

Xin Lu

List of Publications by Year in descending order

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7448
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#	ARTICLE	IF	CITATIONS
1	Insights into the gold-catalyzed intermolecular annulations of alkynes with <i>N</i> -allenamides: a mechanistic DFT study. Dalton Transactions, 2022, 51, 3734-3739.	1.6	3
2	Efficient synthesis of tetracyclic β -lactams via gold-catalyzed oxidative cyclization of alkenyl diynes. Organic Chemistry Frontiers, 2022, 9, 2557-2562.	2.3	5
3	Insights into the Mechanism of Metal-Catalyzed Transformation of Oxime Esters: Metal-Bound Radical Pathway vs Free Radical Pathway. Journal of Organic Chemistry, 2022, 87, 6014-6024.	1.7	5
4	Copper-Catalyzed Asymmetric Diyne Cyclization via [1,2]-Stevens-Type Rearrangement for the Synthesis of Chiral Chromeno[3,4- <i>c</i>]pyrroles. Angewandte Chemie - International Edition, 2022, 61, e202115554.	7.2	44
5	Copper-Catalyzed Asymmetric Diyne Cyclization via [1,2]-Stevens-Type Rearrangement for the Synthesis of Chiral Chromeno[3,4- <i>c</i>]pyrroles. Angewandte Chemie, 2022, 134, .	1.6	9
6	Intermolecular 1,2-Difunctionalization of Alkenes Enabled by Fluoroamide-Directed Remote Benzyl C(sp ³)-H Functionalization. Journal of the American Chemical Society, 2022, 144, 339-348.	6.6	51
7	Catalyst-Dependent Stereospecific [3,3]-Sigmatropic Rearrangement of Sulfoxide- γ -namides: Divergent Synthesis of Chiral Medium-Sized <i>N</i> , <i>S</i> -Heterocycles. Angewandte Chemie, 2022, 134, .	1.6	6
8	Catalyst-Dependent Stereospecific [3,3]-Sigmatropic Rearrangement of Sulfoxide- γ -namides: Divergent Synthesis of Chiral Medium-Sized <i>N</i> , <i>S</i> -Heterocycles. Angewandte Chemie - International Edition, 2022, 61, .	7.2	26
9	Copper-catalyzed asymmetric cyclization of alkenyl diynes: method development and new mechanistic insights. Chemical Science, 2021, 12, 9466-9474.	3.7	41
10	Dynamic Effects in Intramolecular Schmidt Reactions: Entropy, Electrostatic Drag, and Selectivity Prediction. ChemPhysChem, 2021, 22, 649-656.	1.0	2
11	Insights into the mechanism of fatty acid photodecarboxylase: A theoretical investigation. Chemical Physics Letters, 2021, 771, 138550.	1.2	2
12	Carbon Nitride Supported High-Loading Fe Single-Atom Catalyst for Activation of Peroxymonosulfate to Generate ¹ O ₂ with 100% Selectivity. Angewandte Chemie - International Edition, 2021, 60, 21751-21755.	7.2	521
13	Carbon Nitride Supported High-Loading Fe Single-Atom Catalyst for Activation of Peroxymonosulfate to Generate 1 O ₂ with 100% Selectivity. Angewandte Chemie, 2021, 133, 21919-21923.	1.6	18
14	Atroposelective carbonylation of aryl iodides with amides: facile synthesis of enantioenriched cyclic and acyclic amides. Organic Chemistry Frontiers, 2021, 8, 6067-6073.	2.3	20
15	Synthesis and Spectroscopy of Monodispersed, Quantum-Confined FAPbBr ₃ Perovskite Nanocrystals. Chemistry of Materials, 2020, 32, 549-556.	3.2	39
16	Size- and Halide-Dependent Auger Recombination in Lead Halide Perovskite Nanocrystals. Angewandte Chemie - International Edition, 2020, 59, 14292-14295.	7.2	63
17	Size- and Halide-Dependent Auger Recombination in Lead Halide Perovskite Nanocrystals. Angewandte Chemie, 2020, 132, 14398-14401.	1.6	8
