Luigi Cavallo

List of Publications by Citations

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	Selectivity in propene polymerization with metallocene catalysts. *Chemical Reviews*, **2000**, 100, 1253-346	68.1	1202
544	SambVca: A Web Application for the Calculation of the Buried Volume of N-Heterocyclic Carbene Ligands. *European Journal of Inorganic Chemistry*, **2009**, 2009, 1759-1766	2.3	610
543	Understanding the M(NHC) (NHC=N-heterocyclic carbene) bond. *Coordination Chemistry Reviews*, **2009**, 253, 687-703	23.2	567
542	Steric and electronic properties of N-heterocyclic carbenes (NHC): a detailed study on their interaction with Ni(CO)4. *Journal of the American Chemical Society*, **2005**, 127, 2485-95	16.4	512
541	Determination of N-Heterocyclic Carbene (NHC) Steric and Electronic Parameters using the [(NHC)Ir(CO)2Cl] System. *Organometallics*, **2008**, 27, 202-210	3.8	497
540	SambVca 2. A Web Tool for Analyzing Catalytic Pockets with Topographic Steric Maps. *Organometallics*, **2016**, 35, 2286-2293	3.8	468
539	Steric and electronic effects in the bonding of N-heterocyclic ligands to transition metals. *Journal of Organometallic Chemistry*, **2005**, 690, 5407-5413	2.3	394
538	A Combined Experimental and Theoretical Study Examining the Binding of N-Heterocyclic Carbenes (NHC) to the Cp*RuCl (Cp* = □5-C5Me5) Moiety: Insight into Stereoelectronic Differences between Unsaturated and Saturated NHC Ligands. *Organometallics*, **2003**, 22, 4322-4326	3.8	354
537	Towards the online computer-aided design of catalytic pockets. *Nature Chemistry*, **2019**, 11, 872-879	17.6	350
536	A highly selective copper-indium bimetallic electrocatalyst for the electrochemical reduction of aqueous CO2 to CO. *Angewandte Chemie - International Edition*, **2015**, 54, 2146-50	16.4	338
535	(NHC)Copper(I)-catalyzed [3+2] cycloaddition of azides and mono- or disubstituted alkynes. *Chemistry - A European Journal*, **2006**, 12, 7558-64	4.8	315
534	The Role of Bulky Substituents in Brookhart-Type Ni(II) Diimine Catalyzed Olefin Polymerization: A Combined Density Functional Theory and Molecular Mechanics Study. *Journal of the American Chemical Society*, **1997**, 119, 6177-6186	16.4	304
533	Cu□n Bimetallic Catalyst for Selective Aqueous Electroreduction of CO2 to CO. *ACS Catalysis*, **2016**, 6, 2842-2851	13.1	284
532	Synthetic and Structural Studies of (NHC)Pd(allyl)Cl Complexes (NHC = N-heterocyclic carbene). *Organometallics*, **2004**, 23, 1629-1635	3.8	271
531	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. *Journal of the American Chemical Society*, **2005**, 127, 3516-26	16.4	264
530	Golden carousel in catalysis: the cationic gold/propargylic ester cycle. *Angewandte Chemie - International Edition*, **2008**, 47, 718-21	16.4	255
529	Mechanism of ruthenium-catalyzed olefin metathesis reactions from a theoretical perspective. *Journal of the American Chemical Society*, **2002**, 124, 8965-73	16.4	234

528	Communication: An improved linear scaling perturbative triples correction for the domain based local pair-natural orbital based singles and doubles coupled cluster method [DLPNO-CCSD(T)]. *Journal of Chemical Physics*, **2018**, 148, 011101	3.9	224
527	Aqueous Zinc-Ion Storage in MoS by Tuning the Intercalation Energy. *Nano Letters*, **2019**, 19, 3199-3206	11.5	223
526	2D Nanomaterials for Photocatalytic Hydrogen Production. *ACS Energy Letters*, **2019**, 4, 1687-1709	20.1	212
525	Do new century catalysts unravel the mechanism of stereocontrol of old Ziegler-Natta catalysts?. *Accounts of Chemical Research*, **2004**, 37, 231-41	24.3	206
524	What can NMR spectroscopy of selenoureas and phosphinidenes teach us about the accepting abilities of -heterocyclic carbenes?. *Chemical Science*, **2015**, 6, 1895-1904	9.4	201
523	MoS2 Polymorphic Engineering Enhances Selectivity in the Electrochemical Reduction of Nitrogen to Ammonia. *ACS Energy Letters*, **2019**, 4, 430-435	20.1	179
522	POPS: A fast algorithm for solvent accessible surface areas at atomic and residue level. *Nucleic Acids Research*, **2003**, 31, 3364-6	20.1	174
521	Acidity and basicity of N-heterocyclic carbene ligands. A computational assessment. *Journal of Organometallic Chemistry*, **2006**, 691, 4350-4358	2.3	171
520	Thermodynamics of N-Heterocyclic Carbene Dimerization: The Balance of Sterics and Electronics. *Organometallics*, **2008**, 27, 2679-2681	3.8	170
519	Electronic Properties of N-Heterocyclic Carbene (NHC) Ligands: Synthetic, Structural, and Spectroscopic Studies of (NHC)Platinum(II) Complexes. *Organometallics*, **2007**, 26, 5880-5889	3.8	168
518	Lewis pair polymerization by classical and frustrated Lewis pairs: acid, base and monomer scope and polymerization mechanism. *Dalton Transactions*, **2012**, 41, 9119-34	4.3	164
517	Shape and Volume of Cavities in Thermoplastic Molecular Sieves Based on Syndiotactic Polystyrene. *Chemistry of Materials*, **2001**, 13, 1506-1511	9.6	164
516	COCOMAPS: a web application to analyze and visualize contacts at the interface of biomolecular complexes. *Bioinformatics*, **2011**, 27, 2915-6	7.2	159
515	The structure and binding mode of citrate in the stabilization of gold nanoparticles. *Nature Chemistry*, **2017**, 9, 890-895	17.6	158
514	Comparing the enantioselective power of steric and electrostatic effects in transition-metal-catalyzed asymmetric synthesis. *Chemistry - A European Journal*, **2010**, 16, 14348-53	4.8	150
513	High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. *Nature Catalysis*, **2020**, 3, 985-992	36.5	149
512	Flexibility of N-heterocyclic carbene ligands in ruthenium complexes relevant to olefin metathesis and their impact in the first coordination sphere of the metal. *Journal of the American Chemical Society*, **2010**, 132, 4249-58	16.4	148
511	Rational Electrode Electrolyte Design for Efficient Ammonia Electrosynthesis under Ambient Conditions. *ACS Energy Letters*, **2018**, 3, 1219-1224	20.1	146

510	Recognizing the Mechanism of Sulfurized Polyacrylonitrile Cathode Materials for Li–S Batteries and beyond in Al–S Batteries. *ACS Energy Letters*, **2018**, 3, 2899-2907	20.1	146
509	[Pd(IPr*)(cinnamyl)Cl]: an efficient pre-catalyst for the preparation of tetra-ortho-substituted biaryls by Suzuki-Miyaura cross-coupling. *Chemistry - A European Journal*, **2012**, 18, 4517-21	4.8	142
508	A possible model for the stereospecificity in the syndiospecific polymerization of propene with group 4a metallocenes. *Macromolecules*, **1991**, 24, 1784-1790	5.5	138
507	Implementation of the IMOMM methodology for performing combined QM/MM molecular dynamics simulations and frequency calculations. *Theoretical Chemistry Accounts*, **1998**, 100, 307-313	1.9	135
506	New Insights on Graphite Anode Stability in Rechargeable Batteries: Li Ion Coordination Structures Prevail over Solid Electrolyte Interphases. *ACS Energy Letters*, **2018**, 3, 335-340	20.1	134
505	Feasibility of N Binding and Reduction to Ammonia on Fe-Deposited MoS 2D Sheets: A DFT Study. *Chemistry - A European Journal*, **2017**, 23, 8275-8279	4.8	133
504	Key Elements in the Structure and Function Relationship of the MgCl2/TiCl4/Lewis Base Ziegler–Natta Catalytic System. *Macromolecules*, **2007**, 40, 9181-9189	5.5	125
503	Mechanistic features of isomerizing alkoxycarbonylation of methyl oleate. *Journal of the American Chemical Society*, **2012**, 134, 17696-703	16.4	124
502	Gold- and platinum-catalyzed cycloisomerization of enynyl esters versus allenenyl esters: an experimental and theoretical study. *Chemistry - A European Journal*, **2009**, 15, 3243-60	4.8	122
501	The elusive mechanism of olefin metathesis promoted by (NHC)Ru-based catalysts: a trade between steric, electronic, and solvent effects. *Journal of the American Chemical Society*, **2006**, 128, 13352-3	16.4	122
500	Selective Reduction of CO2 to CH4 by Tandem Hydrosilylation with Mixed Al/B Catalysts. *Journal of the American Chemical Society*, **2016**, 138, 5321-33	16.4	122
499	The Comparison between Single Atom Catalysis and Surface Organometallic Catalysis. *Chemical Reviews*, **2020**, 120, 734-813	68.1	120
498	A Highly Selective Copper–Indium Bimetallic Electrocatalyst for the Electrochemical Reduction of Aqueous CO2 to CO. *Angewandte Chemie*, **2015**, 127, 2174-2178	3.6	118
497	Geometry and Stability of Titanium Chloride Species Adsorbed on the (100) and (110) Cuts of the MgCl2 Support of the Heterogeneous Ziegler–Natta Catalysts. *Macromolecules*, **2000**, 33, 8953-8962	5.5	116
496	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. *Journal of the American Chemical Society*, **2018**, 140, 3724-3735	16.4	114
495	Thermoplastic Molecular Sieves. *Chemistry of Materials*, **2000**, 12, 363-368	9.6	112
494	Origin of enantioselectivity in the asymmetric Ru-catalyzed metathesis of olefins. *Journal of the American Chemical Society*, **2004**, 126, 9592-600	16.4	111
493	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111

492	Selectivity Switch in the Synthesis of Vinylgold(I) Intermediates. *Organometallics*, **2011**, 30, 6328-6337	3.8	110
491	Synthesis of 3-fluoro-3-aryl oxindoles: direct enantioselective □arylation of amides. *Angewandte Chemie - International Edition*, **2012**, 51, 2870-3	16.4	106
490	[{Au(IPr)}2(□OH)]X complexes: synthetic, structural and catalytic studies. *Chemistry - A European Journal*, **2011**, 17, 1238-46	4.8	103
489	Cooperative Effect of Monopodal Silica-Supported Niobium Complex Pairs Enhancing Catalytic Cyclic Carbonate Production. *Journal of the American Chemical Society*, **2015**, 137, 7728-39	16.4	100
488	Bifunctional (cyclopentadienone)iron-tricarbonyl complexes: synthesis, computational studies and application in reductive amination. *Chemistry - A European Journal*, **2013**, 19, 17881-90	4.8	100
487	Ascorbic Acid as a Bifunctional Hydrogen Bond Donor for the Synthesis of Cyclic Carbonates from CO2 under Ambient Conditions. *ACS Sustainable Chemistry and Engineering*, **2017**, 5, 6392-6397	8.3	100
486	Mechanisms of Propagation and Termination Reactions in Classical Heterogeneous Ziegler□Natta Catalytic Systems: A Nonlocal Density Functional Study. *Journal of the American Chemical Society*, **1998**, 120, 2428-2436	16.4	100
485	Relationship between Regiospecificity and Type of Stereospecificity in Propene Polymerization with Zirconocene-Based Catalysts1. *Journal of the American Chemical Society*, **1997**, 119, 4394-4403	16.4	99
484	Identification and characterization of a new family of catalytically highly active imidazolin-2-ylidenes. *Journal of the American Chemical Society*, **2008**, 130, 6848-58	16.4	98
483	Mechanistic insights on acrylate insertion polymerization. *Journal of the American Chemical Society*, **2010**, 132, 4418-26	16.4	96
482	A comprehensive mechanistic picture of the isomerizing alkoxycarbonylation of plant oils. *Journal of the American Chemical Society*, **2014**, 136, 16871-81	16.4	95
481	Hydrogenation of CO -Derived Carbonates and Polycarbonates to Methanol and Diols by Metal-Ligand Cooperative Manganese Catalysis. *Angewandte Chemie - International Edition*, **2018**, 57, 13439-13443	16.4	92
480	Energy-Efficient Nitrogen Reduction to Ammonia at Low Overpotential in Aqueous Electrolyte under Ambient Conditions. *ChemSusChem*, **2018**, 11, 3416-3422	8.3	92
479	Electrolyte Engineering Enables High Stability and Capacity Alloying Anodes for Sodium and Potassium Ion Batteries. *ACS Energy Letters*, **2020**, 5, 766-776	20.1	91
478	Blue-emitting dinuclear N-heterocyclic dicarbene gold(I) complex featuring a nearly unit quantum yield. *Inorganic Chemistry*, **2012**, 51, 1778-84	5.1	91
477	New Insight on the Role of Electrolyte Additives in Rechargeable Lithium Ion Batteries. *ACS Energy Letters*, **2019**, 4, 2613-2622	20.1	90
476	The activation mechanism of Ru-indenylidene complexes in olefin metathesis. *Journal of the American Chemical Society*, **2013**, 135, 7073-9	16.4	88
475	Site chirality as a messenger in chain-end stereocontrolled propene polymerization. *Journal of the American Chemical Society*, **2002**, 124, 13368-9	16.4	87

