i>Nature Catalysis</i> , 2019 , 2, 678-687	36.5	65
425	Electronic effects in mixed N-heterocyclic carbene/phosphite indenylidene ruthenium metathesis catalysts. <i>Dalton Transactions</i> , 2019 , 48, 11326-11337	4.3	6
424	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019 , 87, 1200-1221	4.2	58
423	New Insight on the Role of Electrolyte Additives in Rechargeable Lithium Ion Batteries. <i>ACS Energy Letters</i> , 2019 , 4, 2613-2622	20.1	90
422	Asymmetric Hydroboration of Heteroaryl Ketones by Aluminum Catalysis. <i>Journal of the American Chemical Society</i> , 2019 , 141, 19415-19423	16.4	22
421	Asymmetric Magnesium-Catalyzed Hydroboration by Metal-Ligand Cooperative Catalysis. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 17567-17571	16.4	27

420	Revisiting O ₂ Bond Formation through Outer-Sphere Water Molecules versus Bimolecular Mechanisms in Water-Oxidation Catalysis (WOC) by Cp*Ir Based Complexes. <i>European Journal of Inorganic Chemistry</i> , 2019 , 2019, 2093-2100	2.3	4
419	Manganese-Catalyzed Multicomponent Synthesis of Pyrroles through Acceptorless Dehydrogenation Hydrogen Autotransfer Catalysis: Experiment and Computation. <i>ChemSusChem</i> , 2019 , 12, 3083-3088	8.3	41
418	MoS ₂ Polymorphic Engineering Enhances Selectivity in the Electrochemical Reduction of Nitrogen to Ammonia. <i>ACS Energy Letters</i> , 2019 , 4, 430-435	20.1	179
417	Tungsten Catalyst Incorporating a Well-Defined Tetracoordinated Aluminum Surface Ligand for Selective Metathesis of Propane, [(<i>η</i> -SiDBi)(<i>η</i> -SiDBi)Al(<i>η</i> -CtBu)(H) ₂]. <i>ChemCatChem</i> , 2019 , 11, 614-620	5.2	1
416	Roughening of Copper (100) at Elevated CO Pressure: Cu Adatom and Cluster Formation Enable CO Dissociation. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 8112-8121	3.8	15
415	Assessing the pK _a -Dependent Activity of Hydroxyl Hydrogen Bond Donors in the Organocatalyzed Cycloaddition of Carbon Dioxide to Epoxides: Experimental and Theoretical Study. <i>Advanced Synthesis and Catalysis</i> , 2019 , 361, 366-373	5.6	61
414	Oxidative Addition to Palladium(0) Made Easy through Photoexcited-State Metal Catalysis: Experiment and Computation. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 3412-3416	16.4	60
413	Oxidative Addition to Palladium(0) Made Easy through Photoexcited-State Metal Catalysis: Experiment and Computation. <i>Angewandte Chemie</i> , 2019 , 131, 3450-3454	3.6	18
412	Mapping the minimum domain of the fibronectin binding site on transglutaminase 2 (TG2) and its importance in mediating signaling, adhesion, and migration in TG2-expressing cells. <i>FASEB Journal</i> , 2019 , 33, 2327-2342	0.9	7
411	A Robust and Cost-Efficient Scheme for Accurate Conformational Energies of Organic Molecules. <i>ChemPhysChem</i> , 2019 , 20, 92-102	3.2	14
410	Ligand-Controlled Chemoselective C(acyl)-O Bond vs C(aryl)-C Bond Activation of Aromatic Esters in Nickel Catalyzed C(sp)-C(sp) Cross-Couplings. <i>Journal of the American Chemical Society</i> , 2018 , 140, 3724-3735	16.4	114
409	Theoretical characterization of sulfur-to-selenium substitution in an emissive RNA alphabet: impact on H-bonding potential and photophysical properties. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 7678-7685 ¹³	2.6	13
408	Exploiting the interactions between the ruthenium Hoveyda-Grubbs catalyst and Al-modified mesoporous silica: the case of SBA15 KCC-1. <i>Chemical Science</i> , 2018 , 9, 3531-3537	9.4	10
407	Rational Electrode/Electrolyte Design for Efficient Ammonia Electrosynthesis under Ambient Conditions. <i>ACS Energy Letters</i> , 2018 , 3, 1219-1224	20.1	146
406	Mechanistic Study of Suzuki-Miyaura Cross-Coupling Reactions of Amides Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. <i>ChemCatChem</i> , 2018 , 10, 3096-3106	5.2	58
405	A Silica-Supported Monoalkylated Tungsten Dioxo Complex Catalyst for Olefin Metathesis. <i>ACS Catalysis</i> , 2018 , 8, 2715-2729	13.1	26
404	Metal-Free Catalytic Asymmetric Fluorination of Keto Esters Using a Combination of Hydrogen Fluoride (HF) and Oxidant: Experiment and Computation. <i>ACS Catalysis</i> , 2018 , 8, 2582-2588	13.1	44
403	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)]. <i>Journal of Chemical Physics</i> , 2018 , 148, 011101	3.9	224

402	Control of Chain Walking by Weak Neighboring Group Interactions in Unsymmetrical Catalysts. <i>Journal of the American Chemical Society</i> , 2018 , 140, 1305-1312	16.4	54
401	Energetics and dynamics of the non-natural fluorescent 4AP:DAP base pair. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 3699-3709	3.6	9
400	New Insights on Graphite Anode Stability in Rechargeable Batteries: Li Ion Coordination Structures Prevail over Solid Electrolyte Interphases. <i>ACS Energy Letters</i> , 2018 , 3, 335-340	20.1	134
399	Predicting the DNP-SENS efficiency in reactive heterogeneous catalysts from hydrophilicity. <i>Chemical Science</i> , 2018 , 9, 4866-4872	9.4	17
398	Highly Chemo- and Stereoselective Transfer Semihydrogenation of Alkynes Catalyzed by a Stable, Well-Defined Manganese(II) Complex. <i>ACS Catalysis</i> , 2018 , 8, 4103-4109	13.1	64
397	Tailoring the Crystal Structure of Nanoclusters Unveiled High Photoluminescence via Ion Pairing. <i>Chemistry of Materials</i> , 2018 , 30, 2719-2725	9.6	60
396	Insights into the Catalytic Activity of [Pd(NHC)(cin)Cl] (NHC=IPr, IPrCl, IPrBr) Complexes in the Suzuki-Miyaura Reaction. <i>ChemCatChem</i> , 2018 , 10, 601-611	5.2	14
395	Complexation of trichlorosalicylic acid with alkaline and first row transition metals as a switch for their antibacterial activity. <i>Inorganica Chimica Acta</i> , 2018 , 469, 379-386	2.7	14
394	Insights into the Impact of Native Defects on the Conductivity of CuVO Material for Photovoltaic Application: A First-Principles Computational Study. <i>ACS Omega</i> , 2018 , 3, 6605-6610	3.9	3
393	Activity enhancement via borate incorporation into a NiFe (oxy)hydroxide catalyst for electrocatalytic oxygen evolution. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 16959-16964	13	14
392	Determination of the Intrinsic Defect at the Origin of Poor H ₂ Evolution Performance of the Monoclinic BiVO ₄ Photocatalyst Using Density Functional Theory. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 18204-18211	3.8	19
391	Metathetic Oxidation of 2-Butenes to Acetaldehyde by Molecular Oxygen Using the Single-Site Olefin Metathesis Catalyst (SiO) ₂ Mo(O) ₂ . <i>ACS Catalysis</i> , 2018 , 8, 7549-7555	13.1	15
390	Manganese Catalyzed Regioselective C-H Alkylation: Experiment and Computation. <i>Organic Letters</i> , 2018 , 20, 3105-3108	6.2	47
389	Constructing Bridges between Computational Tools in Heterogeneous and Homogeneous Catalysis. <i>ACS Catalysis</i> , 2018 , 8, 5637-5656	13.1	42
388	Hydrogenation of CO ₂ -Derived Carbonates and Polycarbonates to Methanol and Diols by Metal-Ligand Cooperative Manganese Catalysis. <i>Angewandte Chemie</i> , 2018 , 130, 13627-13631	3.6	22
387	Hydrogenation of CO ₂ -Derived Carbonates and Polycarbonates to Methanol and Diols by Metal-Ligand Cooperative Manganese Catalysis. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 13439-13443	16.4	92
386	Energy-Efficient Nitrogen Reduction to Ammonia at Low Overpotential in Aqueous Electrolyte under Ambient Conditions. <i>ChemSusChem</i> , 2018 , 11, 3416-3422	8.3	92
385	Mechanism of Insertion Polymerization of Allyl Ethers. <i>Macromolecules</i> , 2018 , 51, 4525-4531	5.5	14

384	SOMC grafting of vanadium oxytriisopropoxide (VO(O Pr)) on dehydroxylated silica; analysis of surface complexes and thermal restructuring mechanism.. <i>RSC Advances</i> , 2018 , 8, 20801-20808	3.7	8
383	[OSSO]-Type Iron(III) Complexes for the Low-Pressure Reaction of Carbon Dioxide with Epoxides: Catalytic Activity, Reaction Kinetics, and Computational Study. <i>ACS Catalysis</i> , 2018 , 8, 6882-6893	13.1	69
382	Enhanced Carrier Transport and Bandgap Reduction in Sulfur-Modified BiVO ₄ Photoanodes. <i>Chemistry of Materials</i> , 2018 , 30, 8630-8638	9.6	25
381	Recognizing the Mechanism of Sulfurized Polyacrylonitrile Cathode Materials for LiS Batteries and beyond in AlS Batteries. <i>ACS Energy Letters</i> , 2018 , 3, 2899-2907	20.1	146
380	Synthesis and Characterization of Cationic Tetramethyl Tantalum(V) Complex. <i>Catalysts</i> , 2018 , 8, 507	4	1
379	Toward the Design of New Suitable Materials for Solar Water Splitting Using Density Functional Theory. <i>ACS Omega</i> , 2018 , 3, 18117-18123	3.9	10
378	The activity of indenylidene derivatives in olefin metathesis catalysts. <i>Beilstein Journal of Organic Chemistry</i> , 2018 , 14, 2956-2963	2.5	8
377	Apixaban Interacts with Haemoglobin: Effects on Its Plasma Levels. <i>Thrombosis and Haemostasis</i> , 2018 , 118, 1701-1712	7	3
376	Single-Site Molybdenum on Solid Support Materials for Catalytic Hydrogenation of N -into-NH. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 15812-15816	16.4	25
375	Energy-Efficient Nitrogen Reduction to Ammonia at Low Overpotential in Aqueous Electrolyte under Ambient Conditions. <i>ChemSusChem</i> , 2018 , 11, 3356-3356	8.3	
374	Single-Site Molybdenum on Solid Support Materials for Catalytic Hydrogenation of N ₂ -into-NH ₃ . <i>Angewandte Chemie</i> , 2018 , 130, 16038-16042	3.6	5
373	Efficient electrochemical transformation of CO to C/C chemicals on benzimidazole-functionalized copper surfaces. <i>Chemical Communications</i> , 2018 , 54, 11324-11327	5.8	27
372	Imine Metathesis Catalyzed by a Silica-Supported Hafnium Imido Complex. <i>ACS Catalysis</i> , 2018 , 8, 9440-9446	11.4	12
371	Morphology control of anatase TiO ₂ for well-defined surface chemistry. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 14362-14373	3.6	17
370	Application of Semiempirical Methods to Transition Metal Complexes: Fast Results but Hard-to-Predict Accuracy. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 3428-3439	6.4	29
369	Theoretical insights into dehydrogenative chemisorption of alkylaromatics on Pt(1 0 0) and Ni(1 0 0). <i>Journal of Catalysis</i> , 2018 , 363, 197-203	7.3	3
368	Hydrogen atom induced magnetic behaviors in two-dimensional materials: insight on origination in the model of HMoO ₃ . <i>Nanoscale</i> , 2018 , 10, 14100-14106	7.7	3
367	Computational modeling of heterogeneous Ziegler-Natta catalysts for olefins polymerization. <i>Progress in Polymer Science</i> , 2018 , 84, 89-114	29.6	72