18	Copper-Catalyzed Asymmetric Reaction of Alkenyl Diynes with Styrenes by Formal [3 + 2] Cycloaddition via Cu-Containing All-Carbon 1,3-Dipoles: Access to Chiral Pyrrole-Fused Bridged [2.2.1] Skeletons. Journal of the American Chemical Society, 2020, 142, 7618-7626.	6.6	83

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19	Size- and Composition-Dependent Exciton Spin Relaxation in Lead Halide Perovskite Quantum Dots. <i>ACS Energy Letters</i> , 2020, 5, 1701-1708.	8.8	47
20	Strong Spin-Selective Optical Stark Effect in Lead Halide Perovskite Quantum Dots. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3594-3600.	2.1	21
21	Scandium Tetrahedron Supported by H Anion and CN Pentaanion inside Fullerene C ₈₀ . <i>Inorganic Chemistry</i> , 2020, 59, 8284-8290.	1.9	7
22	Organocatalytic Enantioselective Conia-Ene-Type Carbocyclization of Ynamide Cyclohexanones: Regiodivergent Synthesis of Morphans and Normorphans. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 16252-16259.	7.2	72
23	Organocatalytic Enantioselective Conia-Ene-Type Carbocyclization of Ynamide Cyclohexanones: Regiodivergent Synthesis of Morphans and Normorphans. <i>Angewandte Chemie</i> , 2019, 131, 16398-16405.	1.6	21
24	Chemoselectivity in Gold(I)-Catalyzed Propargyl Ester Reactions: Insights From DFT Calculations. <i>Frontiers in Chemistry</i> , 2019, 7, 609.	1.8	3
25	Generation of Donor/Donor Copper Carbenes through Copper-Catalyzed Diyne Cyclization: Enantioselective and Divergent Synthesis of Chiral Polycyclic Pyrroles. <i>Journal of the American Chemical Society</i> , 2019, 141, 16961-16970.	6.6	84
26	On the absence of a phonon bottleneck in strongly confined CsPbBr ₃ perovskite nanocrystals. <i>Chemical Science</i> , 2019, 10, 5983-5989.	3.7	71
27	Sulfur Moiety as a Double-Edged Sword for Realizing Ultrafine Supported Metal Nanoclusters with a Cationic Nature. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 11317-11326.	4.0	15
28	Generation of Endocyclic Vinyl Carbene Complexes via Gold-Catalyzed Oxidative Cyclization of Terminal Dienes: Toward Naphthoquinones and Carbazolequinones. <i>ACS Catalysis</i> , 2019, 9, 1019-1025.	5.5	46
29	Biexciton Auger recombination in mono-dispersed, quantum-confined CsPbBr ₃ perovskite nanocrystals obeys universal volume-scaling. <i>Nano Research</i> , 2019, 12, 619-623.	5.8	63
30	Metal-catalyzed alkyne oxidation/C-H functionalization: Effects of oxidant, temperature, and metal catalyst on chemoselectivity. <i>Journal of Computational Chemistry</i> , 2019, 40, 1038-1044.	1.5	2
31	Dual catalysis for enantioselective convergent synthesis of enantiopure vicinal amino alcohols. <i>Nature Communications</i> , 2018, 9, 410.	5.8	92
32	Electrochemical Synthesis of Imidazo-Fused N-Heteroaromatic Compounds through a C-N Bond-Forming Radical Cascade. <i>Angewandte Chemie</i> , 2018, 130, 1652-1655.	1.6	41
33	Electrochemical Synthesis of Imidazo-Fused N-Heteroaromatic Compounds through a C-N Bond-Forming Radical Cascade. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 1636-1639.	7.2	155
34	Gold-Catalyzed [5+2]- and [5+1]-Annulations between Ynamides and 1,2-Benzisoxazoles with Ligand-Controlled Chemoselectivity. <i>ACS Catalysis</i> , 2018, 8, 9697-9701.	5.5	71
35	Zinc-catalyzed reaction of isoxazoles with thioynol ethers involving an unprecedented 1,2-sulfur migration. <i>Chemical Communications</i> , 2018, 54, 7435-7438.	2.2	28