474	A possible mechanism for enantioselectivity in the chiral epoxidation of olefins with. *Chemistry - A European Journal*, **2001**, 7, 800-7	4.8	86
473	Enantioselectivity in the Regioirregular Placements and Regiospecificity in the Isospecific Polymerization of Propene with Homogeneous Ziegler-Natta Catalysts. *Journal of the American Chemical Society*, **1994**, 116, 2988-2995	16.4	86
472	A Site-Selective Doping Strategy of Carbon Anodes with Remarkable K-Ion Storage Capacity. *Angewandte Chemie - International Edition*, **2020**, 59, 4448-4455	16.4	86
471	Electronic effects in (salen)Mn-based epoxidation catalysts. *Journal of Organic Chemistry*, **2003**, 68, 6202-12	4.2	84
470	Back-Skip of the Growing Chain at Model Complexes for the Metallocene Polymerization Catalysis. *Macromolecules*, **1996**, 29, 4834-4845	5.5	82
469	Nickel-catalyzed C-N bond activation: activated primary amines as alkylating reagents in reductive cross-coupling. *Chemical Science*, **2019**, 10, 4430-4435	9.4	81
468	The isolation of [Pd{OC(O)H}(H)(NHC)(PR3)] (NHC = N-heterocyclic carbene) and its role in alkene and alkyne reductions using formic acid. *Journal of the American Chemical Society*, **2013**, 135, 4588-91	16.4	80
467	Mixed Phosphite/N-Heterocyclic Carbene Complexes: Synthesis, Characterization and Catalytic Studies. *Organometallics*, **2010**, 29, 1443-1450	3.8	80
466	Golden Carousel in Catalysis: The Cationic Gold/Propargylic Ester Cycle. *Angewandte Chemie*, **2008**, 120, 730-733	3.6	80
465	Parameter optimized surfaces (POPS): analysis of key interactions and conformational changes in the ribosome. *Nucleic Acids Research*, **2002**, 30, 2950-60	20.1	80
464	Theoretical Investigation of Active Sites at the Corners of MgCl2 Crystallites in Supported Ziegler□Natta Catalysts. *Macromolecules*, **2012**, 45, 3695-3701	5.5	79
463	Room-temperature synthesis of tetra-ortho-substituted biaryls by NHC-catalyzed Suzuki-Miyaura couplings. *Chemistry - A European Journal*, **2011**, 17, 12886-90	4.8	79
462	Enhancing Charge Carrier Lifetime in Metal Oxide Photoelectrodes through Mild Hydrogen Treatment. *Advanced Energy Materials*, **2017**, 7, 1701536	21.8	78
461	Solution processable metal-organic frameworks for mixed matrix membranes using porous liquids. *Nature Materials*, **2020**, 19, 1346-1353	27	78
460	Generation of Cu□h alloy surfaces from CuInO2 as selective catalytic sites for CO2 electroreduction. *Journal of Materials Chemistry A*, **2015**, 3, 19085-19092	13	77
459	Tuning the properties of visible-light-responsive tantalum (oxy)nitride photocatalysts by non-stoichiometric compositions: a first-principles viewpoint. *Physical Chemistry Chemical Physics*, **2014**, 16, 20548-60	3.6	77
458	Organocatalytic conjugate-addition polymerization of linear and cyclic acrylic monomers by N-heterocyclic carbenes: mechanisms of chain initiation, propagation, and termination. *Journal of the American Chemical Society*, **2013**, 135, 17925-42	16.4	77
457	□living□Propene Polymerization with Bis(phenoxyimine) Group 4 Metal Catalysts:□New Strategies and Old Concepts. *Organometallics*, **2004**, 23, 5989-5993	3.8	77

456	The Quest for Converting Biorenewable Bifunctional α-Methylene-γ-butyrolactone into Degradable and Recyclable Polyester: Controlling Vinyl-Addition/Ring-Opening/Cross-Linking Pathways. *Journal of the American Chemical Society*, **2016**, 138, 14326-14337	16.4	77
455	Toward a Unified Model Explaining Heterogeneous Ziegler–Natta Catalysis. *ACS Catalysis*, **2015**, 5, 5431-5435	11.1	76
454	Chain Propagation and Termination Mechanisms for Polymerization of Conjugated Polar Alkenes by [Al]-Based Frustrated Lewis Pairs. *Macromolecules*, **2014**, 47, 7765-7774	5.5	76
453	Enantioselective polymerization of epoxides using biaryl-linked bimetallic cobalt catalysts: a mechanistic study. *Journal of the American Chemical Society*, **2013**, 135, 18901-11	16.4	76
452	Radical Intermediates in the Jacobsen - Katsuki Epoxidation. *Angewandte Chemie - International Edition*, **2000**, 39, 589-592	16.4	76
451	Model catalytic sites for olefin polymerization and diastereoselectivity in the cyclopolymerization of 1,5-hexadiene. *Macromolecules*, **1993**, 26, 260-267	5.5	75
450	Accuracy of DLPNO-CCSD(T) method for noncovalent bond dissociation enthalpies from coinage metal cation complexes. *Journal of Chemical Theory and Computation*, **2015**, 11, 4664-76	6.4	74
449	Phenanthroline Covalent Organic Framework Electrodes for High-Performance Zinc-Ion Supercapattery. *ACS Energy Letters*, **2020**, 5, 2256-2264	20.1	74
448	The doping effect of fluorinated aromatic solvents on the rate of ruthenium-catalysed olefin metathesis. *Chemistry - A European Journal*, **2011**, 17, 12981-93	4.8	74
447	Origin of the regiochemistry of propene insertion at octahedral column 4 polymerization catalysts: design or serendipity?. *Journal of the American Chemical Society*, **2003**, 125, 7172-3	16.4	74
446	[Pd(NHC)(allyl)Cl] Complexes: Synthesis and Determination of the NHC Percent Buried Volume (%Vbur) Steric Parameter. *European Journal of Inorganic Chemistry*, **2009**, 2009, 1767-1773	2.3	73
445	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 MgCl2Platelets. *Macromolecules*, **2000**, 33, 1134-1140	5.5	73
444	Moving up and down the Titanium Oxidation State in Ziegler–Natta Catalysis. *Macromolecules*, **2011**, 44, 778-783	5.5	72
443	Computational modeling of heterogeneous Ziegler-Natta catalysts for olefins polymerization. *Progress in Polymer Science*, **2018**, 84, 89-114	29.6	72
442	Modeling the structure-property relationships of nanoneedles: A journey toward nanomedicine. *Journal of Computational Chemistry*, **2009**, 30, 275-84	3.5	71
441	Accurate energies of hydrogen bonded nucleic acid base pairs and triplets in tRNA tertiary interactions. *Nucleic Acids Research*, **2006**, 34, 865-79	20.1	71
440	Breaking the regioselectivity rule for acrylate insertion in the Mizoroki-Heck reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 8955-9	11.5	70
439	Mg2+ binding and archaeosine modification stabilize the G15 C48 Levitt base pair in tRNAs. *Rna*, **2007**, 13, 1427-36	5.8	70

438	[OSSO]-Type Iron(III) Complexes for the Low-Pressure Reaction of Carbon Dioxide with Epoxides: Catalytic Activity, Reaction Kinetics, and Computational Study. *ACS Catalysis*, **2018**, 8, 6882-6893	13.1	69
437	Propene Polymerization with the Isospecific, Highly Regioselective rac-Me2C(3-t-Bu-1-Ind)2ZrCl2/MAO Catalyst. 2. Combined DFT/MM Analysis of Chain Propagation and Chain Release Reactions. *Organometallics*, **2001**, 20, 1918-1931	3.8	69
436	Gold(I)-catalyzed synthesis of furans and pyrroles via alkyne hydration. *Catalysis Science and Technology*, **2011**, 1, 58	5.5	68
435	A Density Functional and Molecular Mechanics Study Of β-Hydrogen Transfer in Homogeneous Ziegler−Natta Catalysis. *Macromolecules*, **1996**, 29, 2729-2737	5.5	68
434	Doping-Induced Anisotropic Self-Assembly of Silver Icosahedra in [PtAgCl(PPh)] Nanoclusters. *Journal of the American Chemical Society*, **2017**, 139, 1053-1056	16.4	67
433	Mechanistic insights into the cis-trans isomerization of ruthenium complexes relevant to catalysis of olefin metathesis. *Chemistry - A European Journal*, **2010**, 16, 14354-64	4.8	67
432	Supramolecular water oxidation with Ru-bda-based catalysts. *Chemistry - A European Journal*, **2014**, 20, 17282-6	4.8	66
431	How does the addition of steric hindrance to a typical N-heterocyclic carbene ligand affect catalytic activity in olefin metathesis?. *Dalton Transactions*, **2013**, 42, 7433-9	4.3	66
430	A multicomponent synthesis of stereodefined olefins via nickel catalysis and single electron/triplet energy transfer. *Nature Catalysis*, **2019**, 2, 678-687	36.5	65
429	The Right Computational Recipe for Olefin Metathesis with Ru-Based Catalysts: The Whole Mechanism of Ring-Closing Olefin Metathesis. *Journal of Chemical Theory and Computation*, **2014**, 10, 4442-8	6.4	65
428	Coordinatively Unsaturated Ruthenium Complexes As Efficient Alkyne−Azide Cycloaddition Catalysts. *Organometallics*, **2012**, 31, 756-767	3.8	65
427	Exploring the reactivity of Ru-based metathesis catalysts with a pi-acid ligand trans to the Ru-ylidene bond. *Journal of the American Chemical Society*, **2009**, 131, 9000-6	16.4	65
426	Highly Chemo- and Stereoselective Transfer Semihydrogenation of Alkynes Catalyzed by a Stable, Well-Defined Manganese(II) Complex. *ACS Catalysis*, **2018**, 8, 4103-4109	13.1	64
425	Substrate Lattice-Guided Seed Formation Controls the Orientation of 2D Transition-Metal Dichalcogenides. *ACS Nano*, **2017**, 11, 9215-9222	16.7	64
424	Thermodynamics of Formation of Uncovered and Dimethyl Ether-Covered MgCl2 Crystallites. Consequences in the Structure of Ziegler−Natta Heterogeneous Catalysts. *Journal of Physical Chemistry C*, **2011**, 115, 13322-13328	3.8	63
423	Coupling of Carbon Dioxide with Epoxides Efficiently Catalyzed by Thioether-Triphenolate Bimetallic Iron(III) Complexes: Catalyst Structure−Reactivity Relationship and Mechanistic DFT Study. *Advanced Synthesis and Catalysis*, **2016**, 358, 3231-3243	5.6	62
422	Key Interactions in Heterogeneous Ziegler−Natta Catalytic Systems: Structure and Energetics of TiCl4−Lewis Base Complexes. *Journal of Physical Chemistry C*, **2007**, 111, 4412-4419	3.8	62
421	Manganese-Salen Complexes as Oxygen-Transfer Agents in Catalytic Epoxidations: A Density Functional Study of Mechanistic Aspects. *European Journal of Inorganic Chemistry*, **2003**, 2003, 892-902	2.3	62

420	Molecular-Scale Interfacial Model for Predicting Electrode Performance in Rechargeable Batteries. *ACS Energy Letters*, **2019**, 4, 1584-1593	20.1	61
419	Assessing the pKa-Dependent Activity of Hydroxyl Hydrogen Bond Donors in the Organocatalyzed Cycloaddition of Carbon Dioxide to Epoxides: Experimental and Theoretical Study. *Advanced Synthesis and Catalysis*, **2019**, 361, 366-373	5.6	61
418	In-operando elucidation of bimetallic CoNi nanoparticles during high-temperature CH4/CO2 reaction. *Applied Catalysis B: Environmental*, **2017**, 213, 177-189	21.8	60
417	Tailoring the Crystal Structure of Nanoclusters Unveiled High Photoluminescence via Ion Pairing. *Chemistry of Materials*, **2018**, 30, 2719-2725	9.6	60
416	A Molecular Dynamics Study of the First Five Generations of Poly(Propylene Imine) Dendrimers Modified with N-tBoc-L-Phenylalanine. *Chemistry - A European Journal*, **1998**, 4, 927-934	4.8	60
415	A theoretical study of steric and electronic effects in the rhodium-catalyzed carbonylation reactions. *Journal of the American Chemical Society*, **2001**, 123, 12294-302	16.4	60
414	Oxidative Addition to Palladium(0) Made Easy through Photoexcited-State Metal Catalysis: Experiment and Computation. *Angewandte Chemie - International Edition*, **2019**, 58, 3412-3416	16.4	60
413	Towards more realistic computational modeling of homogenous catalysis by density functional theory: combined QM/MM and ab initio molecular dynamics. *Catalysis Today*, **1999**, 50, 479-500	5.3	59
412	Mechanistic Study of Suzuki–Miyaura Cross-Coupling Reactions of Amides Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. *ChemCatChem*, **2018**, 10, 3096-3106	5.2	58
411	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2019**, 87, 1200-1221	4.2	58
410	Mechanism of racemization of chiral alcohols mediated by 16-electron ruthenium complexes. *Journal of the American Chemical Society*, **2010**, 132, 13146-9	16.4	58
409	Hexafluorobenzene: a powerful solvent for a noncovalent stereoselective organocatalytic Michael addition reaction. *Chemical Communications*, **2012**, 48, 1650-2	5.8	57
408	A computational perspective of olefins metathesis catalyzed by N-heterocyclic carbene ruthenium (pre)catalysts. *Catalysis Science and Technology*, **2011**, 1, 1287	5.5	57
407	Magnesium-Catalyzed Hydroboration of Terminal and Internal Alkynes. *Angewandte Chemie - International Edition*, **2019**, 58, 7025-7029	16.4	56
406	Chemodivergent metathesis of dienynes catalyzed by ruthenium-indenylidene complexes: an experimental and computational study. *Chemistry - A European Journal*, **2009**, 15, 10244-54	4.8	56
405	3D Crumpled Ultrathin 1T MoS for Inkjet Printing of Mg-Ion Asymmetric Micro-supercapacitors. *ACS Nano*, **2020**, 14, 7308-7318	16.7	55
404	Dynamics of the NbCl5-catalyzed cycloaddition of propylene oxide and CO2 : assessing the dual role of the nucleophilic Co-catalysts. *Chemistry - A European Journal*, **2014**, 20, 11870-82	4.8	55
403	Catalyst-site-controlled coordination polymerization of polar vinyl monomers to highly syndiotactic polymers. *Journal of the American Chemical Society*, **2010**, 132, 2695-709	16.4	55