366	Phase Inversion Strategy to Flexible Freestanding Electrode: Critical Coupling of Binders and Electrolytes for High Performance LiB Battery. <i>Advanced Functional Materials</i> , 2018 , 28, 1802244	15.6	48
365	Kinetics on NiZn Bimetallic Catalysts for Hydrogen Evolution via Selective Dehydrogenation of Methylcyclohexane to Toluene. <i>ACS Catalysis</i> , 2017 , 7, 1592-1600	13.1	34
364	Mechanism of Propylene Oxide Polymerization Promoted by N-Heterocyclic Olefins. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 2730-2737	3.8	10
363	Doping-Induced Anisotropic Self-Assembly of Silver Icosahedra in [PtAgCl(PPh)] Nanoclusters. <i>Journal of the American Chemical Society</i> , 2017 , 139, 1053-1056	16.4	67
362	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists 2017 , 225-267		1
361	Accurate Gas Phase Formation Enthalpies of Alloys and Refractories Decomposition Products. <i>Inorganic Chemistry</i> , 2017 , 56, 1386-1401	5.1	13
360	Structure-Activity Relationship To Screen NiBisphosphine Complexes for the Oxidative Coupling of CO ₂ and Ethylene. <i>Organometallics</i> , 2017 , 36, 1107-1112	3.8	15
359	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 9374-9391	3.6	36
358	Guidelines To Select the N-Heterocyclic Carbene for the Organopolymerization of Monomers with a Polar Group. <i>Macromolecules</i> , 2017 , 50, 1394-1401	5.5	19
357	Prediction of Biomolecular Complexes 2017 , 265-292		5
356	In-operando elucidation of bimetallic CoNi nanoparticles during high-temperature CH ₄ /CO ₂ reaction. <i>Applied Catalysis B: Environmental</i> , 2017 , 213, 177-189	21.8	60
355	Ab initio assessment of BiRECuOS (RE = La, Gd, Y, Lu) solid solutions as a semiconductor for photochemical water splitting. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 12321-12330	3.6	19
354	Organocatalytic Coupling of Bromo-Lactide with Cyclic Ethers and Carbonates to Chiral Bromo-Diesters: NHC or Anion Catalysis?. <i>ACS Catalysis</i> , 2017 , 7, 3929-3933	13.1	3
353	Toward better understanding of the support effect: Test cases for CO dissociation on Fe _n /TiO ₂ (1 1 0), n = 4, 5. <i>Chemical Physics Letters</i> , 2017 , 684, 30-35	2.5	1
352	Feasibility of N Binding and Reduction to Ammonia on Fe-Deposited MoS ₂ 2D Sheets: A DFT Study. <i>Chemistry - A European Journal</i> , 2017 , 23, 8275-8279	4.8	133
351	Direct versus ligand-exchange synthesis of [PtAg(BDT)(TPP)] nanoclusters: effect of a single-atom dopant on the optoelectronic and chemical properties. <i>Nanoscale</i> , 2017 , 9, 9529-9536	7.7	47
350	Mechanism of the Suzuki-Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. <i>Organometallics</i> , 2017 , 36, 2088-2095	3.8	53
349	Switchable Diastereoselectivity in the Fluoride-Promoted Vinylogous Mukaiyama-Michael Reaction of 2-[(Trimethylsilyl)oxy]furan Catalyzed by Crown Ethers. <i>Journal of Organic Chemistry</i> , 2017 , 82, 6629-6637	4.2	8

348	Conversion of actual flue gas CO ₂ via cycloaddition to propylene oxide catalyzed by a single-site, recyclable zirconium catalyst. <i>Journal of CO₂ Utilization</i> , 2017 , 20, 243-252	7.6	49
347	The structure and binding mode of citrate in the stabilization of gold nanoparticles. <i>Nature Chemistry</i> , 2017 , 9, 890-895	17.6	158
346	Well-Defined Silica Grafted Molybdenum Bis(imido) Catalysts for Imine Metathesis Reactions. <i>Organometallics</i> , 2017 , 36, 1550-1556	3.8	11
345	Impact of Interfacial Defects on the Properties of Monolayer Transition Metal Dichalcogenide Lateral Heterojunctions. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 1664-1669	6.4	22
344	Theoretical NMR spectroscopy of N-heterocyclic carbenes and their metal complexes. <i>Coordination Chemistry Reviews</i> , 2017 , 344, 101-114	23.2	21
343	Accurate experimental and theoretical enthalpies of association of TiCl ₄ with typical Lewis bases used in heterogeneous Ziegler-Natta catalysis. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 26996-27006	3.6	24
342	Experimental and Computational Study of an Unexpected Iron-Catalyzed Carboetherification by Cooperative Metal and Ligand Substrate Interaction and Proton Shuttling. <i>Angewandte Chemie</i> , 2017 , 129, 15059-15063	3.6	8
341	Investigating the Structure and Reactivity of Azolyl-Based Copper(I)NHC Complexes: The Role of the Anionic Ligand. <i>ACS Catalysis</i> , 2017 , 7, 8176-8183	13.1	12
340	Experimental and Computational Study of an Unexpected Iron-Catalyzed Carboetherification by Cooperative Metal and Ligand Substrate Interaction and Proton Shuttling. <i>Angewandte Chemie - International Edition</i> , 2017 , 56, 14863-14867	16.4	23
339	Enhancing Charge Carrier Lifetime in Metal Oxide Photoelectrodes through Mild Hydrogen Treatment. <i>Advanced Energy Materials</i> , 2017 , 7, 1701536	21.8	78
338	Exploiting Confinement Effects to Tune Selectivity in Cyclooctane Metathesis. <i>ACS Catalysis</i> , 2017 , 7, 6581-6586	13.1	13
337	N-Heterocyclic olefins as initiators for the polymerization of (meth)acrylic monomers: a combined experimental and theoretical approach. <i>Polymer Chemistry</i> , 2017 , 8, 5803-5812	4.9	21
336	Quantum confinement effect of two-dimensional all-inorganic halide perovskites. <i>Science China Materials</i> , 2017 , 60, 811-818	7.1	26
335	Ruthenium-catalysed decomposition of formic acid: Fuel cell and catalytic applications. <i>Molecular Catalysis</i> , 2017 , 440, 184-189	3.3	19
334	Inner-Sphere versus Outer-Sphere Coordination of BF ₄ ⁻ in a NHC-Gold(I) Complex. <i>Organometallics</i> , 2017 , 36, 2861-2869	3.8	19
333	Substrate Lattice-Guided Seed Formation Controls the Orientation of 2D Transition-Metal Dichalcogenides. <i>ACS Nano</i> , 2017 , 11, 9215-9222	16.7	64
332	Cycloaddition of CO ₂ to challenging N-tosyl aziridines using a halogen-free niobium complex: Catalytic activity and mechanistic insights. <i>Molecular Catalysis</i> , 2017 , 443, 280-285	3.3	21
331	Ground-State Gas-Phase Structures of Inorganic Molecules Predicted by Density Functional Theory Methods. <i>ACS Omega</i> , 2017 , 2, 8373-8387	3.9	10

330	Solar Water Splitting: Enhancing Charge Carrier Lifetime in Metal Oxide Photoelectrodes through Mild Hydrogen Treatment (Adv. Energy Mater. 22/2017). <i>Advanced Energy Materials</i> , 2017 , 7,	21.8	1
329	Heats of Formation of Medium-Sized Organic Compounds from Contemporary Electronic Structure Methods. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3537-3560	6.4	29
328	Ascorbic Acid as a Bifunctional Hydrogen Bond Donor for the Synthesis of Cyclic Carbonates from CO ₂ under Ambient Conditions. <i>ACS Sustainable Chemistry and Engineering</i> , 2017 , 5, 6392-6397	8.3	100
327	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 3220-3227	6.4	29
326	Photophysics and electrochemistry relevant to photocatalytic water splitting involved at solid-electrolyte interfaces. <i>Journal of Energy Chemistry</i> , 2017 , 26, 259-269	12	14
325	Real-time observation of intersystem crossing induced by charge recombination during bimolecular electron transfer reactions. <i>Dyes and Pigments</i> , 2017 , 136, 881-886	4.6	1
324	Clean and selective catalytic C-H alkylation of alkenes with environmental friendly alcohols. <i>Molecular Catalysis</i> , 2017 , 435, 69-75	3.3	3
323	Occurrence and stability of lone pair- π -stacking interactions between ribose and nucleobases in functional RNAs. <i>Nucleic Acids Research</i> , 2017 , 45, 11019-11032	20.1	38
322	Pesticides Curbing Soil Fertility: Effect of Complexation of Free Metal Ions. <i>Frontiers in Chemistry</i> , 2017 , 5, 43	5	34
321	Coupling of Carbon Dioxide with Epoxides Efficiently Catalyzed by Thioether-Triphenolate Bimetallic Iron(III) Complexes: Catalyst Structure-Reactivity Relationship and Mechanistic DFT Study. <i>Advanced Synthesis and Catalysis</i> , 2016 , 358, 3231-3243	5.6	62
320	Investigation of Surface Alkylation Strategy in SOMC: In Situ Generation of a Silica-Supported Tungsten Methyl Catalyst for Cyclooctane Metathesis. <i>Organometallics</i> , 2016 , 35, 2524-2531	3.8	4
319	Synthesis and characterization of a homogeneous and silica supported homoleptic cationic tungsten(vi) methyl complex: application in olefin metathesis. <i>Chemical Communications</i> , 2016 , 52, 11270-11273	5.8	1273
318	Mechanistic Insights of a Selective C-H Alkylation of Alkenes by a Ru-Based Catalyst and Alcohols. <i>ChemistrySelect</i> , 2016 , 1, 4218-4228	1.8	2
317	Selective Metathesis of Olefins from Bio-Sourced Fischer-Tropsch Feeds. <i>ACS Catalysis</i> , 2016 , 6, 7970-7976	19.1	54
316	Single-Step Access to Long-Chain α,ω -Dicarboxylic Acids by Isomerizing Hydroxycarbonylation of Unsaturated Fatty Acids. <i>ACS Catalysis</i> , 2016 , 6, 8229-8238	13.1	42
315	Solid-State NMR and DFT Studies on the Formation of Well-Defined Silica-Supported Tantalaziridines: From Synthesis to Catalytic Application. <i>Chemistry - A European Journal</i> , 2016 , 22, 3000-3	4.8	17
314	SambVca 2. A Web Tool for Analyzing Catalytic Pockets with Topographic Steric Maps. <i>Organometallics</i> , 2016 , 35, 2286-2293	3.8	468
313	An Alternative Reaction Pathway for Iridium-Catalyzed Water Oxidation Driven by Cerium Ammonium Nitrate (CAN). <i>ACS Catalysis</i> , 2016 , 6, 4559-4563	13.1	49