36	Benign catalysis with zinc: atom-economical and divergent synthesis of nitrogen heterocycles by formal [3 + 2] annulation of isoxazoles with ynol ethers. <i>Green Chemistry</i> , 2018, 20, 4287-4291.	4.6	45

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37	Transition-metal-free oxidative cyclization of <i>N</i> -propargyl ynamides: stereospecific construction of linear polycyclic N-heterocycles. <i>Green Chemistry</i> , 2018, 20, 3271-3278.	4.6	33
38	Highly Site Selective Formal [5+2] and [4+2] Annulations of Isoxazoles with Heterosubstituted Alkynes by Platinum Catalysis: Rapid Access to Functionalized 1,3-Oxazepines and 2,5-Dihydropyridines. <i>Angewandte Chemie</i> , 2017, 129, 620-624.	1.6	41
39	Conjugated Microporous Polymer as Heterogeneous Ligand for Highly Selective Oxidative Heck Reaction. <i>Journal of the American Chemical Society</i> , 2017, 139, 3966-3969.	6.6	86
40	Reversal of Regioselectivity in Catalytic Arene-Ynamide Cyclization: Direct Synthesis of Valuable Azepino[4,5- <i>b</i>]indoles and β -Carbolines and DFT Calculations. <i>ACS Catalysis</i> , 2017, 7, 4004-4010.	5.5	92
41	Synthesis and Characterization of a Metallocyclic Framework with Three Fused Five-membered Rings. <i>Angewandte Chemie</i> , 2017, 129, 9195-9199.	1.6	13
42	Highly Site Selective Formal [5+2] and [4+2] Annulations of Isoxazoles with Heterosubstituted Alkynes by Platinum Catalysis: Rapid Access to Functionalized 1,3-Oxazepines and 2,5-Dihydropyridines. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 605-609.	7.2	146
43	Divergent synthesis of N-heterocycles via controllable cyclization of azido-diyne catalyzed by copper and gold. <i>Nature Communications</i> , 2017, 8, 1748.	5.8	139
44	Sponge-like quaternary ammonium-based poly(ionic liquid)s for high CO ₂ capture and efficient cycloaddition under mild conditions. <i>Journal of Materials Chemistry A</i> , 2017, 5, 25594-25600.	5.2	60
45	Synthesis and Characterization of a Metallocyclic Framework with Three Fused Five-membered Rings. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9067-9071.	7.2	45
46	Electrochemical C ^α H/N ^α H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. <i>Angewandte Chemie</i> , 2016, 128, 9314-9318.	1.6	56
47	Electrochemical C ^α H/N ^α H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9168-9172.	7.2	215
48	Electrocatalytic Generation of Amidyl Radicals for Olefin Hydroamidation: Use of Solvent Effects to Enable Anilide Oxidation. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2226-2229.	7.2	214
49	Catalytic Ynamide Oxidation Strategy for the Preparation of β -Functionalized Amides. <i>ACS Catalysis</i> , 2016, 6, 6055-6062.	5.5	68
50	Synthesis of 2-Aza-1,3-butadienes through Gold-Catalyzed Intermolecular Ynamide Amination/C ^α H Functionalization. <i>Organic Letters</i> , 2016, 18, 4630-4633.	2.4	35
51	Assembled molecular face-rotating polyhedra to transfer chirality from two to three dimensions. <i>Nature Communications</i> , 2016, 7, 12469.	5.8	90
52	CCCCC pentadentate chelates with planar M ⁺ aromaticity and unique properties. <i>Science Advances</i> , 2016, 2, e1601031.	4.7	74
53	Electrocatalytic Generation of Amidyl Radicals for Olefin Hydroamidation: Use of Solvent Effects to Enable Anilide Oxidation. <i>Angewandte Chemie</i> , 2016, 128, 2266-2269.	1.6	71