402	A versatile gold synthon for acetylene C-H bond activation. *Dalton Transactions*, **2010**, 39, 10382-90	4.3	55
401	Turning a Methanation Co Catalyst into an In Situ Methanol Producer. *ACS Catalysis*, **2019**, 9, 6910-6918	13.1	54
400	Control of Chain Walking by Weak Neighboring Group Interactions in Unsymmetrical Catalysts. *Journal of the American Chemical Society*, **2018**, 140, 1305-1312	16.4	54
399	Selective Metathesis of Olefins from Bio-Sourced Fischer Tropsch Feeds. *ACS Catalysis*, **2016**, 6, 7970-7976	13.1	54
398	Multicomponent synthesis of unsymmetrical unsaturated N-heterocyclic carbene precursors and their related transition-metal complexes. *Angewandte Chemie - International Edition*, **2013**, 52, 14103-7	16.4	54
397	C2-symmetric chiral disulfoxide ligands in rhodium-catalyzed 1,4-addition: from ligand synthesis to the enantioselection pathway. *Chemistry - A European Journal*, **2010**, 16, 14335-47	4.8	54
396	Mechanistic insights into the double CH (de)activation route of a Ru-based olefin metathesis catalyst?. *Journal of Molecular Catalysis A*, **2010**, 324, 75-79		54
395	Complete mechanism of sigma* intramolecular aromatic hydroxylation through O2 activation by a macrocyclic dicopper(I) complex. *Journal of the American Chemical Society*, **2008**, 130, 17710-7	16.4	54
394	Mechanism of the Suzuki Miyaura Cross-Coupling Reaction Mediated by [Pd(NHC)(allyl)Cl] Precatalysts. *Organometallics*, **2017**, 36, 2088-2095	3.8	53
393	On the accuracy of DFT methods in reproducing ligand substitution energies for transition metal complexes in solution: the role of dispersive interactions. *ChemPhysChem*, **2012**, 13, 562-9	3.2	53
392	Activation and Deactivation of Neutral Palladium(II) Phosphinesulfonato Polymerization Catalysts. *Organometallics*, **2012**, 31, 8388-8406	3.8	53
391	Gold Nanoparticle/Polymer Interfaces: All Atom Structures from Molecular Dynamics Simulations. *Journal of Physical Chemistry C*, **2011**, 115, 15154-15163	3.8	53
390	A Theoretical Study of Syndiospecific Styrene Polymerization with Cp-Based and Cp-Free Titanium Catalysts. 2. Mechanism of Chain-End Stereocontrol. *Macromolecules*, **2001**, 34, 5379-5385	5.5	53
389	How phenyl makes a difference: mechanistic insights into the ruthenium(II)-catalysed isomerisation of allylic alcohols. *Chemical Science*, **2014**, 5, 180-188	9.4	52
388	Synthesis and Reactivity of Ruthenium Phosphite Indenylidene Complexes. *Organometallics*, **2012**, 31, 7415-7426	3.8	52
387	Face donation from the aromatic N-substituent of N-heterocyclic carbene ligands to metal and its role in catalysis. *Journal of the American Chemical Society*, **2012**, 134, 8127-35	16.4	52
386	Highly Efficient and Eco-Friendly Gold-Catalyzed Synthesis of Homoallylic Ketones. *ACS Catalysis*, **2014**, 4, 2701-2705	13.1	51
385	Insights into the decomposition of olefin metathesis precatalysts. *Angewandte Chemie - International Edition*, **2014**, 53, 8995-9	16.4	51

384	Concepts for stereoselective acrylate insertion. *Journal of the American Chemical Society*, **2013**, 135, 10266-6	16.4	51
383	Activation of hydrogen by palladium(0): formation of the mononuclear dihydride complex trans-[Pd(H)2(IPr)(PCy3)]. *Angewandte Chemie - International Edition*, **2009**, 48, 5182-6	16.4	51
382	Toward a catalytic cycle for the Mn-salen mediated alkene epoxidation: a computational approach. *Inorganic Chemistry*, **2004**, 43, 2175-82	5.1	51
381	A combined mechanistic and computational study of the gold(I)-catalyzed formation of substituted indenes. *Organic and Biomolecular Chemistry*, **2011**, 9, 101-4	3.9	50
380	Conversion of actual flue gas CO 2 via cycloaddition to propylene oxide catalyzed by a single-site, recyclable zirconium catalyst. *Journal of CO2 Utilization*, **2017**, 20, 243-252	7.6	49
379	An Alternative Reaction Pathway for Iridium-Catalyzed Water Oxidation Driven by Cerium Ammonium Nitrate (CAN). *ACS Catalysis*, **2016**, 6, 4559-4563	13.1	49
378	Stereoselectivity in metallocene-catalyzed coordination polymerization of renewable methylene butyrolactones: from stereo-random to stereo-perfect polymers. *Journal of the American Chemical Society*, **2012**, 134, 7278-81	16.4	49
377	Comparison of different ruthenium-alkylidene bonds in the activation step with N-heterocyclic carbene Ru-catalysts for olefins metathesis. *Dalton Transactions*, **2011**, 40, 11066-9	4.3	49
376	Rationalizing current strategies to protect N-heterocyclic carbene-based ruthenium catalysts active in olefin metathesis from C-H (de)activation. *Chemical Communications*, **2011**, 47, 6674-6	5.8	49
375	Influence of Ligand Substitutions on the Regiospecificity and Stereospecificity in Isospecific Zirconocenes for Propene Polymerization. A Molecular Mechanics Analysis. *Macromolecules*, **1998**, 31, 3431-3438	5.5	49
374	Model-Based Design of Graphite-Compatible Electrolytes in Potassium-Ion Batteries. *ACS Energy Letters*, **2020**, 5, 2651-2661	20.1	49
373	Theoretical Study of Syndiospecific Styrene Polymerization with Cp-Based and Cp-Free Titanium Catalysts. 1. Mechanism of Chain Propagation. *Macromolecules*, **2001**, 34, 2459-2468	5.5	48
372	Electrolyte-Mediated Stabilization of High-Capacity Micro-Sized Antimony Anodes for Potassium-Ion Batteries. *Advanced Materials*, **2021**, 33, e2005993	24	48
371	Phase Inversion Strategy to Flexible Freestanding Electrode: Critical Coupling of Binders and Electrolytes for High Performance Li S Battery. *Advanced Functional Materials*, **2018**, 28, 1802244	15.6	48
370	Direct versus ligand-exchange synthesis of [PtAg(BDT)(TPP)] nanoclusters: effect of a single-atom dopant on the optoelectronic and chemical properties. *Nanoscale*, **2017**, 9, 9529-9536	7.7	47
369	Manganese Catalyzed Regioselective C-H Alkylation: Experiment and Computation. *Organic Letters*, **2018**, 20, 3105-3108	6.2	47
368	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. *Organometallics*, **2002**, 21, 4939-4949	3.8	47
367	Insertion of a N-Heterocyclic Carbene (NHC) into a Platinum Olefin Bond. *Organometallics*, **2007**, 26, 3286-3288	3.8	46

366	Proton-Transfer Polymerization by N-Heterocyclic Carbenes: Monomer and Catalyst Scopes and Mechanism for Converting Dimethacrylates into Unsaturated Polyesters. *Journal of the American Chemical Society*, **2016**, 138, 2021-35	16.4	45
365	Controlling the hydrogenolysis of silica-supported tungsten pentamethyl leads to a class of highly electron deficient partially alkylated metal hydrides. *Chemical Science*, **2016**, 7, 1558-1568	9.4	45
364	From olefin metathesis catalyst to alcohol racemization catalyst in one step. *Angewandte Chemie - International Edition*, **2012**, 51, 1042-5	16.4	45
363	N-heterocyclic carbene complexes of au, pd, and pt as effective catalysts in organic synthesis. *Topics in Current Chemistry*, **2011**, 302, 131-55		45
362	Transition Metal Mediated Epoxidation as Test Case for the Performance of Different Density Functionals: A Computational Study. *Journal of Physical Chemistry A*, **2003**, 107, 5466-5471	2.8	45
361	On the effects of methyl substituents on chelating ligands in models for homogeneous isospecific Ziegler-Natta catalysis. *Polymer*, **1991**, 32, 1329-1335	3.9	45
360	Metal-Free Catalytic Asymmetric Fluorination of Keto Esters Using a Combination of Hydrogen Fluoride (HF) and Oxidant: Experiment and Computation. *ACS Catalysis*, **2018**, 8, 2582-2588	13.1	44
359	Inverting the Diastereoselectivity of the Mukaiyama–Michael Addition with Graphite-Based Catalysts. *ACS Catalysis*, **2014**, 4, 492-496	13.1	44
358	Computational methods to predict the reactivity of nanoparticles through structure-property relationships. *Expert Opinion on Drug Delivery*, **2010**, 7, 295-305	8	44
357	Frequency and effect of the binding of Mg2+, Mn2+, and Co2+ ions on the guanine base in Watson-Crick and reverse Watson-Crick base pairs. *Journal of Physical Chemistry B*, **2009**, 113, 15670-8	3.4	44
356	Buried Volume Analysis for Propene Polymerization Catalysis Promoted by Group 4 Metals: A Tool for Molecular Mass Prediction. *ACS Catalysis*, **2015**, 5, 6815-6822	13.1	43
355	A latent ruthenium based olefin metathesis catalyst with a sterically demanding NHC ligand. *Catalysis Science and Technology*, **2012**, 2, 1640	5.5	43
354	Single-Step Access to Long-Chain α,ω-Dicarboxylic Acids by Isomerizing Hydroxycarbonylation of Unsaturated Fatty Acids. *ACS Catalysis*, **2016**, 6, 8229-8238	13.1	42
353	Constructing Bridges between Computational Tools in Heterogeneous and Homogeneous Catalysis. *ACS Catalysis*, **2018**, 8, 5637-5656	13.1	42
352	Engineering Sodium-Ion Solvation Structure to Stabilize Sodium Anodes: Universal Strategy for Fast-Charging and Safer Sodium-Ion Batteries. *Nano Letters*, **2020**, 20, 3247-3254	11.5	41
351	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). *Organometallics*, **2013**, 32, 3249-3252	3.8	41
350	Probing the mechanism of O2 activation by a copper(I) biomimetic complex of a C-H hydroxylating copper monooxygenase. *Inorganic Chemistry*, **2009**, 48, 4062-6	5.1	41
349	Ligand Mobility and Solution Structures of the Metallocenium Ion Pairs [Me2C(Cp)(fluorenyl)MCH2SiMe3+][X] (M = Zr, Hf; X = MeB(C6F5)3, B(C6F5)4). *Organometallics*, **2008**, 27, 5474-5487	3.8	41