312	Unusual NHC-Iridium(I) Complexes and Their Use in the Intramolecular Hydroamination of Unactivated Aminoalkenes. <i>Chemistry - A European Journal</i> , 2016 , 22, 6939-46	4.8	38
311	Proton-Transfer Polymerization by N-Heterocyclic Carbenes: Monomer and Catalyst Scopes and Mechanism for Converting Dimethacrylates into Unsaturated Polyesters. <i>Journal of the American Chemical Society</i> , 2016 , 138, 2021-35	16.4	45
310	How easy is CO ₂ fixation by M π bond containing complexes (M = Cu, Ni, Co, Rh, Ir)?. <i>Organic Chemistry Frontiers</i> , 2016 , 3, 19-23	5.2	21
309	Controlling the hydrogenolysis of silica-supported tungsten pentamethyl leads to a class of highly electron deficient partially alkylated metal hydrides. <i>Chemical Science</i> , 2016 , 7, 1558-1568	9.4	45
308	Cu π Bimetallic Catalyst for Selective Aqueous Electroreduction of CO ₂ to CO. <i>ACS Catalysis</i> , 2016 , 6, 2842-2851	13.1	284
307	Theoretical Characterization of the H-Bonding and Stacking Potential of Two Nonstandard Nucleobases Expanding the Genetic Alphabet. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 2216-24	3.4	18
306	Nitrite to nitric oxide interconversion by heme FeII complex assisted by [CuI(tmpa)] ⁺ . <i>Structural Chemistry</i> , 2016 , 27, 409-417	1.8	3
305	Simple activation by acid of latent Ru-NHC-based metathesis initiators bearing 8-quinolinolate co-ligands. <i>Beilstein Journal of Organic Chemistry</i> , 2016 , 12, 154-65	2.5	12
304	The D173G mutation in ADAMTS-13 causes a severe form of congenital thrombotic thrombocytopenic purpura. A clinical, biochemical and in silico study. <i>Thrombosis and Haemostasis</i> , 2016 , 115, 51-62	7	10
303	Introducing a Clustering Step in a Consensus Approach for the Scoring of Protein-Protein Docking Models. <i>PLoS ONE</i> , 2016 , 11, e0166460	3.7	12
302	Robust Cross-Linked Stereocomplexes and C60 Inclusion Complexes of Vinyl-Functionalized Stereoregular Polymers Derived from Chemo/Stereoselective Coordination Polymerization. <i>Journal of the American Chemical Society</i> , 2016 , 138, 9533-47	16.4	26
301	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016 , 84 Suppl 1, 323-48	4.2	111
300	On the Mechanism of the Digold(I)-Hydroxide-Catalysed Hydrophenoxylation of Alkynes. <i>Chemistry - A European Journal</i> , 2016 , 22, 1125-32	4.8	41
299	In Silico Olefin Metathesis with Ru-Based Catalysts Containing N-Heterocyclic Carbenes Bearing C60 Fullerenes. <i>Chemistry - A European Journal</i> , 2016 , 22, 6617-23	4.8	9
298	Structural and energetic characterization of the emissive RNA alphabet based on the isothiazolo[4,3-d]pyrimidine heterocycle core. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 18045-53	3.6	18
297	Insights into the Halogen Oxidative Addition Reaction to Dinuclear Gold(I) Di(NHC) Complexes. <i>Chemistry - A European Journal</i> , 2016 , 22, 10211-24	4.8	21
296	NHC-Copper(I) Halide-Catalyzed Direct Alkynylation of Trifluoromethyl Ketones on Water. <i>Chemistry - A European Journal</i> , 2016 , 22, 8089-94	4.8	20
295	Suitable Fundamental Properties of TaVON Material for Visible-Light-Driven Photocatalysis: A DFT Study. <i>ACS Omega</i> , 2016 , 1, 1041-1048	3.9	12

294	Determination of the electronic, dielectric, and optical properties of sillenite Bi ₁₂ TiO ₂₀ and perovskite-like Bi ₄ Ti ₃ O ₁₂ materials from hybrid first-principle calculations. <i>Journal of Chemical Physics</i> , 2016 , 144, 134702	3.9	38
293	Catalytic β -Arylation of Imines Leading to N-Unprotected Indoles and Azaindoles. <i>ACS Catalysis</i> , 2016 , 6, 2930-2938	13.1	23
292	Troubles in the Systematic Prediction of Transition Metal Thermochemistry with Contemporary Out-of-the-Box Methods. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 1542-60	6.4	37
291	Selective Reduction of CO ₂ to CH ₄ by Tandem Hydrosilylation with Mixed A/B Catalysts. <i>Journal of the American Chemical Society</i> , 2016 , 138, 5321-33	16.4	122
290	Single-Site Tetracoordinated Aluminum Hydride Supported on Mesoporous Silica. From Dream to Reality!. <i>Organometallics</i> , 2016 , 35, 3288-3294	3.8	10
289	Mechanistic Insights into the Organopolymerization of N-Methyl N-Carboxyanhydrides Mediated by N-Heterocyclic Carbenes. <i>Macromolecules</i> , 2016 , 49, 7777-7784	5.5	5
288	The Quest for Converting Biorenewable Bifunctional β -Methylene- β -butyrolactone into Degradable and Recyclable Polyester: Controlling Vinyl-Addition/Ring-Opening/Cross-Linking Pathways. <i>Journal of the American Chemical Society</i> , 2016 , 138, 14326-14337	16.4	77
287	Synthesis, Structure and Catalytic Activity of NHC-Ag(I) Carboxylate Complexes. <i>Chemistry - A European Journal</i> , 2016 , 22, 13320-7	4.8	22
286	Tungsten(VI) Carbyne/Bis(carbene) Tautomerization Enabled by N-Donor SBA15 Surface Ligands: A Solid-State NMR and DFT Study. <i>Angewandte Chemie - International Edition</i> , 2016 , 55, 11162-6	16.4	11
285	Mechanism of the Transmetalation of Organosilanes to Gold. <i>ChemistryOpen</i> , 2016 , 5, 60-4	2.3	9
284	What can NMR spectroscopy of selenoureas and phosphinidenes teach us about the β -accepting abilities of β -heterocyclic carbenes?. <i>Chemical Science</i> , 2015 , 6, 1895-1904	9.4	201
283	A theoretical view on the thermodynamic cis/trans equilibrium of dihalo ruthenium olefin metathesis (pre-)catalysts. <i>Monatshefte für Chemie</i> , 2015 , 146, 1131-1141	1.4	21
282	Non-precious bimetallic catalysts for selective dehydrogenation of an organic chemical hydride system. <i>Chemical Communications</i> , 2015 , 51, 12931-4	5.8	22
281	Well-defined silica supported aluminum hydride: another step towards the utopian single site dream?. <i>Chemical Science</i> , 2015 , 6, 5456-5465	9.4	15
280	Mechanistic insights into the reductive dehydroxylation pathway for the biosynthesis of isoprenoids promoted by the IspH enzyme. <i>Chemical Science</i> , 2015 , 6, 5643-5651	9.4	9
279	Mechanism of the Ru π -Allenylidene to Ru π -Indenylidene Rearrangement in Ruthenium Precatalysts for Olefin Metathesis. <i>Organometallics</i> , 2015 , 34, 3107-3111	3.8	23
278	Insights into functional-group-tolerant polymerization catalysis with phosphine-sulfonamide palladium(II) complexes. <i>Chemistry - A European Journal</i> , 2015 , 21, 2062-75	4.8	21
277	Cooperative Effect of Monopodal Silica-Supported Niobium Complex Pairs Enhancing Catalytic Cyclic Carbonate Production. <i>Journal of the American Chemical Society</i> , 2015 , 137, 7728-39	16.4	100