54	Copper-Catalyzed Intramolecular Oxidative Amination of Unactivated Internal Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 4379-4383.	1.7	52

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55	Gold-Catalyzed Intermolecular Ynamide Amination-Initiated Aza-Nazarov Cyclization: Access to Functionalized 2-Aminopyrroles. <i>Organic Letters</i> , 2016, 18, 3254-3257.	2.4	97
56	Zinc-Catalyzed Alkyne Oxidation/C ₁₂ H Functionalization: Highly Site-Selective Synthesis of Versatile Isoquinolones and β -Carbolines. <i>Angewandte Chemie</i> , 2015, 127, 8363-8367.	1.6	35
57	Zinc-Catalyzed Alkyne Oxidation/C ₁₂ H Functionalization: Highly Site-Selective Synthesis of Versatile Isoquinolones and β -Carbolines. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 8245-8249.	7.2	154
58	Pristine graphene dispersion in solvents and its application as a catalyst support: a combined theoretical and experimental study. <i>Journal of Materials Chemistry A</i> , 2015, 3, 6282-6285.	5.2	26
59	Generation of λ^5 -Imino Gold Carbenes through Gold-Catalyzed Intermolecular Reaction of Azides with Ynamides. <i>Journal of the American Chemical Society</i> , 2015, 137, 9567-9570.	6.6	245
60	Atom-economic generation of gold carbenes: gold-catalyzed formal [3+2] cycloaddition between ynamides and isoxazoles. <i>Chemical Science</i> , 2015, 6, 1265-1271.	3.7	251
61	Practical, Modular, and General Synthesis of β -Coumaranones through Gold-Catalyzed Intermolecular Alkyne Oxidation Strategy. <i>Chemistry - an Asian Journal</i> , 2015, 10, 91-95.	1.7	39
62	Planar Möbius aromatic pentalenes incorporating 16 and 18 valence electron osmiums. <i>Nature Communications</i> , 2014, 5, 3265.	5.8	169
63	Mechanism of Lewis-acid-catalyzed intramolecular coupling of sp^3 -C-H bond and alkene: A theoretical investigation. <i>Journal of Theoretical and Computational Chemistry</i> , 2014, 13, 1450015.	1.8	0
64	Hydrogen bonding in microsolvation: photoelectron imaging and theoretical studies on $Aux^+(H_2O)_n$ and $Aux^+(CH_3OH)_n$ ($x = 1, 2; n = 1, 2$) complexes. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 4771.	1.3	11
65	Real-time analysis of self-assembled nucleobases by Venturi easy ambient sonic-spray ionization mass spectrometry. <i>Talanta</i> , 2014, 128, 366-372.	2.9	15
66	Control of the Charge Distribution and Modulation of the Class II ^{III} Transition in Weakly Coupled Mo ₂ Systems. <i>Inorganic Chemistry</i> , 2013, 52, 12624-12633.	1.9	37
67	Exohedrally stabilized C ₇₀ isomer with adjacent pentagons characterized by crystallography. <i>Chemical Science</i> , 2013, 4, 2967.	3.7	22
68	Stabilization of anti-aromatic and strained five-membered rings with a transition metal. <i>Nature Chemistry</i> , 2013, 5, 698-703.	6.6	244
69	Vibrationally resolved photoelectron imaging of platinum carbonyl anion $Pt(CO)_n^-$ ($n = 1, 2$). <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 505-525.	1.8	6
70	CHAMELEON GROUND STATE AND EXCITED STATES OF EDT-TTF-IM-F4TCNQ RADICAL DYAD IN DIFFERENT ENVIRONMENTS. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 505-525.	1.8	6
71	INSIGHTS INTO THE SOLVATO-/THERMO-PROMOTED INTRAMOLECULAR ELECTRON TRANSFER IN A TTF-f-TCNQ DYAD WITH AN EXTREMELY LOW HOMO-LUMO GAP. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 599-609.	1.8	5
72	Is C ₆₀ buckminsterfullerene aromatic?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14886.	1.3	58