348	On the Mechanism of the Digold(I)-Hydroxide-Catalysed Hydrophenoxylation of Alkynes. *Chemistry - A European Journal*, **2016**, 22, 1125-32	4.8	41
347	Manganese-Catalyzed Multicomponent Synthesis of Pyrroles through Acceptorless Dehydrogenation Hydrogen Autotransfer Catalysis: Experiment and Computation. *ChemSusChem*, **2019**, 12, 3083-3088	8.3	41
346	Unraveling the New Role of an Ethylene Carbonate Solvation Shell in Rechargeable Metal Ion Batteries. *ACS Energy Letters*, **2021**, 6, 69-78	20.1	41
345	The pivotal role of symmetry in the ruthenium-catalyzed ring-closing metathesis of olefins. *Chemistry - A European Journal*, **2011**, 17, 8618-29	4.8	40
344	Molecular Mechanics and Stereospecificity in Ziegler□Natta 1,2 and Cis-1,4 Polymerizations of Conjugated Dienes. *Macromolecules*, **1997**, 30, 677-684	5.5	39
343	Parametrization of an empirical correction term to density functional theory for an accurate description of pi-stacking interactions in nucleic acids. *Journal of Physical Chemistry B*, **2007**, 111, 13124-34	3.4	39
342	Stereoselectivity and Chemoselectivity in Ziegler□Natta Polymerizations of Conjugated Dienes. 1. Monomers with Low-Energy s-Cis □4 Coordination§. *Macromolecules*, **2001**, 34, 7952-7960	5.5	39
341	Nickel-catalyzed Suzuki-Miyaura cross-couplings of aldehydes. *Nature Communications*, **2019**, 10, 1957	17.4	38
340	Amino acid ionic liquids as potential candidates for CO2 capture: Combined density functional theory and molecular dynamics simulations. *Chemical Physics Letters*, **2020**, 745, 137239	2.5	38
339	Unusual NHC-Iridium(I) Complexes and Their Use in the Intramolecular Hydroamination of Unactivated Aminoalkenes. *Chemistry - A European Journal*, **2016**, 22, 6939-46	4.8	38
338	Occurrence and stability of lone pair-□stacking interactions between ribose and nucleobases in functional RNAs. *Nucleic Acids Research*, **2017**, 45, 11019-11032	20.1	38
337	Determination of the electronic, dielectric, and optical properties of sillenite Bi12TiO20 and perovskite-like Bi4Ti3O12 materials from hybrid first-principle calculations. *Journal of Chemical Physics*, **2016**, 144, 134702	3.9	38
336	Tandem Conversion of CO2 to Valuable Hydrocarbons in Highly Concentrated Potassium Iron Catalysts. *ChemCatChem*, **2019**, 11, 2879-2886	5.2	37
335	An atlas of RNA base pairs involving modified nucleobases with optimal geometries and accurate energies. *Nucleic Acids Research*, **2015**, 43, 6714-29	20.1	37
334	Dynamic properties of metallocenium ion pairs in solution by atomistic simulations. *Journal of the American Chemical Society*, **2006**, 128, 10952-9	16.4	37
333	Additives Engineered Nonflammable Electrolyte for Safer Potassium Ion Batteries. *Advanced Functional Materials*, **2020**, 30, 2001934	15.6	37
332	Troubles in the Systematic Prediction of Transition Metal Thermochemistry with Contemporary Out-of-the-Box Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 1542-60	6.4	37
331	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. *Physical Chemistry Chemical Physics*, **2017**, 19, 9374-9391	3.6	36

330	Investigating Phthalate and 1,3-Diether Coverage and Dynamics on the (104) and (110) Surfaces of MgCl2-Supported Ziegler□Natta Catalysts. *Journal of Physical Chemistry C*, **2014**, 118, 8050-8058	3.8	36
329	Structural analogies between homogeneous and heterogeneous catalysts for the stereospecific polymerization of 1-alkenes. *Journal of Molecular Catalysis*, **1992**, 74, 433-442		36
328	Controlled Acrylate Insertion Regioselectivity in Diazaphospholidine-Sulfonato Palladium(II) Complexes. *Organometallics*, **2012**, 31, 8505-8515	3.8	35
327	Buchwald□Hartwig cross-coupling of amides (transamidation) by selective N□C(O) cleavage mediated by air- and moisture-stable [Pd(NHC)(allyl)Cl] precatalysts: catalyst evaluation and mechanism. *Catalysis Science and Technology*, **2020**, 10, 710-716	5.5	35
326	Kinetics on NiZn Bimetallic Catalysts for Hydrogen Evolution via Selective Dehydrogenation of Methylcyclohexane to Toluene. *ACS Catalysis*, **2017**, 7, 1592-1600	13.1	34
325	Comparing Ru and Fe-catalyzed olefin metathesis. *Dalton Transactions*, **2014**, 43, 11216-20	4.3	34
324	How Well Can DFT Reproduce Key Interactions in Ziegler□Natta Systems?. *Macromolecular Chemistry and Physics*, **2013**, 214, 1980-1989	2.6	34
323	Pesticides Curbing Soil Fertility: Effect of Complexation of Free Metal Ions. *Frontiers in Chemistry*, **2017**, 5, 43	5	34
322	Hydration-Effect-Promoting Ni-Fe Oxyhydroxide Catalysts for Neutral Water Oxidation. *Advanced Materials*, **2020**, 32, e1906806	24	33
321	Synthesis of 3-Fluoro-3-aryl Oxindoles: Direct Enantioselective □Arylation of Amides. *Angewandte Chemie*, **2012**, 124, 2924-2927	3.6	33
320	Exploring electronic and steric effects on the insertion and polymerization reactivity of phosphinesulfonato Pd(II) catalysts. *Chemistry - A European Journal*, **2013**, 19, 17773-88	4.8	33
319	Interfacial Model Deciphering High-Voltage Electrolytes for High Energy Density, High Safety, and Fast-Charging Lithium-Ion Batteries. *Advanced Materials*, **2021**, 33, e2102964	24	33
318	Exploring the mechanism of Grignard metathesis polymerization of 3-alkylthiophenes. *Dalton Transactions*, **2014**, 43, 15143-50	4.3	32
317	Major Difference in Visible-Light Photocatalytic Features between Perfect and Self-Defective Ta3N5 Materials: A Screened Coulomb Hybrid DFT Investigation. *Journal of Physical Chemistry C*, **2014**, 118, 20784-20790	3.8	32
316	Catalytic deuteration of silanes mediated by N-heterocyclic carbene-Ir(III) complexes. *Chemical Communications*, **2011**, 47, 9723-5	5.8	32
315	Stability and cations coordination of DNA and RNA 14-mer G-quadruplexes: a multiscale computational approach. *Journal of Physical Chemistry B*, **2008**, 112, 12115-23	3.4	32
314	Model-Based Design of Stable Electrolytes for Potassium Ion Batteries. *ACS Energy Letters*, **2020**, 5, 3124-3131	23.1	32
313	Well-Defined Surface Species [(?Si□O□)W(?O)Me3] Prepared by Direct Methylation of [(?Si□O□)W(?O)Cl3], a Catalyst for Cycloalkane Metathesis and Transformation of Ethylene to Propylene. *ACS Catalysis*, **2015**, 5, 2164-2171	13.1	31

312	Impact of Electronic Modification of the Chelating Benzylidene Ligand in cis-Dichloro-Configured Second-Generation Olefin Metathesis Catalysts on Their Activity. *Organometallics*, **2014**, 33, 2806-2813	3.8	31
311	Higher order structural effects stabilizing the reverse Watson-Crick Guanine-Cytosine base pair in functional RNAs. *Nucleic Acids Research*, **2014**, 42, 714-26	20.1	31
310	Neutral Square-Planar Olefin/Alkyl Platinum(II) Complexes Containing a N,N-Iminoamide Ligand. Experimental and Theoretical Evidence of Relevant π-Back-Donation in the Platinum-Olefin Bond. *Organometallics*, **2004**, 23, 2137-2145	3.8	31
309	High-performance pan-tactic polythioesters with intrinsic crystallinity and chemical recyclability. *Science Advances*, **2020**, 6, eabc0495	14.3	31
308	Molecular Engineering of Covalent Organic Framework Cathodes for Enhanced Zinc-Ion Batteries. *Advanced Materials*, **2021**, 33, e2103617	24	31
307	A Mechanistically and Operationally Simple Route to Metal-N-Heterocyclic Carbene (NHC) Complexes. *Chemistry - A European Journal*, **2020**, 26, 4515-4519	4.8	31
306	Investigating Alkoxysilane Coverage and Dynamics on the (104) and (110) Surfaces of MgCl2-Supported Ziegler-Natta Catalysts. *Journal of Physical Chemistry C*, **2012**, 116, 22980-22986	3.8	30
305	Heats of Formation of Medium-Sized Organic Compounds from Contemporary Electronic Structure Methods. *Journal of Chemical Theory and Computation*, **2017**, 13, 3537-3560	6.4	29
304	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. *Journal of Chemical Theory and Computation*, **2017**, 13, 3220-3227	6.4	29
303	Regiochemistry of propene insertion with group 4 polymerization catalysts from a theoretical perspective. *Journal of Organometallic Chemistry*, **2007**, 692, 4519-4527	2.3	29
302	Application of Semiempirical Methods to Transition Metal Complexes: Fast Results but Hard-to-Predict Accuracy. *Journal of Chemical Theory and Computation*, **2018**, 14, 3428-3439	6.4	29
301	CONSRANK: a server for the analysis, comparison and ranking of docking models based on inter-residue contacts. *Bioinformatics*, **2015**, 31, 1481-3	7.2	28
300	Dinuclear Ru-aqua complexes for selective epoxidation catalysis based on supramolecular substrate orientation effects. *Chemistry - A European Journal*, **2014**, 20, 3898-902	4.8	28
299	Ranking multiple docking solutions based on the conservation of inter-residue contacts. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1571-84	4.2	28
298	Energetics of the ruthenium-halide bond in olefin metathesis (pre)catalysts. *Dalton Transactions*, **2013**, 42, 7312-7	4.3	28
297	The intriguing modeling of cis-trans selectivity in ruthenium-catalyzed olefin metathesis. *Beilstein Journal of Organic Chemistry*, **2011**, 7, 40-5	2.5	28
296	Comparing families of olefin polymerization precatalysts using the percentage of buried volume. *Dalton Transactions*, **2009**, 8885-90	4.3	28
295	Effects of pathological mutations on the stability of a conserved amino acid triad in retinoschisin. *FEBS Letters*, **2003**, 544, 21-6	3.8	28

294	Density functional study on the electronic and molecular structure of the hydroformylation catalyst HCo(CO)3. *Organometallics*, **1993**, 12, 3586-3593	3.8	28
293	Catalysis of silica-based anode (de-)lithiation: compositional design within a hollow structure for accelerated conversion reaction kinetics. *Journal of Materials Chemistry A*, **2020**, 8, 12306-12313	13	27
292	Asymmetric Magnesium-Catalyzed Hydroboration by Metal-Ligand Cooperative Catalysis. *Angewandte Chemie - International Edition*, **2019**, 58, 17567-17571	16.4	27
291	Combined experimental□heoretical study of the optoelectronic properties of non-stoichiometric pyrochlore bismuth titanate. *Journal of Materials Chemistry C*, **2015**, 3, 12032-12039	7.1	27
290	Coordination□Addition Polymerization and Kinetic Resolution of Methacrylamides by Chiral Metallocene Catalysts. *Macromolecules*, **2009**, 42, 1462-1471	5.5	27
289	A combined QM/MM study of ligand substitution enthalpies in the L2Fe(CO)3, RuCpL2Cl, and RuCp*L2Cl systems. *Canadian Journal of Chemistry*, **1998**, 76, 1457-1466	0.9	27
288	Olefin Polymerizations with Group IV Metal Catalysts **2007**, 1005-1166		27
287	(E)-(Z) Selectivity in 2-Butene Copolymerization by Group 4 Metallocenes. A Combined Density Functional Theory and Molecular Mechanics Study. *Journal of the American Chemical Society*, **1999**, 121, 8651-8652	16.4	27
286	Mechanistic Insight into the Photoredox-Nickel-HAT Triple Catalyzed Arylation and Alkylation of □Amino C-H Bonds. *Journal of the American Chemical Society*, **2020**, 142, 16942-16952	16.4	27
285	Efficient electrochemical transformation of CO to C/C chemicals on benzimidazole-functionalized copper surfaces. *Chemical Communications*, **2018**, 54, 11324-11327	5.8	27
284	Stereoselectivity and chiral recognition in copper(I) olefin complexes with a chiral diamine. *Chemistry - A European Journal*, **2000**, 6, 1127-39	4.8	27
283	A Site-Selective Doping Strategy of Carbon Anodes with Remarkable K-Ion Storage Capacity. *Angewandte Chemie*, **2020**, 132, 4478-4485	3.6	26
282	A Silica-Supported Monoalkylated Tungsten Dioxo Complex Catalyst for Olefin Metathesis. *ACS Catalysis*, **2018**, 8, 2715-2729	13.1	26
281	Cycloalkyl-based unsymmetrical unsaturated (U)□NHC ligands: flexibility and dissymmetry in ruthenium-catalysed olefin metathesis. *Dalton Transactions*, **2014**, 43, 7044-9	4.3	26
280	The activation mechanism of Fe-based olefin metathesis catalysts. *Chemical Physics Letters*, **2014**, 610-611, 29-32	2.5	26
279	Exploring new generations of ruthenium olefin metathesis catalysts: the reactivity of a bis-ylidene ruthenium complex by DFT. *Dalton Transactions*, **2013**, 42, 7271-5	4.3	26
278	Quantum confinement effect of two-dimensional all-inorganic halide perovskites. *Science China Materials*, **2017**, 60, 811-818	7.1	26
277	Stereospecificity in metallocene catalyzed acrylate polymerizations: the chiral orientation of the growing chain selects its own chain end enantioface. *Journal of the American Chemical Society*, **2006** , 128, 16649-54	16.4	26