276	Well-Defined Surface Species [(?SiD)W(?O)Me3] Prepared by Direct Methylation of [(?SiD)W(?O)Cl3], a Catalyst for Cycloalkane Metathesis and Transformation of Ethylene to Propylene. <i>ACS Catalysis</i> , 2015 , 5, 2164-2171	13.1	31
275	CONSRANK: a server for the analysis, comparison and ranking of docking models based on inter-residue contacts. <i>Bioinformatics</i> , 2015 , 31, 1481-3	7.2	28
274	Structural and Energetic Impact of Non-Natural 7-Deaza-8-Azaadenine and Its 7-Substituted Derivatives on H-Bonding Potential with Uracil in RNA Molecules. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 12982-9	3.4	13
273	An atlas of RNA base pairs involving modified nucleobases with optimal geometries and accurate energies. <i>Nucleic Acids Research</i> , 2015 , 43, 6714-29	20.1	37
272	Buried Volume Analysis for Propene Polymerization Catalysis Promoted by Group 4 Metals: A Tool for Molecular Mass Prediction. <i>ACS Catalysis</i> , 2015 , 5, 6815-6822	13.1	43
271	Generation of CuIn alloy surfaces from CuInO2 as selective catalytic sites for CO2 electroreduction. <i>Journal of Materials Chemistry A</i> , 2015 , 3, 19085-19092	13	77
270	Toward a Unified Model Explaining Heterogeneous Ziegler-Natta Catalysis. <i>ACS Catalysis</i> , 2015 , 5, 5431-5435	4.3	76
269	Accuracy of DLPNO-CCSD(T) method for noncovalent bond dissociation enthalpies from coinage metal cation complexes. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 4664-76	6.4	74
268	Vibrational Fingerprints of Low-Lying Pt(n)P(2n) (n = 1-5) Cluster Structures from Global Optimization Based on Density Functional Theory Potential Energy Surfaces. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 11711-8	2.8	2
267	Variation of the Sterical Properties of the N-Heterocyclic Carbene Coligand in Thermally Triggerable Ruthenium-Based Olefin Metathesis Precatalysts/Initiators. <i>Organometallics</i> , 2015 , 34, 5383-5392	3.8	21
266	A highly selective copper-indium bimetallic electrocatalyst for the electrochemical reduction of aqueous CO2 to CO. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 2146-50	16.4	338
265	Structural stability, acidity, and halide selectivity of the fluoride riboswitch recognition site. <i>Journal of the American Chemical Society</i> , 2015 , 137, 299-306	16.4	18
264	Mechanism of CO2 Fixation by IrIX Bonds (X = OH, OR, N, C). <i>European Journal of Inorganic Chemistry</i> , 2015 , 2015, 4653-4657	2.3	17
263	Mechanism of Intramolecular Rhodium- and Palladium-Catalyzed Alkene Alkoxyfunctionalizations. <i>Organometallics</i> , 2015 , 34, 5549-5554	3.8	6
262	Consequences of the electronic tuning of latent ruthenium-based olefin metathesis catalysts on their reactivity. <i>Beilstein Journal of Organic Chemistry</i> , 2015 , 11, 1458-68	2.5	9
261	Analysis and Ranking of Protein-Protein Docking Models Using Inter-Residue Contacts and Inter-Molecular Contact Maps. <i>Molecules</i> , 2015 , 20, 12045-60	4.8	12
260	A comprehensive study of olefin metathesis catalyzed by Ru-based catalysts. <i>Beilstein Journal of Organic Chemistry</i> , 2015 , 11, 1767-80	2.5	21
259	Ruthenium Olefin Metathesis Catalysts Containing Fluoride. <i>ACS Catalysis</i> , 2015 , 5, 3932-3939	13.1	16

258	A Highly Selective Copper/Indium Bimetallic Electrocatalyst for the Electrochemical Reduction of Aqueous CO ₂ to CO. <i>Angewandte Chemie</i> , 2015 , 127, 2174-2178	3.6	118
257	Combined experimental/theoretical study of the optoelectronic properties of non-stoichiometric pyrochlore bismuth titanate. <i>Journal of Materials Chemistry C</i> , 2015 , 3, 12032-12039	7.1	27
256	Silica-Supported Tungsten Carbynes (SiO) _x W(CH)(Me) _y (x = 1, y = 2; x = 2, y = 1): New Efficient Catalysts for Alkyne Cyclotrimerization. <i>Organometallics</i> , 2015 , 34, 690-695	3.8	21
255	The driving force role of ruthenacyclobutanes. <i>Theoretical Chemistry Accounts</i> , 2015 , 134, 1	1.9	6
254	Synthesis, structural studies and ligand influence on the stability of aryl-NHC stabilised trimethylaluminium complexes. <i>Dalton Transactions</i> , 2015 , 44, 15166-74	4.3	14
253	Fluxional Behavior of Molecular WMe ₆ and of Silica Grafted WMe ₆ . <i>Organometallics</i> , 2015 , 34, 663-668	3.8	3
252	Evaluation of an olefin metathesis pre-catalyst with a bulky and electron-rich N-heterocyclic carbene. <i>Journal of Organometallic Chemistry</i> , 2015 , 780, 43-48	2.3	24
251	Cycloalkyl-based unsymmetrical unsaturated (U)-NHC ligands: flexibility and dissymmetry in ruthenium-catalysed olefin metathesis. <i>Dalton Transactions</i> , 2014 , 43, 7044-9	4.3	26
250	A recurrent Gly43Asp substitution in coagulation Factor X rigidifies its catalytic pocket and impairs catalytic activity and intracellular trafficking. <i>Thrombosis Research</i> , 2014 , 133, 481-7	8.2	7
249	Theoretical Attempts: In Silico Olefin Metathesis How Can Computers Help in the Understanding of Metathesis Mechanisms and in Catalysts Development? 2014 , 483-494		3
248	Impact of Electronic Modification of the Chelating Benzylidene Ligand in cis-Dichloro-Configured Second-Generation Olefin Metathesis Catalysts on Their Activity. <i>Organometallics</i> , 2014 , 33, 2806-2813	3.8	31
247	From ruthenium olefin metathesis catalyst to (E)-3-phenylindenyl)hydrido complex via alcoholysis. <i>Chemical Communications</i> , 2014 , 50, 2205-7	5.8	19
246	Inverting the Diastereoselectivity of the Mukaiyama-Michael Addition with Graphite-Based Catalysts. <i>ACS Catalysis</i> , 2014 , 4, 492-496	13.1	44
245	Chain Propagation and Termination Mechanisms for Polymerization of Conjugated Polar Alkenes by [Al]-Based Frustrated Lewis Pairs. <i>Macromolecules</i> , 2014 , 47, 7765-7774	5.5	76
244	Supramolecular water oxidation with Ru-bda-based catalysts. <i>Chemistry - A European Journal</i> , 2014 , 20, 17282-6	4.8	66
243	A comprehensive mechanistic picture of the isomerizing alkoxyacylation of plant oils. <i>Journal of the American Chemical Society</i> , 2014 , 136, 16871-81	16.4	95
242	Tuning the properties of visible-light-responsive tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first-principles viewpoint. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 20548-60	3.6	77
241	How phenyl makes a difference: mechanistic insights into the ruthenium(II)-catalysed isomerisation of allylic alcohols. <i>Chemical Science</i> , 2014 , 5, 180-188	9.4	52

240	Molecular dynamics characterization of five pathogenic Factor X mutants associated with decreased catalytic activity. <i>Biochemistry</i> , 2014 , 53, 6992-7001	3.2	13
239	Comparing Ru and Fe-catalyzed olefin metathesis. <i>Dalton Transactions</i> , 2014 , 43, 11216-20	4.3	34
238	The "innocent" role of Sc(3+) on a non-heme Fe catalyst in an O ₂ environment. <i>Dalton Transactions</i> , 2014 , 43, 11190-4	4.3	2
237	Exploring the mechanism of Grignard metathesis polymerization of 3-alkylthiophenes. <i>Dalton Transactions</i> , 2014 , 43, 15143-50	4.3	32
236	High-speed organocatalytic polymerization of a renewable methylene butyrolactone by a phosphazene superbases. <i>Polymer Chemistry</i> , 2014 , 5, 3261	4.9	23
235	Major Difference in Visible-Light Photocatalytic Features between Perfect and Self-Defective Ta ₃ N ₅ Materials: A Screened Coulomb Hybrid DFT Investigation. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 20784-20790	3.8	32
234	Investigating Phthalate and 1,3-Diether Coverage and Dynamics on the (104) and (110) Surfaces of MgCl ₂ -Supported Ziegler-Natta Catalysts. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 8050-8058	3.8	36
233	Unusual C-C Bond Cleavage in the Formation of Amine-Bis(phenoxy) Group 4 Benzyl Complexes: Mechanism of Formation and Application to Stereospecific Polymerization. <i>Organometallics</i> , 2014 , 33, 4118-4130	3.8	9
232	Tuning and Quantifying Steric and Electronic Effects of N-Heterocyclic Carbenes 2014 , 25-38		
231	The activation mechanism of Fe-based olefin metathesis catalysts. <i>Chemical Physics Letters</i> , 2014 , 610-611, 29-32	2.5	26
230	The Right Computational Recipe for Olefin Metathesis with Ru-Based Catalysts: The Whole Mechanism of Ring-Closing Olefin Metathesis. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4442-8	6.4	65
229	Mechanism of n-Butane Hydrogenolysis Promoted by Ta-Hydrides Supported on Silica. <i>ACS Catalysis</i> , 2014 , 4, 1868-1874	13.1	21
228	Deconstructing Selectivity in the Gold-Promoted Cyclization of Alkynyl Benzothioamides to Six-Membered Mesoionic Carbene or Acyclic Carbene Complexes. <i>ACS Catalysis</i> , 2014 , 4, 1287-1291	13.1	16
227	MDcons: Intermolecular contact maps as a tool to analyze the interface of protein complexes from molecular dynamics trajectories. <i>BMC Bioinformatics</i> , 2014 , 15 Suppl 5, S1	3.6	21
226	Tethering metal ions to photocatalyst particulate surfaces by bifunctional molecular linkers for efficient hydrogen evolution. <i>ChemSusChem</i> , 2014 , 7, 2575-83	8.3	17
225	Dynamics of the NbCl ₅ -catalyzed cycloaddition of propylene oxide and CO ₂ : assessing the dual role of the nucleophilic Co-catalysts. <i>Chemistry - A European Journal</i> , 2014 , 20, 11870-82	4.8	55
224	Highly Efficient and Eco-Friendly Gold-Catalyzed Synthesis of Homoallylic Ketones. <i>ACS Catalysis</i> , 2014 , 4, 2701-2705	13.1	51
223	cis/trans Coordination in Olefin Metathesis by Static and Molecular Dynamic DFT Calculations. <i>Chemistry of Heterocyclic Compounds</i> , 2014 , 50, 389-395	1.4	6