276	Quantum Mechanics Calculations on Rhodamine Dyes Require Inclusion of Solvent Water for Accurate Representation of the Structure. *Journal of Physical Chemistry A*, **2004**, 108, 7744-7751	2.8	26
275	Mechanism ofUnlikeStereoselectivity in 1-Alkene Primary Insertions:Syndiospecific Propene Polymerization by Brookhart-Type Nickel(II) Catalysts. *Organometallics*, **2000**, 19, 1343-1349	3.8	26
274	Robust Cross-Linked Stereocomplexes and C60 Inclusion Complexes of Vinyl-Functionalized Stereoregular Polymers Derived from Chemo/Stereoselective Coordination Polymerization. *Journal of the American Chemical Society*, **2016**, 138, 9533-47	16.4	26
273	Re-evaluation of the Mn(salen) mediated epoxidation of alkenes by means of the B3LYP* density functional. *Physical Chemistry Chemical Physics*, **2004**, 6, 3747	3.6	25
272	Enhanced Carrier Transport and Bandgap Reduction in Sulfur-Modified BiVO4 Photoanodes. *Chemistry of Materials*, **2018**, 30, 8630-8638	9.6	25
271	Single-Site Molybdenum on Solid Support Materials for Catalytic Hydrogenation of N -into-NH. *Angewandte Chemie - International Edition*, **2018**, 57, 15812-15816	16.4	25
270	Accurate experimental and theoretical enthalpies of association of TiCl with typical Lewis bases used in heterogeneous Ziegler-Natta catalysis. *Physical Chemistry Chemical Physics*, **2017**, 19, 26996-27006	3.6	24
269	Closed-Loop Polymer Upcycling by Installing Property-Enhancing Comonomer Sequences and Recyclability. *Macromolecules*, **2019**, 52, 4570-4578	5.5	24
268	Significant Impact of Exposed Facets on the BiVO Material Performance for Photocatalytic Water Splitting Reactions. *Journal of Physical Chemistry Letters*, **2020**, 11, 5497-5503	6.4	24
267	Evaluation of an olefin metathesis pre-catalyst with a bulky and electron-rich N-heterocyclic carbene. *Journal of Organometallic Chemistry*, **2015**, 780, 43-48	2.3	24
266	Role of Oxidized Mo Species on the Active Surface of NiMo Electrocatalysts for Hydrogen Evolution under Alkaline Conditions. *ACS Catalysis*, **2020**, 10, 12858-12866	13.1	24
265	[Pd(NHC)(Cl)Cl]: Versatile and Highly Reactive Complexes for Cross-Coupling Reactions that Avoid Formation of Inactive Pd(I) Off-Cycle Products. *IScience*, **2020**, 23, 101377	6.1	24
264	Experimental and Computational Study of an Unexpected Iron-Catalyzed Carboetherification by Cooperative Metal and Ligand Substrate Interaction and Proton Shuttling. *Angewandte Chemie - International Edition*, **2017**, 56, 14863-14867	16.4	23
263	Mechanism of the RuAllenylidene to RuIndenylidene Rearrangement in Ruthenium Precatalysts for Olefin Metathesis. *Organometallics*, **2015**, 34, 3107-3111	3.8	23
262	High-speed organocatalytic polymerization of a renewable methylene butyrolactone by a phosphazene superbase. *Polymer Chemistry*, **2014**, 5, 3261	4.9	23
261	Cationic bis-N-heterocyclic carbene (NHC) ruthenium complex: structure and application as latent catalyst in olefin metathesis. *Chemistry - A European Journal*, **2014**, 20, 13716-21	4.8	23
260	Catalytic Arylation of Imines Leading to N-Unprotected Indoles and Azaindoles. *ACS Catalysis*, **2016**, 6, 2930-2938	13.1	23
259	Impact of Interfacial Defects on the Properties of Monolayer Transition Metal Dichalcogenide Lateral Heterojunctions. *Journal of Physical Chemistry Letters*, **2017**, 8, 1664-1669	6.4	22

258	Non-precious bimetallic catalysts for selective dehydrogenation of an organic chemical hydride system. *Chemical Communications*, **2015**, 51, 12931-4	5.8	22
257	Hydrogenation of CO2-Derived Carbonates and Polycarbonates to Methanol and Diols by Metal□ligand Cooperative Manganese Catalysis. *Angewandte Chemie*, **2018**, 130, 13627-13631	3.6	22
256	Asymmetric Hydroboration of Heteroaryl Ketones by Aluminum Catalysis. *Journal of the American Chemical Society*, **2019**, 141, 19415-19423	16.4	22
255	CONS-COCOMAPS: a novel tool to measure and visualize the conservation of inter-residue contacts in multiple docking solutions. *BMC Bioinformatics*, **2012**, 13 Suppl 4, S19	3.6	22
254	Donor-Ligand Effect on the Product Distribution in the Manganese-Catalyzed Epoxidation of Olefins:□A Computational Assessment. *Organometallics*, **2006**, 25, 177-183	3.8	22
253	Reactivity ofZandEIsomers, Growing Chain Isomerization, and Chain Transfer Reactions in Ethene/2-Butene Copolymerization by Metallocene-Based Catalysts. *Macromolecules*, **2000**, 33, 4647-4659	5.5	22
252	Synthesis, Structure and Catalytic Activity of NHC-Ag(I) Carboxylate Complexes. *Chemistry - A European Journal*, **2016**, 22, 13320-7	4.8	22
251	Theoretical NMR spectroscopy of N-heterocyclic carbenes and their metal complexes. *Coordination Chemistry Reviews*, **2017**, 344, 101-114	23.2	21
250	A theoretical view on the thermodynamic cis□trans equilibrium of dihalo ruthenium olefin metathesis (pre-)catalysts. *Monatshefte F□ Chemie*, **2015**, 146, 1131-1141	1.4	21
249	Insights into functional-group-tolerant polymerization catalysis with phosphine-sulfonamide palladium(II) complexes. *Chemistry - A European Journal*, **2015**, 21, 2062-75	4.8	21
248	Variation of the Sterical Properties of the N-Heterocyclic Carbene Coligand in Thermally Triggerable Ruthenium-Based Olefin Metathesis Precatalysts/Initiators. *Organometallics*, **2015**, 34, 5383-5392	3.8	21
247	How easy is CO2 fixation by M□□ bond containing complexes (M = Cu, Ni, Co, Rh, Ir)?. *Organic Chemistry Frontiers*, **2016**, 3, 19-23	5.2	21
246	Mechanism of n-Butane Hydrogenolysis Promoted by Ta-Hydrides Supported on Silica. *ACS Catalysis*, **2014**, 4, 1868-1874	13.1	21
245	MDcons: Intermolecular contact maps as a tool to analyze the interface of protein complexes from molecular dynamics trajectories. *BMC Bioinformatics*, **2014**, 15 Suppl 5, S1	3.6	21
244	N-Heterocyclic olefins as initiators for the polymerization of (meth)acrylic monomers: a combined experimental and theoretical approach. *Polymer Chemistry*, **2017**, 8, 5803-5812	4.9	21
243	Cycloaddition of CO2 to challenging N-tosyl aziridines using a halogen-free niobium complex: Catalytic activity and mechanistic insights. *Molecular Catalysis*, **2017**, 443, 280-285	3.3	21
242	A comprehensive study of olefin metathesis catalyzed by Ru-based catalysts. *Beilstein Journal of Organic Chemistry*, **2015**, 11, 1767-80	2.5	21
241	Silica-Supported Tungsten Carbynes (?SiO)xW(?CH)(Me)y (x = 1, y = 2; x = 2, y = 1): New Efficient Catalysts for Alkyne Cyclotrimerization. *Organometallics*, **2015**, 34, 690-695	3.8	21

240	Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	21
239	Rare-Earth Half-Sandwich Dialkyl and Homoleptic Trialkyl Complexes for Rapid and Stereoselective Polymerization of a Conjugated Polar Olefin. *Organometallics*, **2013**, 32, 1459-1465	3.8	21
238	Syndioselective MMA Polymerization by Group 4 Constrained Geometry Catalysts: A Combined Experimental and Theoretical Study. *Macromolecules*, **2008**, 41, 6910-6919	5.5	21
237	Insights into the Halogen Oxidative Addition Reaction to Dinuclear Gold(I) Di(NHC) Complexes. *Chemistry - A European Journal*, **2016**, 22, 10211-24	4.8	21
236	Lithium dendrite-free plating/stripping: a new synergistic lithium ion solvation structure effect for reliable lithium-sulfur full batteries. *Chemical Communications*, **2019**, 55, 5713-5716	5.8	20
235	Precision Molecular Threading/Dethreading. *Angewandte Chemie - International Edition*, **2020**, 59, 14825-14834	16.1	20
234	Mechanism of Stereocontrol in Methyl Methacrylate Polymerization Promoted by C1-Symmetric Metallocenes. *Macromolecules*, **2008**, 41, 3439-3445	5.5	20
233	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 □4 coordination. *Polymer*, **2004**, 45, 467-485	3.9	20
232	NHC-Copper(I) Halide-Catalyzed Direct Alkynylation of Trifluoromethyl Ketones on Water. *Chemistry - A European Journal*, **2016**, 22, 8089-94	4.8	20
231	Guidelines To Select the N-Heterocyclic Carbene for the Organopolymerization of Monomers with a Polar Group. *Macromolecules*, **2017**, 50, 1394-1401	5.5	19
230	Ab initio assessment of BiRECuOS (RE = La, Gd, Y, Lu) solid solutions as a semiconductor for photochemical water splitting. *Physical Chemistry Chemical Physics*, **2017**, 19, 12321-12330	3.6	19
229	Biodegradable Polyhydroxyalkanoates by Stereoselective Copolymerization of Racemic Diolides: Stereocontrol and Polyolefin-Like Properties. *Angewandte Chemie - International Edition*, **2020**, 59, 7881-7890	16.1	19
228	Determination of the Intrinsic Defect at the Origin of Poor H2 Evolution Performance of the Monoclinic BiVO4 Photocatalyst Using Density Functional Theory. *Journal of Physical Chemistry C*, **2018**, 122, 18204-18211	3.8	19
227	From ruthenium olefin metathesis catalyst to (□5-3-phenylindenyl)hydrido complex via alcoholysis. *Chemical Communications*, **2014**, 50, 2205-7	5.8	19
226	Catalytic Role of Nickel in the Decarbonylative Addition of Phthalimides to Alkynes. *Organometallics*, **2013**, 32, 6330-6336	3.8	19
225	Ruthenium-catalysed decomposition of formic acid: Fuel cell and catalytic applications. *Molecular Catalysis*, **2017**, 440, 184-189	3.3	19
224	Inner-Sphere versus Outer-Sphere Coordination of BF_4^- in a NHC-Gold(I) Complex. *Organometallics*, **2017**, 36, 2861-2869	3.8	19
223	Understanding Tantalum-Catalyzed Ethylene Trimerization: When Things Go Wrong. *ACS Catalysis*, **2013**, 3, 1360-1364	13.1	19

222	Insertion of Imine into Palladium Methyl and Palladium Acyl Bonds. A Density Functional Study. *Journal of the American Chemical Society*, **1999**, 121, 4238-4241	16.4	19
221	A model for the homogeneous isospecific Ziegler Natta polymerization of olefins: Enantioselectivity in the deuteration and deuteriooligomerization of 1-alkenes. *Chirality*, **1991**, 3, 299-306	2.1	19
220	Regiodivergent Hydroborative Ring Opening of Epoxides via Selective C-O Bond Activation. *Journal of the American Chemical Society*, **2020**, 142, 14286-14294	16.4	19
219	Extension of Surface Organometallic Chemistry to Metal-Organic Frameworks: Development of a Well-Defined Single Site [(?Zr-O-)W(?O)(CHBu)] Olefin Metathesis Catalyst. *Journal of the American Chemical Society*, **2020**, 142, 16690-16703	16.4	19
218	Structural stability, acidity, and halide selectivity of the fluoride riboswitch recognition site. *Journal of the American Chemical Society*, **2015**, 137, 299-306	16.4	18
217	Theoretical Characterization of the H-Bonding and Stacking Potential of Two Nonstandard Nucleobases Expanding the Genetic Alphabet. *Journal of Physical Chemistry B*, **2016**, 120, 2216-24	3.4	18
216	Promotion of selective pathways in isomerizing functionalization of plant oils by rigid framework substituents. *ChemSusChem*, **2014**, 7, 3491-5	8.3	18
215	Structural and energetic characterization of the emissive RNA alphabet based on the isothiazolo[4,3-d]pyrimidine heterocycle core. *Physical Chemistry Chemical Physics*, **2016**, 18, 18045-53	3.6	18
214	Oxidative Addition to Palladium(0) Made Easy through Photoexcited-State Metal Catalysis: Experiment and Computation. *Angewandte Chemie*, **2019**, 131, 3450-3454	3.6	18
213	Synthesis and reactivity of [Au(NHC)(Bpin)] complexes. *Chemical Communications*, **2019**, 55, 6799-6802	5.8	17
212	Predicting the DNP-SENS efficiency in reactive heterogeneous catalysts from hydrophilicity. *Chemical Science*, **2018**, 9, 4866-4872	9.4	17
211	Solid-State NMR and DFT Studies on the Formation of Well-Defined Silica-Supported Tantallaaziridines: From Synthesis to Catalytic Application. *Chemistry - A European Journal*, **2016**, 22, 3000-8	4.8	17
210	Tethering metal ions to photocatalyst particulate surfaces by bifunctional molecular linkers for efficient hydrogen evolution. *ChemSusChem*, **2014**, 7, 2575-83	8.3	17
209	Mechanism of CO2 Fixation by Ir X Bonds (X = OH, OR, N, C). *European Journal of Inorganic Chemistry*, **2015**, 2015, 4653-4657	2.3	17
208	Simple ligand modifications as a key to playing with the stability of Cu(I), Cu(II), and Cu(III) organometallic complexes. *Inorganic Chemistry*, **2009**, 48, 2340-2	5.1	17
207	. *Chemistry - A European Journal*, **2000**, 6, 1127-1139	4.8	17
206	Iridium-Catalyzed Enantioselective Hydroarylation of Alkenes through C-H bond Activation: Experiment and Computation. *Chemistry - A European Journal*, **2020**, 26, 8308-8313	4.8	17
205	Morphology control of anatase TiO for well-defined surface chemistry. *Physical Chemistry Chemical Physics*, **2018**, 20, 14362-14373	3.6	17

204	Au???H-C Hydrogen Bonds as Design Principle in Gold(I) Catalysis. *Angewandte Chemie - International Edition*, **2021**, 60, 21014-21024	16.4	17
203	Prediction of protein assemblies, the next frontier: The CASP14-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2021**, 89, 1800-1823	4.2	17
202	Bio-inspired heteroatom-doped hollow aurilave-like structured carbon for high-performance sodium-ion batteries and supercapacitors. *Journal of Power Sources*, **2020**, 461, 228128	8.9	16
201	Deconstructing Selectivity in the Gold-Promoted Cyclization of Alkynyl Benzothioamides to Six-Membered Mesoionic Carbene or Acyclic Carbene Complexes. *ACS Catalysis*, **2014**, 4, 1287-1291	13.1	16
200	Using a consensus approach based on the conservation of inter-residue contacts to rank CAPRI models. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 2210-20	4.2	16
199	Ruthenium Olefin Metathesis Catalysts Containing Fluoride. *ACS Catalysis*, **2015**, 5, 3932-3939	13.1	16
198	Multicomponent Synthesis of Unsymmetrical Unsaturated N-Heterocyclic Carbene Precursors and Their Related Transition-Metal Complexes. *Angewandte Chemie*, **2013**, 125, 14353-14357	3.6	16
197	Hydride-shuttling chain-transfer polymerization of methacrylates catalyzed by metallocenium enolate metallacycle-hydridoborate ion pairs. *Journal of the American Chemical Society*, **2011**, 133, 1572-88	16.4	16
196	(E)/(Z) Selectivity in the Polymerization of 2-Butene Promoted by Ni(II) Brookhart-Type Catalysts. *Macromolecules*, **2005**, 38, 2072-2075	5.5	16
195	Doubly Bridged ansa-Zirconocenes Based on the Norbornadiene Skeleton: A Quantum Mechanical and Molecular Mechanics Study. *Organometallics*, **1996**, 15, 2254-2263	3.8	16
194	Adsorptive Molecular Sieving of Styrene over Ethylbenzene by Trianglimine Crystals. *Journal of the American Chemical Society*, **2021**, 143, 4090-4094	16.4	16
193	Structure–Activity Relationship To Screen Ni–Bisphosphine Complexes for the Oxidative Coupling of CO2 and Ethylene. *Organometallics*, **2017**, 36, 1107-1112	3.8	15
192	Well-defined silica supported aluminum hydride: another step towards the utopian single site dream?. *Chemical Science*, **2015**, 6, 5456-5465	9.4	15
191	Metathetic Oxidation of 2-Butenes to Acetaldehyde by Molecular Oxygen Using the Single-Site Olefin Metathesis Catalyst (?SiO)2Mo(?O)2. *ACS Catalysis*, **2018**, 8, 7549-7555	13.1	15
190	Tuning the electronic properties by width and length modifications of narrow- diameter carbon nanotubes for nanomedicine. *Current Medicinal Chemistry*, **2012**, 19, 5219-25	4.3	15
189	Highly Active Heterogeneous Catalyst for Ethylene Dimerization Prepared by Selectively Doping Ni on the Surface of a Zeolitic Imidazolate Framework. *Journal of the American Chemical Society*, **2021**, 143, 7144-7153	16.4	15
188	Simple Synthetic Routes to Carbene-M-Amido (M=Cu, Ag, Au) Complexes for Luminescence and Photocatalysis Applications. *Chemistry - A European Journal*, **2021**, 27, 11904-11911	4.8	15
187	Roughening of Copper (100) at Elevated CO Pressure: Cu Adatom and Cluster Formation Enable CO Dissociation. *Journal of Physical Chemistry C*, **2019**, 123, 8112-8121	3.8	15

186	Using sodium acetate for the synthesis of [Au(NHC)X] complexes. *Dalton Transactions*, **2020**, 49, 9694-9709	4.9	14
185	Insights into the Catalytic Activity of [Pd(NHC)(cin)Cl] (NHC=IPr, IPrCl, IPrBr) Complexes in the Suzuki–Miyaura Reaction. *ChemCatChem*, **2018**, 10, 601-611	5.2	14
184	Complexation of trichlorosalicylic acid with alkaline and first row transition metals as a switch for their antibacterial activity. *Inorganica Chimica Acta*, **2018**, 469, 379-386	2.7	14
183	Activity enhancement via borate incorporation into a NiFe (oxy)hydroxide catalyst for electrocatalytic oxygen evolution. *Journal of Materials Chemistry A*, **2018**, 6, 16959-16964	13	14
182	Mechanism of Insertion Polymerization of Allyl Ethers. *Macromolecules*, **2018**, 51, 4525-4531	5.5	14
181	Photophysics and electrochemistry relevant to photocatalytic water splitting involved at solid–electrolyte interfaces. *Journal of Energy Chemistry*, **2017**, 26, 259-269	12	14
180	Synthesis, structural studies and ligand influence on the stability of aryl-NHC stabilised trimethylaluminium complexes. *Dalton Transactions*, **2015**, 44, 15166-74	4.3	14
179	Molecular Modeling of Stereo- and Regioselectivity of Group 4 Heterocenes in the Polymerization of Propene. *Macromolecules*, **2005**, 38, 3973-3976	5.5	14
178	Radikalische Zwischenstufen in der Jacobsen-Katsuki-Epoxidierung. *Angewandte Chemie*, **2000**, 112, 602-604	3.6	14
177	Models for the Explanation of the Stereospecific Behaviour of Ziegler–Natta Catalysts **1995**, 237-249		14
176	Nature of Nitrogen Incorporation in BiVO4 Photoanodes through Chemical and Physical Methods. *Solar Rrl*, **2020**, 4, 1900290	7.1	14
175	The anticancer activity of an air-stable Pd(I)-NHC (NHC = N-heterocyclic carbene) dimer. *Chemical Communications*, **2020**, 56, 12238-12241	5.8	14
174	A Robust and Cost-Efficient Scheme for Accurate Conformational Energies of Organic Molecules. *ChemPhysChem*, **2019**, 20, 92-102	3.2	14
173	Accurate Gas Phase Formation Enthalpies of Alloys and Refractories Decomposition Products. *Inorganic Chemistry*, **2017**, 56, 1386-1401	5.1	13
172	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. *Journal of Physical Chemistry B*, **2015**, 119, 12982-9	3.4	13
171	Theoretical characterization of sulfur-to-selenium substitution in an emissive RNA alphabet: impact on H-bonding potential and photophysical properties. *Physical Chemistry Chemical Physics*, **2018**, 20, 7676-7685	3.6	13
170	Molecular dynamics characterization of five pathogenic Factor X mutants associated with decreased catalytic activity. *Biochemistry*, **2014**, 53, 6992-7001	3.2	13
169	Exploiting Confinement Effects to Tune Selectivity in Cyclooctane Metathesis. *ACS Catalysis*, **2017**, 7, 6581-6586	13.1	13

168	From Olefin Metathesis Catalyst to Alcohol Racemization Catalyst in One Step. *Angewandte Chemie* , **2012**, 124, 1066-1069	3.6	13
167	Probing the Validity of the CH2SiMe3 Group as a Model of the Growing Chain in Mechanistic Studies of Olefin Polymerization with Group 4 Catalysts. *Organometallics*, **2006**, 25, 1431-1433	3.8	13
166	From Capsule to Helix: Guest-Induced Superstructures of Chiral Macrocycle Crystals. *Journal of the American Chemical Society*, **2020**, 142, 15823-15829	16.4	13
165	Preferred Orientation of TiN Coatings Enables Stable Zinc Anodes. *ACS Energy Letters*, **2022**, 7, 197-203	20.1	13
164	Investigating the Structure and Reactivity of Azolyl-Based Copper(I)NHC Complexes: The Role of the Anionic Ligand. *ACS Catalysis*, **2017**, 7, 8176-8183	13.1	12
163	Analysis and Ranking of Protein-Protein Docking Models Using Inter-Residue Contacts and Inter-Molecular Contact Maps. *Molecules*, **2015**, 20, 12045-60	4.8	12
162	Pentacoordinated Organoaluminum Complexes: A Computational Insight. *Organometallics*, **2012**, 31, 8498-8504	3.8	12
161	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 *ChemPhysChem*, **2012**, 13, 1405-1406	3.2	12
160	Electronic Effects on Regioselectivity in Styrene Polyinsertion Promoted by Group 4 Catalysts. *Organometallics*, **2008**, 27, 1028-1029	3.8	12
159	Optically Pure -Symmetric Cyclic(alkyl)(amino)carbene Ruthenium Complexes for Asymmetric Olefin Metathesis. *Journal of the American Chemical Society*, **2020**, 142, 19895-19901	16.4	12
158	Simple activation by acid of latent Ru-NHC-based metathesis initiators bearing 8-quinolinolate co-ligands. *Beilstein Journal of Organic Chemistry*, **2016**, 12, 154-65	2.5	12
157	Introducing a Clustering Step in a Consensus Approach for the Scoring of Protein-Protein Docking Models. *PLoS ONE*, **2016**, 11, e0166460	3.7	12
156	Suitable Fundamental Properties of TaVON Material for Visible-Light-Driven Photocatalysis: A DFT Study. *ACS Omega*, **2016**, 1, 1041-1048	3.9	12
155	Imine Metathesis Catalyzed by a Silica-Supported Hafnium Imido Complex. *ACS Catalysis*, **2018**, 8, 9440-9446	13.1	12
154	Well-Defined Silica Grafted Molybdenum Bis(imido) Catalysts for Imine Metathesis Reactions. *Organometallics*, **2017**, 36, 1550-1556	3.8	11
153	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O2. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	11
152	Activation of Hydrogen by Palladium(0): Formation of the Mononuclear Dihydride Complex trans-[Pd(H)2(IPr)(PCy3)]. *Angewandte Chemie*, **2009**, 121, 5284-5288	3.6	11
151	Methane dry reforming on supported cobalt nanoparticles promoted by boron. *Journal of Catalysis*, **2020**, 392, 126-134	7.3	11