222	Insights into the decomposition of olefin metathesis precatalysts. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 8995-9	16.4	51
221	Quantifying the Impact of Relativity and of Dispersion Interactions on the Activation of Molecular Oxygen Promoted by Noble Metal Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 13707-13714	3.8	10
220	Promotion of selective pathways in isomerizing functionalization of plant oils by rigid framework substituents. <i>ChemSusChem</i> , 2014 , 7, 3491-5	8.3	18
219	Dinuclear Ru-aqua complexes for selective epoxidation catalysis based on supramolecular substrate orientation effects. <i>Chemistry - A European Journal</i> , 2014 , 20, 3898-902	4.8	28
218	Structural basis for the recognition in an idiotype-anti-idiotype antibody complex related to celiac disease. <i>PLoS ONE</i> , 2014 , 9, e102839	3.7	9
217	Cationic bis-N-heterocyclic carbene (NHC) ruthenium complex: structure and application as latent catalyst in olefin metathesis. <i>Chemistry - A European Journal</i> , 2014 , 20, 13716-21	4.8	23
216	Insights into the Decomposition of Olefin Metathesis Precatalysts. <i>Angewandte Chemie</i> , 2014 , 126, 9141-9145	3.7	7
215	Higher order structural effects stabilizing the reverse Watson-Crick Guanine-Cytosine base pair in functional RNAs. <i>Nucleic Acids Research</i> , 2014 , 42, 714-26	20.1	31
214	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . <i>Highlights in Theoretical Chemistry</i> , 2014 , 143-155		
213	Organometallic copper I, II or III species in an intramolecular dechlorination reaction. <i>Highlights in Theoretical Chemistry</i> , 2014 , 105-110		
212	Organometallic copper I, II or III species in an intramolecular dechlorination reaction. <i>Theoretical Chemistry Accounts</i> , 2013 , 132, 1	1.9	1
211	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O ₂ . <i>Theoretical Chemistry Accounts</i> , 2013 , 132, 1	1.9	11
210	Electronic bond tuning with heterocyclic carbenes. <i>Dalton Transactions</i> , 2013 , 42, 7281-6	4.3	2
209	How Well Can DFT Reproduce Key Interactions in Ziegler-Natta Systems?. <i>Macromolecular Chemistry and Physics</i> , 2013 , 214, 1980-1989	2.6	34
208	Simple and cheap steric and electronic characterization of the reactivity of Ru(II) complexes containing oxazoline ligands as epoxidation catalysts. <i>Chemical Physics Letters</i> , 2013 , 577, 142-146	2.5	5
207	Steric Maps to Evaluate the Role of Steric Hindrance on the IPr NHC Ligand. <i>Procedia Computer Science</i> , 2013 , 18, 845-854	1.6	5
206	Bifunctional (cyclopentadienone)iron-tricarbonyl complexes: synthesis, computational studies and application in reductive amination. <i>Chemistry - A European Journal</i> , 2013 , 19, 17881-90	4.8	100
205	Catalytic Role of Nickel in the Decarbonylative Addition of Phthalimides to Alkynes. <i>Organometallics</i> , 2013 , 32, 6330-6336	3.8	19

204	Multicomponent synthesis of unsymmetrical unsaturated N-heterocyclic carbene precursors and their related transition-metal complexes. <i>Angewandte Chemie - International Edition</i> , 2013 , 52, 14103-7	16.4	54
203	Exploring new generations of ruthenium olefin metathesis catalysts: the reactivity of a bis-ylidene ruthenium complex by DFT. <i>Dalton Transactions</i> , 2013 , 42, 7271-5	4.3	26
202	Using a consensus approach based on the conservation of inter-residue contacts to rank CAPRI models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 2210-20	4.2	16
201	The isolation of [Pd{OC(O)H}(H)(NHC)(PR ₃)] (NHC = N-heterocyclic carbene) and its role in alkene and alkyne reductions using formic acid. <i>Journal of the American Chemical Society</i> , 2013 , 135, 4588-91	16.4	80
200	The activation mechanism of Ru-indenylidene complexes in olefin metathesis. <i>Journal of the American Chemical Society</i> , 2013 , 135, 7073-9	16.4	88
199	How does the addition of steric hindrance to a typical N-heterocyclic carbene ligand affect catalytic activity in olefin metathesis?. <i>Dalton Transactions</i> , 2013 , 42, 7433-9	4.3	66
198	Ranking multiple docking solutions based on the conservation of inter-residue contacts. <i>Proteins: Structure, Function and Bioinformatics</i> , 2013 , 81, 1571-84	4.2	28
197	Understanding Tantalum-Catalyzed Ethylene Trimerization: When Things Go Wrong. <i>ACS Catalysis</i> , 2013 , 3, 1360-1364	13.1	19
196	Steric and Electronic Parameters of a Bulky yet Flexible N-Heterocyclic Carbene: 1,3-Bis(2,6-bis(1-ethylpropyl)phenyl)imidazol-2-ylidene (IPent). <i>Organometallics</i> , 2013 , 32, 3249-3252	3.8	41
195	Energetics of the ruthenium-halide bond in olefin metathesis (pre)catalysts. <i>Dalton Transactions</i> , 2013 , 42, 7312-7	4.3	28
194	Organocatalytic conjugate-addition polymerization of linear and cyclic acrylic monomers by N-heterocyclic carbenes: mechanisms of chain initiation, propagation, and termination. <i>Journal of the American Chemical Society</i> , 2013 , 135, 17925-42	16.4	77
193	Rare-Earth Half-Sandwich Dialkyl and Homoleptic Trialkyl Complexes for Rapid and Stereoselective Polymerization of a Conjugated Polar Olefin. <i>Organometallics</i> , 2013 , 32, 1459-1465	3.8	21
192	Enantioselective polymerization of epoxides using biaryl-linked bimetallic cobalt catalysts: a mechanistic study. <i>Journal of the American Chemical Society</i> , 2013 , 135, 18901-11	16.4	76
191	Concepts for stereoselective acrylate insertion. <i>Journal of the American Chemical Society</i> , 2013 , 135, 10263-6	16.4	51
190	Multicomponent Synthesis of Unsymmetrical Unsaturated N-Heterocyclic Carbene Precursors and Their Related Transition-Metal Complexes. <i>Angewandte Chemie</i> , 2013 , 125, 14353-14357	3.6	16
189	Exploring electronic and steric effects on the insertion and polymerization reactivity of phosphinesulfonato Pd(II) catalysts. <i>Chemistry - A European Journal</i> , 2013 , 19, 17773-88	4.8	33
188	Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis. <i>Highlights in Theoretical Chemistry</i> , 2013 , 129-134		
187	On the accuracy of DFT methods in reproducing ligand substitution energies for transition metal complexes in solution: the role of dispersive interactions. <i>ChemPhysChem</i> , 2012 , 13, 562-9	3.2	53

186	From olefin metathesis catalyst to alcohol racemization catalyst in one step. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 1042-5	16.4	45
185	Mechanistic features of isomerizing alkoxyacylation of methyl oleate. <i>Journal of the American Chemical Society</i> , 2012 , 134, 17696-703	16.4	124
184	Mechanism of Isotactic Styrene Polymerization with a C ₆ F ₅ -Substituted Bis(phenoxyimine) Titanium System. <i>Macromolecules</i> , 2012 , 45, 8588-8597	5.5	10
183	Activation and Deactivation of Neutral Palladium(II) Phosphinesulfonato Polymerization Catalysts. <i>Organometallics</i> , 2012 , 31, 8388-8406	3.8	53
182	Controlled Acrylate Insertion Regioselectivity in Diazaphospholidine-Sulfonato Palladium(II) Complexes. <i>Organometallics</i> , 2012 , 31, 8505-8515	3.8	35
181	Stereoselectivity in metallocene-catalyzed coordination polymerization of renewable methylene butyrolactones: from stereo-random to stereo-perfect polymers. <i>Journal of the American Chemical Society</i> , 2012 , 134, 7278-81	16.4	49
180	Lewis pair polymerization by classical and frustrated Lewis pairs: acid, base and monomer scope and polymerization mechanism. <i>Dalton Transactions</i> , 2012 , 41, 9119-34	4.3	164
179	Investigating Alkoxysilane Coverage and Dynamics on the (104) and (110) Surfaces of MgCl ₂ -Supported Ziegler-Natta Catalysts. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 22980-22986	3.8	30
178	Synthesis and Reactivity of Ruthenium Phosphite Indenylidene Complexes. <i>Organometallics</i> , 2012 , 31, 7415-7426	3.8	52
177	CONS-COCOMAPS: a novel tool to measure and visualize the conservation of inter-residue contacts in multiple docking solutions. <i>BMC Bioinformatics</i> , 2012 , 13 Suppl 4, S19	3.6	22
176	Pentacoordinated Organoaluminum Complexes: A Computational Insight. <i>Organometallics</i> , 2012 , 31, 8498-8504	3.8	12
175	A latent ruthenium based olefin metathesis catalyst with a sterically demanding NHC ligand. <i>Catalysis Science and Technology</i> , 2012 , 2, 1640	5.5	43
174	Coordinatively Unsaturated Ruthenium Complexes As Efficient Alkyne-N ₃ Cycloaddition Catalysts. <i>Organometallics</i> , 2012 , 31, 756-767	3.8	65
173	Theoretical Investigation of Active Sites at the Corners of MgCl ₂ Crystallites in Supported Ziegler-Natta Catalysts. <i>Macromolecules</i> , 2012 , 45, 3695-3701	5.5	79
172	Hexafluorobenzene: a powerful solvent for a noncovalent stereoselective organocatalytic Michael addition reaction. <i>Chemical Communications</i> , 2012 , 48, 1650-2	5.8	57
171	Blue-emitting dinuclear N-heterocyclic dicarbene gold(I) complex featuring a nearly unit quantum yield. <i>Inorganic Chemistry</i> , 2012 , 51, 1778-84	5.1	91
170	σ-Donation from the aromatic N-substituent of N-heterocyclic carbene ligands to metal and its role in catalysis. <i>Journal of the American Chemical Society</i> , 2012 , 134, 8127-35	16.4	52
169	From Olefin Metathesis Catalyst to Alcohol Racemization Catalyst in One Step. <i>Angewandte Chemie</i> , 2012 , 124, 1066-1069	3.6	13

168	Synthesis of 3-Fluoro-3-aryl Oxindoles: Direct Enantioselective Arylation of Amides. <i>Angewandte Chemie</i> , 2012 , 124, 2924-2927	3.6	33
167	Synthesis of 3-fluoro-3-aryl oxindoles: direct enantioselective arylation of amides. <i>Angewandte Chemie - International Edition</i> , 2012 , 51, 2870-3	16.4	106
166	[Pd(IPr*)(cinnamyl)Cl]: an efficient pre-catalyst for the preparation of tetra-ortho-substituted biaryls by Suzuki-Miyaura cross-coupling. <i>Chemistry - A European Journal</i> , 2012 , 18, 4517-21	4.8	142
165	Reply to the Comment by Grimme on: On the Accuracy of DFT Methods in Reproducing Ligand Substitution Energies for Transition Metal Complexes in Solution: The Role of Dispersive Interactions <i>ChemPhysChem</i> , 2012 , 13, 1405-1406	3.2	12
164	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists 2012 , 95-133		2
163	Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	21
162	Tuning the electronic properties by width and length modifications of narrow-diameter carbon nanotubes for nanomedicine. <i>Current Medicinal Chemistry</i> , 2012 , 19, 5219-25	4.3	15
161	Catalytic deuteration of silanes mediated by N-heterocyclic carbene-Ir(III) complexes. <i>Chemical Communications</i> , 2011 , 47, 9723-5	5.8	32
160	Comparison of different ruthenium-alkylidene bonds in the activation step with N-heterocyclic carbene Ru-catalysts for olefins metathesis. <i>Dalton Transactions</i> , 2011 , 40, 11066-9	4.3	49
159	Gold(I)-catalyzed synthesis of furans and pyrroles via alkyne hydration. <i>Catalysis Science and Technology</i> , 2011 , 1, 58	5.5	68
158	Thermodynamics of Formation of Uncovered and Dimethyl Ether-Covered MgCl ₂ Crystallites. Consequences in the Structure of Ziegler-Natta Heterogeneous Catalysts. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 13322-13328	3.8	63
157	Selectivity Switch in the Synthesis of Vinylgold(I) Intermediates. <i>Organometallics</i> , 2011 , 30, 6328-6337	3.8	110
156	A combined mechanistic and computational study of the gold(I)-catalyzed formation of substituted indenones. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 101-4	3.9	50
155	The intriguing modeling of cis-trans selectivity in ruthenium-catalyzed olefin metathesis. <i>Beilstein Journal of Organic Chemistry</i> , 2011 , 7, 40-5	2.5	28
154	Mechanism of Stereospecific Propene Polymerization Promoted by Metallocene and Nonmetallocene Catalysts 2011 , 299-322		
153	N-heterocyclic carbene complexes of au, pd, and pt as effective catalysts in organic synthesis. <i>Topics in Current Chemistry</i> , 2011 , 302, 131-55		45
152	[[Au(IPr)] ₂ (EOH)]X complexes: synthetic, structural and catalytic studies. <i>Chemistry - A European Journal</i> , 2011 , 17, 1238-46	4.8	103
151	The doping effect of fluorinated aromatic solvents on the rate of ruthenium-catalysed olefin metathesis. <i>Chemistry - A European Journal</i> , 2011 , 17, 12981-93	4.8	74