150	D936Y and Other Mutations in the Fusion Core of the SARS-CoV-2 Spike Protein Heptad Repeat 1: Frequency, Geographical Distribution, and Structural Effect. *Molecules*, **2021**, 26,	4.8	11
149	Electrolyte Chemistry in 3D Metal Oxide Nanorod Arrays Deciphers Lithium Dendrite-Free Plating/Stripping Behaviors for High-Performance Lithium Batteries. *Journal of Physical Chemistry Letters*, **2021**, 12, 4857-4866	6.4	11
148	Tungsten(VI) Carbyne/Bis(carbene) Tautomerization Enabled by N-Donor SBA15 Surface Ligands: A Solid-State NMR and DFT Study. *Angewandte Chemie - International Edition*, **2016**, 55, 11162-6	16.4	11
147	Mechanism of Propylene Oxide Polymerization Promoted by N-Heterocyclic Olefins. *Journal of Physical Chemistry C*, **2017**, 121, 2730-2737	3.8	10
146	Occurrence and stability of lone pair-π and OH-π interactions between water and nucleobases in functional RNAs. *Nucleic Acids Research*, **2020**, 48, 5825-5838	20.1	10
145	Exploiting the interactions between the ruthenium Hoveyda-Grubbs catalyst and Al-modified mesoporous silica: the case of SBA15 KCC-1. *Chemical Science*, **2018**, 9, 3531-3537	9.4	10
144	Quantifying the Impact of Relativity and of Dispersion Interactions on the Activation of Molecular Oxygen Promoted by Noble Metal Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 13707-13714	4.8	10
143	Ground-State Gas-Phase Structures of Inorganic Molecules Predicted by Density Functional Theory Methods. *ACS Omega*, **2017**, 2, 8373-8387	3.9	10
142	Mechanism of Isotactic Styrene Polymerization with a C6F5-Substituted Bis(phenoxyimine) Titanium System. *Macromolecules*, **2012**, 45, 8588-8597	5.5	10
141	Enzymatic Formation of an Artificial Base Pair Using a Modified Purine Nucleoside Triphosphate. *ACS Chemical Biology*, **2020**, 15, 2872-2884	4.9	10
140	The D173G mutation in ADAMTS-13 causes a severe form of congenital thrombotic thrombocytopenic purpura. A clinical, biochemical and in silico study. *Thrombosis and Haemostasis*, **2016**, 115, 51-62	7	10
139	Single-Site Tetracoordinated Aluminum Hydride Supported on Mesoporous Silica. From Dream to Reality!. *Organometallics*, **2016**, 35, 3288-3294	3.8	10
138	Toward the Design of New Suitable Materials for Solar Water Splitting Using Density Functional Theory. *ACS Omega*, **2018**, 3, 18117-18123	3.9	10
137	Mechanistic insights into the reductive dehydroxylation pathway for the biosynthesis of isoprenoids promoted by the IspH enzyme. *Chemical Science*, **2015**, 6, 5643-5651	9.4	9
136	Energetics and dynamics of the non-natural fluorescent 4AP:DAP base pair. *Physical Chemistry Chemical Physics*, **2018**, 20, 3699-3709	3.6	9
135	Synthesis and characterization of a homogeneous and silica supported homoleptic cationic tungsten(vi) methyl complex: application in olefin metathesis. *Chemical Communications*, **2016**, 52, 11270-11273	5.8	9
134	Unusual C–H Bond Cleavage in the Formation of Amine-Bis(phenoxy) Group 4 Benzyl Complexes: Mechanism of Formation and Application to Stereospecific Polymerization. *Organometallics*, **2014**, 33, 4118-4130	3.8	9
133	Consequences of the electronic tuning of latent ruthenium-based olefin metathesis catalysts on their reactivity. *Beilstein Journal of Organic Chemistry*, **2015**, 11, 1458-68	2.5	9

132	Structural basis for the recognition in an idiotype-anti-idiotype antibody complex related to celiac disease. *PLoS ONE*, **2014**, 9, e102839	3.7	9
131	A molecular model for H(2) interactions in aliphatic and aromatic hydrocarbons. *Physical Chemistry Chemical Physics*, **2009**, 11, 3935-42	3.6	9
130	In Silico Olefin Metathesis with Ru-Based Catalysts Containing N-Heterocyclic Carbenes Bearing C60 Fullerenes. *Chemistry - A European Journal*, **2016**, 22, 6617-23	4.8	9
129	Mechanism of the Transmetalation of Organosilanes to Gold. *ChemistryOpen*, **2016**, 5, 60-4	2.3	9
128	Switchable Diastereoselectivity in the Fluoride-Promoted Vinylogous Mukaiyama-Michael Reaction of 2-[(Trimethylsilyl)oxy]furan Catalyzed by Crown Ethers. *Journal of Organic Chemistry*, **2017**, 82, 6629-6637	4.3	8
127	Experimental and Computational Study of an Unexpected Iron-Catalyzed Carboetherification by Cooperative Metal and Ligand Substrate Interaction and Proton Shuttling. *Angewandte Chemie*, **2017**, 129, 15059-15063	3.6	8
126	SOMC grafting of vanadium oxytriisopropoxide (VO(O Pr)) on dehydroxylated silica; analysis of surface complexes and thermal restructuring mechanism.. *RSC Advances*, **2018**, 8, 20801-20808	3.7	8
125	Mechanistic Study of Hydroamination of Alkyne through Tantalum-Based Silica-Supported Surface Species. *ACS Catalysis*, **2019**, 9, 8719-8725	13.1	8
124	Chirality of Catalysts for Stereospecific Polymerizations. *Topics in Stereochemistry*, **2004**, 1-69		8
123	A possible unified mechanism of like and unlike chain-end stereocontrol for primary propene-coordinated polymerizations. *Macromolecular Chemistry and Physics*, **2002**, 203, 1564-1572	2.6	8
122	Nickel Mediated Enantioselective Photoredox Allylation of Aldehydes with Visible Light.. *Angewandte Chemie - International Edition*, **2021**,	16.4	8
121	D936Y and Other Mutations in the Fusion Core of the SARS-Cov-2 Spike Protein Heptad Repeat 1 Undermine the Post-Fusion Assembly		8
120	Tungsten Blue Oxide as a Reusable Electrocatalyst for Acidic Water Oxidation by Plasma-Induced Vacancy Engineering. *CCS Chemistry*, **2021**, 3, 1553-1561	7.2	8
119	Suzuki-Miyaura Cross-Coupling of Esters by Selective O-C(O) Cleavage Mediated by Air- and Moisture-Stable [Pd(NHC)(□Cl)Cl] Precatalysts: Catalyst Evaluation and Mechanism. *Catalysis Science and Technology*, **2021**, 11, 3189-3197	5.5	8
118	CO2 hydrogenation to methanol and hydrocarbons over bifunctional Zn-doped ZrO2/zeolite catalysts. *Catalysis Science and Technology*, **2021**, 11, 1249-1268	5.5	8
117	The activity of indenylidene derivatives in olefin metathesis catalysts. *Beilstein Journal of Organic Chemistry*, **2018**, 14, 2956-2963	2.5	8
116	Quantifying electronic similarities between NHC-gold(i) complexes and their isolobal imidazolium precursors. *Physical Chemistry Chemical Physics*, **2019**, 21, 15615-15622	3.6	7
115	A recurrent Gly43Asp substitution in coagulation Factor X rigidifies its catalytic pocket and impairs catalytic activity and intracellular trafficking. *Thrombosis Research*, **2014**, 133, 481-7	8.2	7

114	Insights into the Decomposition of Olefin Metathesis Precatalysts. *Angewandte Chemie*, **2014**, 126, 9141-9145	3.6	7
113	Mechanism of dihydride formation and hydrogen/deuterium exchange in a cationic iridium(III) complex. *Canadian Journal of Chemistry*, **2009**, 87, 1362-1368	0.9	7
112	Molecular modeling of the regiochemistry of olefin insertion with single-site polymerization catalysts. *Kinetics and Catalysis*, **2006**, 47, 170-175	1.5	7
111	Molecular mechanics and mechanisms of regulation of the stereospecificity in Ziegler-Natta catalysis. *Macromolecular Symposia*, **1995**, 89, 307-319	0.8	7
110	Selectivity descriptors for the direct hydrogenation of CO to hydrocarbons during zeolite-mediated bifunctional catalysis. *Nature Communications*, **2021**, 12, 5914	17.4	7
109	A Multivariate Linear Regression Approach to Predict Ethene/1-Olefin Copolymerization Statistics Promoted by Group 4 Catalysts. *ACS Catalysis*, **2021**, 11, 4061-4070	13.1	7
108	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. *FASEB Journal*, **2019**, 33, 2327-2342	0.9	7
107	A Novel [OSSO]-Type Chromium(III) Complex as a Versatile Catalyst for Copolymerization of Carbon Dioxide with Epoxides. *Chemistry - A European Journal*, **2020**, 26, 5347-5353	4.8	7
106	Electrochemical Conversion of CO2 to 2-Bromoethanol in a Membraneless Cell. *ACS Energy Letters*, **2019**, 4, 600-605	20.1	6
105	Electronic effects in mixed N-heterocyclic carbene/phosphite indenylidene ruthenium metathesis catalysts. *Dalton Transactions*, **2019**, 48, 11326-11337	4.3	6
104	cis/trans Coordination in Olefin Metathesis by Static and Molecular Dynamic DFT Calculations. *Chemistry of Heterocyclic Compounds*, **2014**, 50, 389-395	1.4	6
103	Mechanism of Intramolecular Rhodium- and Palladium-Catalyzed Alkene Alkoxyfunctionalizations. *Organometallics*, **2015**, 34, 5549-5554	3.8	6
102	The driving force role of ruthenacyclobutanes. *Theoretical Chemistry Accounts*, **2015**, 134, 1	1.9	6
101	Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis. *Procedia Computer Science*, **2011**, 4, 1222-1229	1.6	6
100	A Preliminary Study of Host-Guest Interactions in Polymeric Clathrates An Ab Initio Study of the Model Complexes Benzene/X2 (X = F, Cl, Br, I). *European Journal of Inorganic Chemistry*, **1998**, 1998, 1513-1517	2.3	6
99	Molecular mechanics and the polymerization mechanism of homogeneous and heterogeneous Ziegler-Natta catalysts. *Makromolekulare Chemie Macromolecular Symposia*, **1993**, 69, 237-246		6
98	Regio, stereo and chemoselectivity of 2nd generation Grubbs ruthenium-catalyzed olefin metathesis. *Catalysis Today*, **2020**, 388-389, 394-394	5.3	6
97	In silico design of novel NRR electrocatalysts: cobalt-molybdenum alloys. *Chemical Communications*, **2020**, 56, 13343-13346	5.8	6

96	Remarkable Influence of β-SnWO4 Exposed Facets on Their Photocatalytic Performance for H2 and O2 Evolution Reactions. *Journal of Physical Chemistry C*, **2020**, 124, 18684-18689	3.8	6
95	Operando Elucidation on the Working State of Immobilized Fluorinated Iron Porphyrin for Selective Aqueous Electroreduction of CO2 to CO. *ACS Catalysis*, **2021**, 11, 6499-6509	13.1	6
94	Adsorption of industrial dyes on functionalized and nonfunctionalized asphaltene: A combined molecular dynamics and quantum mechanics study. *Journal of Molecular Liquids*, **2021**, 337, 116433	6	6
93	Prediction of Biomolecular Complexes **2017**, 265-292		5
92	Gas Phase Silver Thermochemistry from First Principles. *Inorganic Chemistry*, **2019**, 58, 7873-7885	5.1	5
91	Unravelling the reaction mechanism for the Claisen–Tishchenko condensation catalysed by Mn(I)-PNN complexes: a DFT study. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	5
90	Unprecedented Diastereoselective Arylogous Michael Addition of Unactivated Phthalides. *Chemistry - A European Journal*, **2019**, 25, 7131-7141	4.8	5
89	Evaluation of experimental alkali metal ion-ligand noncovalent bond strengths with DLPNO-CCSD(T) method. *Journal of Chemical Physics*, **2019**, 151, 014301	3.9	5
88	Simple and cheap steric and electronic characterization of the reactivity of Ru(II) complexes containing oxazoline ligands as epoxidation catalysts. *Chemical Physics Letters*, **2013**, 577, 142-146	2.5	5
87	Steric Maps to Evaluate the Role of Steric Hindrance on the IPr NHC Ligand. *Procedia Computer Science*, **2013**, 18, 845-854	1.6	5
86	Structure and bonding in monomeric iron(III) complexes with terminal oxo and hydroxo ligands. *Inorganic Chemistry*, **2006**, 45, 1732-8	5.1	5
85	Living propene polymerization with Bis(phenoxy-imine) group 4 metal catalysts: A theoretical study. *Kinetics and Catalysis*, **2006**, 47, 289-294	1.5	5
84	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. *Macromolecular Theory and Simulations*, **2001**, 10, 349-354	1.5	5
83	Olefin Polymerization by Early Transition Metal Catalysts. *Catalysis By Metal Complexes*, **2002**, 23-56		5
82	A Density Functional Theory Study of the Syndiotactic-Specific Polymerization of Styrene **2001**, 299-306		5
81	Mechanistic Insights into the Organopolymerization of N-Methyl N-Carboxyanhydrides Mediated by N-Heterocyclic Carbenes. *Macromolecules*, **2016**, 49, 7777-7784	5.5	5
80	Designing an active TaN photocatalyst for H and O evolution reactions by specific exposed facet engineering: a first-principles study. *Physical Chemistry Chemical Physics*, **2020**, 22, 10295-10304	3.6	5
79	Single-Site Molybdenum on Solid Support Materials for Catalytic Hydrogenation of N2-into-NH3. *Angewandte Chemie*, **2018**, 130, 16038-16042	3.6	5