150	The pivotal role of symmetry in the ruthenium-catalyzed ring-closing metathesis of olefins. <i>Chemistry - A European Journal</i> , 2011 , 17, 8618-29	4.8	40
149	Room-temperature synthesis of tetra-ortho-substituted biaryls by NHC-catalyzed Suzuki-Miyaura couplings. <i>Chemistry - A European Journal</i> , 2011 , 17, 12886-90	4.8	79
148	Moving up and down the Titanium Oxidation State in Ziegler-Natta Catalysis. <i>Macromolecules</i> , 2011 , 44, 778-783	5.5	72
147	A computational perspective of olefins metathesis catalyzed by N-heterocyclic carbene ruthenium (pre)catalysts. <i>Catalysis Science and Technology</i> , 2011 , 1, 1287	5.5	57
146	Hydride-shuttling chain-transfer polymerization of methacrylates catalyzed by metallocenium enolate metallacycle-hydridoborate ion pairs. <i>Journal of the American Chemical Society</i> , 2011 , 133, 1572-88	16.4	16
145	Rationalizing current strategies to protect N-heterocyclic carbene-based ruthenium catalysts active in olefin metathesis from C-H (de)activation. <i>Chemical Communications</i> , 2011 , 47, 6674-6	5.8	49
144	Gold Nanoparticle/Polymer Interfaces: All Atom Structures from Molecular Dynamics Simulations. <i>Journal of Physical Chemistry C</i> , 2011 , 115, 15154-15163	3.8	53
143	Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis. <i>Procedia Computer Science</i> , 2011 , 4, 1222-1229	1.6	6
142	COCOMAPS: a web application to analyze and visualize contacts at the interface of biomolecular complexes. <i>Bioinformatics</i> , 2011 , 27, 2915-6	7.2	159
141	Breaking the regioselectivity rule for acrylate insertion in the Mizoroki-Heck reaction. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011 , 108, 8955-9	11.5	70
140	N-Heterocyclic Carbenes: An Introductory Overview. <i>Catalysis By Metal Complexes</i> , 2010 , 1-22		2
139	Computational methods to predict the reactivity of nanoparticles through structure-property relationships. <i>Expert Opinion on Drug Delivery</i> , 2010 , 7, 295-305	8	44
138	Flexibility of N-heterocyclic carbene ligands in ruthenium complexes relevant to olefin metathesis and their impact in the first coordination sphere of the metal. <i>Journal of the American Chemical Society</i> , 2010 , 132, 4249-58	16.4	148
137	Mechanistic insights on acrylate insertion polymerization. <i>Journal of the American Chemical Society</i> , 2010 , 132, 4418-26	16.4	96
136	Catalyst-site-controlled coordination polymerization of polar vinyl monomers to highly syndiotactic polymers. <i>Journal of the American Chemical Society</i> , 2010 , 132, 2695-709	16.4	55
135	Mixed Phosphite/N-Heterocyclic Carbene Complexes: Synthesis, Characterization and Catalytic Studies. <i>Organometallics</i> , 2010 , 29, 1443-1450	3.8	80
134	A versatile gold synthon for acetylene C-H bond activation. <i>Dalton Transactions</i> , 2010 , 39, 10382-90	4.3	55
133	Mechanism of racemization of chiral alcohols mediated by 16-electron ruthenium complexes. <i>Journal of the American Chemical Society</i> , 2010 , 132, 13146-9	16.4	58

132	C2-symmetric chiral disulfoxide ligands in rhodium-catalyzed 1,4-addition: from ligand synthesis to the enantioselection pathway. <i>Chemistry - A European Journal</i> , 2010 , 16, 14335-47	4.8	54
131	Mechanistic insights into the cis-trans isomerization of ruthenium complexes relevant to catalysis of olefin metathesis. <i>Chemistry - A European Journal</i> , 2010 , 16, 14354-64	4.8	67
130	Comparing the enantioselective power of steric and electrostatic effects in transition-metal-catalyzed asymmetric synthesis. <i>Chemistry - A European Journal</i> , 2010 , 16, 14348-53	4.8	150
129	Mechanistic insights into the double C \equiv H (de)activation route of a Ru-based olefin metathesis catalyst?. <i>Journal of Molecular Catalysis A</i> , 2010 , 324, 75-79		54
128	Probing the Mechanism of the Double C \equiv H (De)Activation Route of a Ru-Based Olefin Metathesis Catalyst. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2010 , 275-280	0.1	2
127	A Comparison of the Performance of the Semiempirical PM6 Method Versus DFT Methods in Ru-Catalyzed Olefin Metathesis. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2010 , 281-292	0.1	2
126	Mechanism of Gold-Catalyzed Cycloisomerization of Enynyl Esters. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2010 , 293-303	0.1	
125	Activation of Hydrogen by Palladium(0): Formation of the Mononuclear Dihydride Complex trans-[Pd(H) ₂ (IPr)(PCy ₃)]. <i>Angewandte Chemie</i> , 2009 , 121, 5284-5288	3.6	11
124	Gold- and platinum-catalyzed cycloisomerization of enynyl esters versus allenyl esters: an experimental and theoretical study. <i>Chemistry - A European Journal</i> , 2009 , 15, 3243-60	4.8	122
123	Chemodivergent metathesis of dienyne catalyzed by ruthenium-indenylidene complexes: an experimental and computational study. <i>Chemistry - A European Journal</i> , 2009 , 15, 10244-54	4.8	56
122	SambVca: A Web Application for the Calculation of the Buried Volume of N-Heterocyclic Carbene Ligands. <i>European Journal of Inorganic Chemistry</i> , 2009 , 2009, 1759-1766	2.3	610
121	[Pd(NHC)(allyl)Cl] Complexes: Synthesis and Determination of the NHC Percent Buried Volume (%V _{bur}) Steric Parameter. <i>European Journal of Inorganic Chemistry</i> , 2009 , 2009, 1767-1773	2.3	73
120	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. <i>Journal of Computational Chemistry</i> , 2009 , 30, 275-84	3.5	71
119	Activation of hydrogen by palladium(0): formation of the mononuclear dihydride complex trans-[Pd(H) ₂ (IPr)(PCy ₃)]. <i>Angewandte Chemie - International Edition</i> , 2009 , 48, 5182-6	16.4	51
118	Understanding the M(NHC) (NHC=N-heterocyclic carbene) bond. <i>Coordination Chemistry Reviews</i> , 2009 , 253, 687-703	23.2	567
117	Exploring the reactivity of Ru-based metathesis catalysts with a pi-acid ligand trans to the Ru-ylidene bond. <i>Journal of the American Chemical Society</i> , 2009 , 131, 9000-6	16.4	65
116	Frequency and effect of the binding of Mg ²⁺ , Mn ²⁺ , and Co ²⁺ ions on the guanine base in Watson-Crick and reverse Watson-Crick base pairs. <i>Journal of Physical Chemistry B</i> , 2009 , 113, 15670-8	3.4	44
115	Coordination-Addition Polymerization and Kinetic Resolution of Methacrylamides by Chiral Metallocene Catalysts. <i>Macromolecules</i> , 2009 , 42, 1462-1471	5.5	27

114	Probing the mechanism of O ₂ activation by a copper(I) biomimetic complex of a C-H hydroxylating copper monoxygenase. <i>Inorganic Chemistry</i> , 2009 , 48, 4062-6	5.1	41
113	A molecular model for H(2) interactions in aliphatic and aromatic hydrocarbons. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 3935-42	3.6	9
112	Simple ligand modifications as a key to playing with the stability of Cu(I), Cu(II), and Cu(III) organometallic complexes. <i>Inorganic Chemistry</i> , 2009 , 48, 2340-2	5.1	17
111	Comparing families of olefin polymerization precatalysts using the percentage of buried volume. <i>Dalton Transactions</i> , 2009 , 8885-90	4.3	28
110	Mechanism of dihydride formation and hydrogen/deuterium exchange in a cationic iridium(III) complex. <i>Canadian Journal of Chemistry</i> , 2009 , 87, 1362-1368	0.9	7
109	Electronic Effects on Regioselectivity in Styrene Polyinsertion Promoted by Group 4 Catalysts. <i>Organometallics</i> , 2008 , 27, 1028-1029	3.8	12
108	Complete mechanism of sigma* intramolecular aromatic hydroxylation through O ₂ activation by a macrocyclic dicopper(I) complex. <i>Journal of the American Chemical Society</i> , 2008 , 130, 17710-7	16.4	54
107	Ligand Mobility and Solution Structures of the Metallocenium Ion Pairs [Me ₂ C(Cp)(fluorenyl)MCH ₂ SiMe ₃ +X ⁺] (M = Zr, Hf; X = MeB(C ₆ F ₅) ₃ , B(C ₆ F ₅) ₄). <i>Organometallics</i> , 2008 , 27, 5474-5487	3.8	41
106	Determination of N-Heterocyclic Carbene (NHC) Steric and Electronic Parameters using the [(NHC)Ir(CO)2Cl] System. <i>Organometallics</i> , 2008 , 27, 202-210	3.8	497
105	Stability and cations coordination of DNA and RNA 14-mer G-quadruplexes: a multiscale computational approach. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 12115-23	3.4	32
104	Thermodynamics of N-Heterocyclic Carbene Dimerization: The Balance of Sterics and Electronics. <i>Organometallics</i> , 2008 , 27, 2679-2681	3.8	170
103	Syndioselective MMA Polymerization by Group 4 Constrained Geometry Catalysts: A Combined Experimental and Theoretical Study. <i>Macromolecules</i> , 2008 , 41, 6910-6919	5.5	21
102	Identification and characterization of a new family of catalytically highly active imidazolin-2-ylidenes. <i>Journal of the American Chemical Society</i> , 2008 , 130, 6848-58	16.4	98
101	Mechanism of Stereocontrol in Methyl Methacrylate Polymerization Promoted by C ₁ -Symmetric Metallocenes. <i>Macromolecules</i> , 2008 , 41, 3439-3445	5.5	20
100	Ziegler-Natta catalytic systems. <i>Journal of Thermal Analysis and Calorimetry</i> , 2008 , 91, 101-106	4.1	4
99	Golden carousel in catalysis: the cationic gold/propargylic ester cycle. <i>Angewandte Chemie - International Edition</i> , 2008 , 47, 718-21	16.4	255
98	Golden Carousel in Catalysis: The Cationic Gold/Propargylic Ester Cycle. <i>Angewandte Chemie</i> , 2008 , 120, 730-733	3.6	80
97	Parametrization of an empirical correction term to density functional theory for an accurate description of pi-stacking interactions in nucleic acids. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 13124-34	3.4	39

96	Key Interactions in Heterogeneous Ziegler-Natta Catalytic Systems: Structure and Energetics of TiCl ₄ -Lewis Base Complexes. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 4412-4419	3.8	62
95	Regiochemistry of propene insertion with group 4 polymerization catalysts from a theoretical perspective. <i>Journal of Organometallic Chemistry</i> , 2007 , 692, 4519-4527	2.3	29
94	Key Elements in the Structure and Function Relationship of the MgCl ₂ /TiCl ₄ /Lewis Base Ziegler-Natta Catalytic System. <i>Macromolecules</i> , 2007 , 40, 9181-9189	5.5	125
93	Mg ²⁺ binding and archaeosine modification stabilize the G15 C48 Levitt base pair in tRNAs. <i>Rna</i> , 2007 , 13, 1427-36	5.8	70
92	An Empirical Correction Term to Density Functional Theory for the Description of the TiCl ₄ -Lewis Base Complexes. <i>Macromolecular Symposia</i> , 2007 , 260, 122-126	0.8	3
91	Insertion of a N-Heterocyclic Carbene (NHC) into a Platinum-Olefin Bond. <i>Organometallics</i> , 2007 , 26, 3286-3288	3.8	46
90	Electronic Properties of N-Heterocyclic Carbene (NHC) Ligands: Synthetic, Structural, and Spectroscopic Studies of (NHC)Platinum(II) Complexes. <i>Organometallics</i> , 2007 , 26, 5880-5889	3.8	168
89	Olefin Polymerizations with Group IV Metal Catalysts 2007 , 1005-1166		27
88	(NHC)Copper(I)-catalyzed [3+2] cycloaddition of azides and mono- or disubstituted alkynes. <i>Chemistry - A European Journal</i> , 2006 , 12, 7558-64	4.8	315
87	Accurate energies of hydrogen bonded nucleic acid base pairs and triplets in tRNA tertiary interactions. <i>Nucleic Acids Research</i> , 2006 , 34, 865-79	20.1	71
86	Donor-Ligand Effect on the Product Distribution in the Manganese-Catalyzed Epoxidation of Olefins: A Computational Assessment. <i>Organometallics</i> , 2006 , 25, 177-183	3.8	22
85	Stereospecificity in metallocene catalyzed acrylate polymerizations: the chiral orientation of the growing chain selects its own chain end enantioface. <i>Journal of the American Chemical Society</i> , 2006 , 128, 16649-54	16.4	26
84	Structure and bonding in monomeric iron(III) complexes with terminal oxo and hydroxo ligands. <i>Inorganic Chemistry</i> , 2006 , 45, 1732-8	5.1	5
83	The elusive mechanism of olefin metathesis promoted by (NHC)Ru-based catalysts: a trade between steric, electronic, and solvent effects. <i>Journal of the American Chemical Society</i> , 2006 , 128, 13352-3	16.4	122
82	Dynamic properties of metallocenium ion pairs in solution by atomistic simulations. <i>Journal of the American Chemical Society</i> , 2006 , 128, 10952-9	16.4	37
81	Probing the Validity of the CH ₂ SiMe ₃ Group as a Model of the Growing Chain in Mechanistic Studies of Olefin Polymerization with Group 4 Catalysts. <i>Organometallics</i> , 2006 , 25, 1431-1433	3.8	13
80	Molecular modeling of the regiochemistry of olefin insertion with single-site polymerization catalysts. <i>Kinetics and Catalysis</i> , 2006 , 47, 170-175	1.5	7
79	Living propene polymerization with Bis(phenoxy-imine) group 4 metal catalysts: A theoretical study. <i>Kinetics and Catalysis</i> , 2006 , 47, 289-294	1.5	5

78	Acidity and Basicity of N-heterocyclic carbene ligands. A computational assessment. <i>Journal of Organometallic Chemistry</i> , 2006 , 691, 4350-4358	2.3	171
77	Molecular Modeling of Stereo- and Regioselectivity of Group 4 Heterocenes in the Polymerization of Propene. <i>Macromolecules</i> , 2005 , 38, 3973-3976	5.5	14
76	Interaction of a bulky N-heterocyclic carbene ligand with Rh(I) and Ir(I). Double C-H activation and isolation of bare 14-electron Rh(III) and Ir(III) complexes. <i>Journal of the American Chemical Society</i> , 2005 , 127, 3516-26	16.4	264
75	Steric and electronic properties of N-heterocyclic carbenes (NHC): a detailed study on their interaction with Ni(CO) ₄ . <i>Journal of the American Chemical Society</i> , 2005 , 127, 2485-95	16.4	512
74	(E/Z) Selectivity in the Polymerization of 2-Butene Promoted by Ni(II) Brookhart-Type Catalysts. <i>Macromolecules</i> , 2005 , 38, 2072-2075	5.5	16
73	Steric and electronic effects in the bonding of N-heterocyclic ligands to transition metals. <i>Journal of Organometallic Chemistry</i> , 2005 , 690, 5407-5413	2.3	394
72	Synthetic and Structural Studies of (NHC)Pd(allyl)Cl Complexes (NHC = N-heterocyclic carbene). <i>Organometallics</i> , 2004 , 23, 1629-1635	3.8	271
71	Do new century catalysts unravel the mechanism of stereocontrol of old Ziegler-Natta catalysts?. <i>Accounts of Chemical Research</i> , 2004 , 37, 231-41	24.3	206
70	Chirality of Catalysts for Stereospecific Polymerizations. <i>Topics in Stereochemistry</i> , 2004 , 1-69		8
69	Stereoselectivity and chemoselectivity in Ziegler-Natta polymerization of conjugated dienes. 2. Mechanism for 1,2 syndiotactic polymerization of diene monomers with high energy s-cis π coordination. <i>Polymer</i> , 2004 , 45, 467-485	3.9	20
68	Re-evaluation of the Mn(salen) mediated epoxidation of alkenes by means of the B3LYP* density functional. <i>Physical Chemistry Chemical Physics</i> , 2004 , 6, 3747	3.6	25
67	Quantum Mechanics Calculations on Rhodamine Dyes Require Inclusion of Solvent Water for Accurate Representation of the Structure. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 7744-7751	2.8	26
66	Toward a catalytic cycle for the Mn-salen mediated alkene epoxidation: a computational approach. <i>Inorganic Chemistry</i> , 2004 , 43, 2175-82	5.1	51
65	Living Propene Polymerization with Bis(phenoxyimine) Group 4 Metal Catalysts: New Strategies and Old Concepts. <i>Organometallics</i> , 2004 , 23, 5989-5993	3.8	77
64	Origin of enantioselectivity in the asymmetric Ru-catalyzed metathesis of olefins. <i>Journal of the American Chemical Society</i> , 2004 , 126, 9592-600	16.4	111
63	Neutral Square-Planar Olefin/Alkyl Platinum(II) Complexes Containing a N,N'-aminoamide Ligand. Experimental and Theoretical Evidence of Relevant Back-Donation in the Platinum-Olefin Bond. <i>Organometallics</i> , 2004 , 23, 2137-2145	3.8	31
62	Manganese-Salen Complexes as Oxygen-Transfer Agents in Catalytic Epoxidations A Density Functional Study of Mechanistic Aspects. <i>European Journal of Inorganic Chemistry</i> , 2003 , 2003, 892-902	2.3	62
61	A Combined Experimental and Theoretical Study Examining the Binding of N-Heterocyclic Carbenes (NHC) to the Cp*RuCl (Cp* = η -5-C ₅ Me ₅) Moiety: Insight into Stereoelectronic Differences between Unsaturated and Saturated NHC Ligands. <i>Organometallics</i> , 2003 , 22, 4322-4326	3.8	354

60	Transition Metal Mediated Epoxidation as Test Case for the Performance of Different Density Functionals: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 5466-5471	2.8	45
59	Origin of the regiochemistry of propene insertion at octahedral column 4 polymerization catalysts: design or serendipity?. <i>Journal of the American Chemical Society</i> , 2003 , 125, 7172-3	16.4	74
58	Effects of pathological mutations on the stability of a conserved amino acid triad in retinoschisin. <i>FEBS Letters</i> , 2003 , 544, 21-6	3.8	28
57	Electronic effects in (salen)Mn-based epoxidation catalysts. <i>Journal of Organic Chemistry</i> , 2003 , 68, 6202-7	4.7	84
56	POPS: A fast algorithm for solvent accessible surface areas at atomic and residue level. <i>Nucleic Acids Research</i> , 2003 , 31, 3364-6	20.1	174
55	A possible unified mechanism of like and unlike chain-end stereocontrol for primary propene-coordinated polymerizations. <i>Macromolecular Chemistry and Physics</i> , 2002 , 203, 1564-1572	2.6	8
54	Mechanism of ruthenium-catalyzed olefin metathesis reactions from a theoretical perspective. <i>Journal of the American Chemical Society</i> , 2002 , 124, 8965-73	16.4	234
53	Parameter optimized surfaces (POPS): analysis of key interactions and conformational changes in the ribosome. <i>Nucleic Acids Research</i> , 2002 , 30, 2950-60	20.1	80
52	Olefin Polymerization by Early Transition Metal Catalysts. <i>Catalysis By Metal Complexes</i> , 2002 , 23-56		5
51	Site chirality as a messenger in chain-end stereocontrolled propene polymerization. <i>Journal of the American Chemical Society</i> , 2002 , 124, 13368-9	16.4	87
50	Comparison of ab Initio and DFT Methods for Studying Chain Propagation and Chain Termination Processes with Group 4 Polymerization Catalysts. 1. The ansa-Bis(cyclopentadienyl)zirconium Catalyst. <i>Organometallics</i> , 2002 , 21, 4939-4949	3.8	47
49	A possible mechanism for enantioselectivity in the chiral epoxidation of olefins with. <i>Chemistry - A European Journal</i> , 2001 , 7, 800-7	4.8	86
48	Ab Initio and Molecular Mechanics Study of Conformational Selectivity of Chlorinated Compounds Adsorbed in the Clathrate Phase of Syndiotactic Polystyrene. The Role of Electrostatic Host-Guest Interactions. <i>Macromolecular Theory and Simulations</i> , 2001 , 10, 349-354	1.5	5
47	Theoretical Study of Syndiospecific Styrene Polymerization with Cp-Based and Cp-Free Titanium Catalysts. 1. Mechanism of Chain Propagation. <i>Macromolecules</i> , 2001 , 34, 2459-2468	5.5	48
46	Shape and Volume of Cavities in Thermoplastic Molecular Sieves Based on Syndiotactic Polystyrene. <i>Chemistry of Materials</i> , 2001 , 13, 1506-1511	9.6	164
45	A theoretical study of steric and electronic effects in the rhodium-catalyzed carbonylation reactions. <i>Journal of the American Chemical Society</i> , 2001 , 123, 12294-302	16.4	60
44	Stereoselectivity and Chemoselectivity in Ziegler-Natta Polymerizations of Conjugated Dienes. 1. Monomers with Low-Energy s-Cis π Coordination. <i>Macromolecules</i> , 2001 , 34, 7952-7960	5.5	39
43	A Theoretical Study of Syndiospecific Styrene Polymerization with Cp-Based and Cp-Free Titanium Catalysts. 2. Mechanism of Chain-End Stereocontrol. <i>Macromolecules</i> , 2001 , 34, 5379-5385	5.5	53