78	Structural Insights in Mammalian Sialyltransferases and Fucosyltransferases: We Have Come a Long Way, but It Is Still a Long Way Down. *Molecules*, **2021**, 26,	4.8	5
77	Regression analysis of properties of [Au(IPr)(CHR)] complexes. *Dalton Transactions*, **2019**, 48, 7693-7703	4.3	4
76	Investigation of Surface Alkylation Strategy in SOMC: In Situ Generation of a Silica-Supported Tungsten Methyl Catalyst for Cyclooctane Metathesis. *Organometallics*, **2016**, 35, 2524-2531	3.8	4
75	Ziegler-Natta catalytic systems. *Journal of Thermal Analysis and Calorimetry*, **2008**, 91, 101-106	4.1	4
74	Phenoxylation of Alkynes through Mono- and Dual Activation Using Group 11 (Cu, Ag, Au) Catalysts. *European Journal of Inorganic Chemistry*, **2020**, 2020, 1123-1134	2.3	4
73	Barium-Catalysed Dehydrocoupling of Hydrosilanes and Borinic Acids: A Mechanistic Insight. *Chemistry - A European Journal*, **2020**, 26, 3535-3544	4.8	4
72	?Plasticity of NHCs on the Ruthenium?Phosphine and Ruthenium?Ylidene Bonds in Olefin Metathesis Catalysts. *Organometallics*, **2020**, 39, 3972-3982	3.8	4
71	Metathesis of Classical and Functionalized Olefins Catalyzed by Silica-Supported Single-Site Well-Defined W and Mo Pre-catalysts. *ChemCatChem*, **2020**, 12, 6067-6075	5.2	4
70	Chemically Induced Mismatch of Rings and Stations in [3]Rotaxanes. *Journal of the American Chemical Society*, **2021**, 143, 8046-8055	16.4	4
69	Need for Rationally Designed SnWO4 Photo(electro)catalysts to Overcome the Performance Limitations for O2 and H2 Evolution Reactions. *Journal of Physical Chemistry C*, **2021**, 125, 8488-8496	3.8	4
68	Revisiting O Bond Formation through Outer-Sphere Water Molecules versus Bimolecular Mechanisms in Water-Oxidation Catalysis (WOC) by Cp*Ir Based Complexes. *European Journal of Inorganic Chemistry*, **2019**, 2019, 2093-2100	2.3	4
67	Ambiguities in solvation free energies from cluster-continuum quasichemical theory: lithium cation in protic and aprotic solvents. *Physical Chemistry Chemical Physics*, **2021**, 23, 16077-16088	3.6	4
66	Au???H Hydrogen Bonds as Design Principle in Gold(I) Catalysis. *Angewandte Chemie*, **2021**, 133, 21182-21192	3.6	4
65	Illuminating the Intrinsic Effect of Water Co-feeding on Methane Dehydroaromatization: A Comprehensive Study. *ACS Catalysis*, **2021**, 11, 11671-11684	13.1	4
64	Mechanistic insights into photochemical nickel-catalyzed cross-couplings enabled by energy transfer.. *Nature Communications*, **2022**, 13, 2737	17.4	4
63	Organocatalytic Coupling of Bromo-Lactide with Cyclic Ethers and Carbonates to Chiral Bromo-Diesters: NHC or Anion Catalysis?. *ACS Catalysis*, **2017**, 7, 3929-3933	13.1	3
62	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. *ChemBioChem*, **2019**, 20, 2262-2270	3.8	3
61	Precision Molecular Threading/Dethreading. *Angewandte Chemie*, **2020**, 132, 14935-14944	3.6	3

60	Tricyclic Sulfoxide–Alkene Hybrid Ligands for Chiral Rh(I) Complexes: The "Matched" Diastereomer Catalyzes Asymmetric C–C Bond Formations. *Organometallics*, **2020**, 39, 1348-1359	3.8	3
59	Conversion of racemic alcohols to optically pure amine precursors enabled by catalyst dynamic kinetic resolution: experiment and computation. *Chemical Communications*, **2020**, 56, 9094-9097	5.8	3
58	Nitrite to nitric oxide interconversion by heme FeII complex assisted by [CuI(tmpa)]+. *Structural Chemistry*, **2016**, 27, 409-417	1.8	3
57	Insights into the Impact of Native Defects on the Conductivity of CuVO Material for Photovoltaic Application: A First-Principles Computational Study. *ACS Omega*, **2018**, 3, 6605-6610	3.9	3
56	Theoretical Attempts: "In Silico Olefin Metathesis" How Can Computers Help in the Understanding of Metathesis Mechanisms and in Catalysts Development? **2014**, 483-494		3
55	Clean and selective catalytic C-H alkylation of alkenes with environmental friendly alcohols. *Molecular Catalysis*, **2017**, 435, 69-75	3.3	3
54	Fluxional Behavior of Molecular WMe6 and of Silica Grafted WMe6. *Organometallics*, **2015**, 34, 663-668	3.8	3
53	An Empirical Correction Term to Density Functional Theory for the Description of the TiCl4-Lewis Base Complexes. *Macromolecular Symposia*, **2007**, 260, 122-126	0.8	3
52	Mechanistic Understanding of Arylation vs Alkylation of Aliphatic Csp3–H Bonds by Decatungstate–Nickel Catalysis. *ACS Catalysis*,13973-13982	13.1	3
51	Thermochemistry of 5,10,15,20-tetraphenylporphyrin. *Journal of Chemical Thermodynamics*, **2020**, 151, 106244	2.9	3
50	[Ag(1,2-BDT)]: How Square-Pyramidal Building Blocks Self-Assemble into the Smallest Silver Nanocluster. *Inorganic Chemistry*, **2021**, 60, 4306-4312	5.1	3
49	Chelation enforcing a dual gold configuration in the catalytic hydroxyphenoxylation of alkynes. *Applied Organometallic Chemistry*, **2021**, 35, e6362	3.1	3
48	Molecular recognition and adsorptive separation of -xylene by trianglimine crystals. *Chemical Communications*, **2021**, 57, 9124-9127	5.8	3
47	Apixaban Interacts with Haemoglobin: Effects on Its Plasma Levels. *Thrombosis and Haemostasis*, **2018**, 118, 1701-1712	7	3
46	Theoretical insights into dehydrogenative chemisorption of alkylaromatics on Pt(1 0 0) and Ni(1 0 0). *Journal of Catalysis*, **2018**, 363, 197-203	7.3	3
45	Hydrogen atom induced magnetic behaviors in two-dimensional materials: insight on origination in the model of –MoO. *Nanoscale*, **2018**, 10, 14100-14106	7.7	3
44	Design, scope and mechanism of highly active and selective chiral NHC-iridium catalysts for the intramolecular hydroamination of a variety of unactivated aminoalkenes. *Chemical Science*, **2021**, 12, 3751-3767	9.4	3
43	Conversion of Pd(I) off-cycle species into highly efficient cross-coupling catalysts. *Dalton Transactions*, **2021**, 50, 5420-5427	4.3	3

42	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. *Journal of Physical Chemistry A*, **2015**, 119, 11711-8	2.8	2
41	Mechanistic Insights of a Selective C-H Alkylation of Alkenes by a Ru-Based Catalyst and Alcohols. *ChemistrySelect*, **2016**, 1, 4218-4228	1.8	2
40	The "innocent" role of Sc(3+) on a non-heme Fe catalyst in an O2 environment. *Dalton Transactions*, **2014**, 43, 11190-4	4.3	2
39	Electronic bond tuning with heterocyclic carbenes. *Dalton Transactions*, **2013**, 42, 7281-6	4.3	2
38	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists **2012**, 95-133		2
37	N-Heterocyclic Carbenes: An Introductory Overview. *Catalysis By Metal Complexes*, **2010**, 1-22		2
36	Gold N-Heterocyclic Carbene Catalysts for the Hydrofluorination of Alkynes Using Hydrofluoric Acid: Reaction Scope, Mechanistic Studies and the Tracking of Elusive Intermediates. *Chemistry - A European Journal*, **2021**,	4.8	2
35	Probing the Mechanism of the Double C-H (De)Activation Route of a Ru-Based Olefin Metathesis Catalyst. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2010**, 275-280	0.1	2
34	A Comparison of the Performance of the Semiempirical PM6 Method Versus DFT Methods in Ru-Catalyzed Olefin Metathesis. *NATO Science for Peace and Security Series A: Chemistry and Biology* , **2010**, 281-292	0.1	2
33	The role of noncovalent interactions in olefin polymerization catalysis: a further look to the fluorinated ligand effect. *Molecular Catalysis*, **2020**, 494, 111118	3.3	2
32	Synthesis of Gold(I)-Trifluoromethyl Complexes and their Role in Generating Spectroscopic Evidence for a Gold(I)-Difluorocarbene Species. *Chemistry - A European Journal*, **2021**, 27, 8461-8467	4.8	2
31	Active and stable Fe-based catalyst, mechanism, and key role of alkali promoters in ammonia synthesis. *Journal of Catalysis*, **2021**, 394, 353-365	7.3	2
30	Replacing thymine with a strongly pairing fifth Base: A combined quantum mechanics and molecular dynamics study. *Computational and Structural Biotechnology Journal*, **2021**, 19, 1312-1324	6.8	2
29	Spontaneous Production of Ultrastable Reactive Oxygen Species on Titanium Oxide Surfaces Modified with Organic Ligands. *Advanced Materials Interfaces*, **2021**, 8, 2100629	4.6	2
28	Iron-Cobalt-Based Materials: An Efficient Bimetallic Catalyst for Ammonia Synthesis at Low Temperatures. *ACS Catalysis*, **2022**, 12, 587-599	13.1	2
27	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists **2017**, 225-267		1
26	Toward better understanding of the support effect: Test cases for CO dissociation on Fen/TiO2(1 1 0), n = 4, 5. *Chemical Physics Letters*, **2017**, 684, 30-35	2.5	1
25	Ligand Effects in Pd-Catalyzed Intermolecular Alkyne Hydroarylations. *Organometallics*, **2019**, 38, 3730-3789	3.8	1

24	Evidence for Silica Surface Three- and Five-Membered Metallacycle Intermediates in the Catalytic Cycle of Hydroaminoalkylation of Olefins Using Single-Ti-Metal Catalysts. *Organometallics*, **2020**, 39, 2438-2445	3.8	1
23	Barium-Catalysed Dehydrocoupling of Hydrosilanes and Borinic Acids: A Mechanistic Insight. *Chemistry - A European Journal*, **2020**, 26, 3445	4.8	1
22	Organometallic copper I, II or III species in an intramolecular dechlorination reaction. *Theoretical Chemistry Accounts*, **2013**, 132, 1	1.9	1
21	Solar Water Splitting: Enhancing Charge Carrier Lifetime in Metal Oxide Photoelectrodes through Mild Hydrogen Treatment (Adv. Energy Mater. 22/2017). *Advanced Energy Materials*, **2017**, 7,	21.8	1
20	Real-time observation of intersystem crossing induced by charge recombination during bimolecular electron transfer reactions. *Dyes and Pigments*, **2017**, 136, 881-886	4.6	1
19	Vapour pressures of fluorocarbons in polyols, polyamines and polycarboxyls. *Journal of Fluorine Chemistry*, **1996**, 78, 167-175	2.1	1
18	Gas-Phase Thermochemistry of MX and MX (M = Sc, Y; X = F, Cl, Br, I) from a Composite Reaction-Based Approach: Homolytic versus Heterolytic Cleavage. *Inorganic Chemistry*, **2020**, 59, 17084-17095	5.1	1
17	The CASP13-CAPRI targets as case studies to illustrate a novel scoring pipeline integrating CONSRANK with clustering and interface analyses. *BMC Bioinformatics*, **2020**, 21, 262	3.6	1
16	Influence of the anionic ligands on properties and reactivity of Hoveyda-Grubbs catalysts. *Molecular Catalysis*, **2021**, 509, 111612	3.3	1
15	Tungsten Catalyst Incorporating a Well-Defined Tetracoordinated Aluminum Surface Ligand for Selective Metathesis of Propane, [(?SiOSi?)(?SiO)2AlOW(?CtBu) (H)2]. *ChemCatChem*, **2019**, 11, 614-620	5.2	1
14	Superconductivity and High-Pressure Performance of 2D MoC Crystals. *Journal of Physical Chemistry Letters*, **2021**, 12, 2219-2225	6.4	1
13	Synthesis and Characterization of Cationic Tetramethyl Tantalum(V) Complex. *Catalysts*, **2018**, 8, 507	4	1
12	A Career in Catalysis: Jean-Marie M. Basset. *ACS Catalysis*,4961-4977	13.1	0
11	Titelbild: Oxidative Addition to Palladium(0) Made Easy through Photoexcited-State Metal Catalysis: Experiment and Computation (Angew. Chem. 11/2019). *Angewandte Chemie*, **2019**, 131, 3263-3263	3.6	
10	Unprecedented Diastereoselective Arylogous Michael Addition of Unactivated Phthalides. *Chemistry - A European Journal*, **2019**, 25, 7043-7043	4.8	
9	Tuning and Quantifying Steric and Electronic Effects of N-Heterocyclic Carbenes **2014**, 25-38		
8	Mechanism of Stereospecific Propene Polymerization Promoted by Metallocene and Nonmetallocene Catalysts **2011**, 299-322		
7	Mechanism of Gold-Catalyzed Cycloisomerization of Enynyl Esters. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2010**, 293-303	0.1	

6	Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis. *Highlights in Theoretical Chemistry*, **2013**, 129-134	
5	Dancing multiplicity states supported by a carboxylated group in dicopper structures bonded to O2. *Highlights in Theoretical Chemistry*, **2014**, 143-155	
4	Organometallic copper I, II or III species in an intramolecular dechlorination reaction. *Highlights in Theoretical Chemistry*, **2014**, 105-110	
3	Fluxional bis(phenoxy-imine) Zr and Ti catalysts for polymerization. *Theoretical Chemistry Accounts*, **2021**, 140, 1	1.9
2	Energy-Efficient Nitrogen Reduction to Ammonia at Low Overpotential in Aqueous Electrolyte under Ambient Conditions. *ChemSusChem*, **2018**, 11, 3356-3356	8.3
1	Selection of Low-Dimensional 3-D Geometric Descriptors for Accurate Enantioselectivity Prediction. *ACS Catalysis*,6934-6945	13.1