42	Propene Polymerization with the Isospecific, Highly Regioselective rac-Me ₂ C(3-t-Bu-1-Ind) ₂ ZrCl ₂ /MAO Catalyst. 2. Combined DFT/MM Analysis of Chain Propagation and Chain Release Reactions. <i>Organometallics</i> , 2001 , 20, 1918-1931	3.8	69
41	A Density Functional Theory Study of the Syndiotactic-Specific Polymerization of Styrene 2001 , 299-306		5
40	Radikalische Zwischenstufen in der Jacobsen-Katsuki-Epoxidierung. <i>Angewandte Chemie</i> , 2000 , 112, 602-604	3.6	14
39	. <i>Chemistry - A European Journal</i> , 2000 , 6, 1127-1139	4.8	17
38	Radical Intermediates in the Jacobsen - Katsuki Epoxidation. <i>Angewandte Chemie - International Edition</i> , 2000 , 39, 589-592	16.4	76
37	Influence of 1,3-Diethers on the Stereospecificity of Propene Polymerization by Supported Ziegler-Natta Catalysts. A Theoretical Investigation on Their Adsorption on (110) and (100) Lateral Cuts of MgCl ₂ Platelets. <i>Macromolecules</i> , 2000 , 33, 1134-1140	5.5	73
36	Mechanism of Unlike Stereoselectivity in 1-Alkene Primary Insertions: Syndiospecific Propene Polymerization by Brookhart-Type Nickel(II) Catalysts. <i>Organometallics</i> , 2000 , 19, 1343-1349	3.8	26
35	Geometry and Stability of Titanium Chloride Species Adsorbed on the (100) and (110) Cuts of the MgCl ₂ Support of the Heterogeneous Ziegler-Natta Catalysts. <i>Macromolecules</i> , 2000 , 33, 8953-8962	5.5	116
34	Thermoplastic Molecular Sieves. <i>Chemistry of Materials</i> , 2000 , 12, 363-368	9.6	112
33	Selectivity in propene polymerization with metallocene catalysts. <i>Chemical Reviews</i> , 2000 , 100, 1253-3466	18.1	1202
32	Reactivity of Z and Isomers, Growing Chain Isomerization, and Chain Transfer Reactions in Ethene/2-Butene Copolymerization by Metallocene-Based Catalysts. <i>Macromolecules</i> , 2000 , 33, 4647-4659	5.5	22
31	Stereoselectivity and chiral recognition in copper(I) olefin complexes with a chiral diamine. <i>Chemistry - A European Journal</i> , 2000 , 6, 1127-39	4.8	27
30	Towards more realistic computational modeling of homogenous catalysis by density functional theory: combined QM/MM and ab initio molecular dynamics. <i>Catalysis Today</i> , 1999 , 50, 479-500	5.3	59
29	Insertion of Imine into Palladium-Methyl and Palladium-Acyl Bonds. A Density Functional Study. <i>Journal of the American Chemical Society</i> , 1999 , 121, 4238-4241	16.4	19
28	(E)-(Z) Selectivity in 2-Butene Copolymerization by Group 4 Metallocenes. A Combined Density Functional Theory and Molecular Mechanics Study. <i>Journal of the American Chemical Society</i> , 1999 , 121, 8651-8652	16.4	27
27	A Preliminary Study of Host-Guest Interactions in Polymeric Clathrates [An Ab Initio Study of the Model Complexes Benzene/X ₂ (X = F, Cl, Br, I). <i>European Journal of Inorganic Chemistry</i> , 1998 , 1998, 1513-1517	2.3	6
26	A Molecular Dynamics Study of the First Five Generations of Poly(Propylene Imine) Dendrimers Modified with N-tBoc-L-Phenylalanine. <i>Chemistry - A European Journal</i> , 1998 , 4, 927-934	4.8	60
25	Implementation of the IMOMM methodology for performing combined QM/MM molecular dynamics simulations and frequency calculations. <i>Theoretical Chemistry Accounts</i> , 1998 , 100, 307-313	1.9	135

24	A combined QM/MM study of ligand substitution enthalpies in the L ₂ Fe(CO) ₃ , RuCpL ₂ Cl, and RuCp*L ₂ Cl systems. <i>Canadian Journal of Chemistry</i> , 1998 , 76, 1457-1466	0.9	27
23	Influence of Ligand Substitutions on the Regiospecificity and Stereospecificity in Isospecific Zirconocenes for Propene Polymerization. A Molecular Mechanics Analysis. <i>Macromolecules</i> , 1998 , 31, 3431-3438	5.5	49
22	Mechanisms of Propagation and Termination Reactions in Classical Heterogeneous Ziegler-Natta Catalytic Systems: A Nonlocal Density Functional Study. <i>Journal of the American Chemical Society</i> , 1998 , 120, 2428-2436	16.4	100
21	Molecular Mechanics and Stereospecificity in Ziegler-Natta 1,2 and Cis-1,4 Polymerizations of Conjugated Dienes. <i>Macromolecules</i> , 1997 , 30, 677-684	5.5	39
20	Relationship between Regiospecificity and Type of Stereospecificity in Propene Polymerization with Zirconocene-Based Catalysts ¹ . <i>Journal of the American Chemical Society</i> , 1997 , 119, 4394-4403	16.4	99
19	The Role of Bulky Substituents in Brookhart-Type Ni(II) Diimine Catalyzed Olefin Polymerization: A Combined Density Functional Theory and Molecular Mechanics Study. <i>Journal of the American Chemical Society</i> , 1997 , 119, 6177-6186	16.4	304
18	A Density Functional and Molecular Mechanics Study Of β -Hydrogen Transfer in Homogeneous Ziegler-Natta Catalysis. <i>Macromolecules</i> , 1996 , 29, 2729-2737	5.5	68
17	Doubly Bridged ansa-Zirconocenes Based on the Norbornadiene Skeleton: A Quantum Mechanical and Molecular Mechanics Study. <i>Organometallics</i> , 1996 , 15, 2254-2263	3.8	16
16	Back-Skip of the Growing Chain at Model Complexes for the Metallocene Polymerization Catalysis. <i>Macromolecules</i> , 1996 , 29, 4834-4845	5.5	82
15	Vapour pressures of fluorocarbons in polyols, polyamines and polycarboxyls. <i>Journal of Fluorine Chemistry</i> , 1996 , 78, 167-175	2.1	1
14	Molecular mechanics and mechanisms of regulation of the stereospecificity in Ziegler-Natta catalysis. <i>Macromolecular Symposia</i> , 1995 , 89, 307-319	0.8	7
13	Models for the Explanation of the Stereospecific Behaviour of Ziegler Natta Catalysts 1995 , 237-249		14
12	Enantioselectivity in the Regioirregular Placements and Regiospecificity in the Isospecific Polymerization of Propene with Homogeneous Ziegler-Natta Catalysts. <i>Journal of the American Chemical Society</i> , 1994 , 116, 2988-2995	16.4	86
11	Density functional study on the electronic and molecular structure of the hydroformylation catalyst HCo(CO) ₃ . <i>Organometallics</i> , 1993 , 12, 3586-3593	3.8	28
10	Model catalytic sites for olefin polymerization and diastereoselectivity in the cyclopolymerization of 1,5-hexadiene. <i>Macromolecules</i> , 1993 , 26, 260-267	5.5	75
9	Molecular mechanics and the polymerization mechanism of homogeneous and heterogeneous Ziegler-Natta catalysts. <i>Makromolekulare Chemie Macromolecular Symposia</i> , 1993 , 69, 237-246		6
8	Structural analogies between homogeneous and heterogeneous catalysts for the stereospecific polymerization of 1-alkenes. <i>Journal of Molecular Catalysis</i> , 1992 , 74, 433-442		36
7	A model for the homogeneous isospecific Ziegler-Natta polymerization of olefins: Enantioselectivity in the deuteration and deuteriooligomerization of 1-alkenes. <i>Chirality</i> , 1991 , 3, 299-306 ^{2,1}		19

6	On the effects of methyl substituents on chelating ligands in models for homogeneous isospecific Ziegler-Natta catalysis. <i>Polymer</i> , 1991 , 32, 1329-1335	3.9	45
5	A possible model for the stereospecificity in the syndiospecific polymerization of propene with group 4a metallocenes. <i>Macromolecules</i> , 1991 , 24, 1784-1790	5.5	138
4	Mechanistic Understanding of Arylation vs Alkylation of Aliphatic Csp ³ Bonds by Decatungstate-Nickel Catalysis. <i>ACS Catalysis</i> , 13973-13982	13.1	3
3	D936Y and Other Mutations in the Fusion Core of the SARS-Cov-2 Spike Protein Heptad Repeat 1 Undermine the Post-Fusion Assembly		8
2	A Career in Catalysis: Jean-Marie M. Basset. <i>ACS Catalysis</i> , 4961-4977	13.1	0
1	Selection of Low-Dimensional 3-D Geometric Descriptors for Accurate Enantioselectivity Prediction. <i>ACS Catalysis</i> , 6934-6945	13.1	