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73	Identification of the Most Stable Sc ₂ C ₈₀ Isomers: Structure, Electronic Property, and Molecular Spectra Investigations. Chinese Journal of Chemistry, 2012, 30, 765-770.	2.6	5
74	Combustion Synthesis and Electrochemical Properties of the Small Hydrofullerene C ₅₀ H ₁₀ . Chemistry - A European Journal, 2012, 18, 3408-3415.	1.7	15
75	Separation and Characterization of C ₇₀ (C ₁₄ H ₁₀) and C ₇₀ (C ₅ H ₆) from an Acetylene-Benzene-Oxygen Flame. Journal of Physical Chemistry C, 2011, 115, 11016-11022.	1.5	7
76	Photoelectron Imaging and Theoretical Studies of Silver Monohalides AgX ⁺ (X = Cl, Br, I) and AuCl ⁺ . Journal of Physical Chemistry A, 2011, 115, 6321-6326.	1.1	8
77	The Dinitrogen-Ligated Triaurum Cation, Aurodiazenylium, Auronitrenium, Auroammonia, and Auroammonium. Angewandte Chemie - International Edition, 2011, 50, 2166-2170.	7.2	7
78	Experimental and Theoretical Evidence of Aromatic Behavior in Heterobenzene-Like Molecules with Metal-Metal Multiple Bonds. Chemistry - A European Journal, 2011, 17, 10288-10296.	1.7	21
79	Carbon arc production of heptagon-containing fullerene [68]. Nature Communications, 2011, 2, 420.	5.8	69
80	Mononuclear Bis(imino)arylcopper(I) N-Heterocyclic Carbene Complex: Synthesis, Structure, and Reaction with Organic Azide. European Journal of Inorganic Chemistry, 2010, 2010, 4506-4512.	1.0	12
81	Addition of Carbene to the Equator of C ₇₀ To Produce the Most Stable C ₇₁ H ₂ Isomer: 2a-H(12)-Homo(C ₇₀ -D₅H₆)[5,6]fullerene. Angewandte Chemie - International Edition, 2010, 49, 962-966.	7.2	25
82	Spin Divergence Induced by Exohedral Modification: ESR Study of Sc ₃ C ₂ @C ₈₀ Fulleropyrrolidine. Angewandte Chemie - International Edition, 2010, 49, 1786-1789.	7.2	65
83	The odd-even alternation of heteroatom-doped carbon clusters AuC _n ⁺ (n = 1/2, 12): Experimental observations and density functional studies. Journal of Molecular Structure, 2010, 967, 153-158.	1.8	6
84	Design, synthesis and discovery of 5-hydroxyaurone derivatives as growth inhibitors against HUVEC and some cancer cell lines. European Journal of Medicinal Chemistry, 2010, 45, 5950-5957.	2.6	65
85	Chlorofullerenes featuring triple sequentially fused pentagons. Nature Chemistry, 2010, 2, 269-273.	6.6	107
86	Synthesis, Properties, and Bishomoaromaticity of the First Tetrahalogenated Derivative of a 1, 5-Diphosphadithiatetrazocine: A Combined Experimental and Computational Investigation. Inorganic Chemistry, 2010, 49, 3810-3815.	1.9	16
87	Pentagon-Fused Hollow Fullerene in C ₇₈ Family Retrieved by Chlorination. Journal of the American Chemical Society, 2010, 132, 12648-12652.	6.6	37
88	Simple Combustion Production and Characterization of Octahydro[60]fullerene with a Non-IPR C ₆₀ Cage. Journal of the American Chemical Society, 2010, 132, 15093-15095.	6.6	32
89	NC unit trapped by fullerenes: a density functional theory study on Sc ₃ NC@C _{2n} (2n = 68, 78 and 80). Physical Chemistry Chemical Physics, 2010, 12, 12442.	1.3	35
90	Planar Quinary Cluster inside a Fullerene Cage: Synthesis and Structural Characterizations of Sc ₃ NC@C ₈₀ -I₅H₆. Journal of the American Chemical Society, 2010, 132, 16362-16364.	6.6	147

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91	Russian-Doll-Type Metal Carbide Endofullerene: Synthesis, Isolation, and Characterization of Sc ₄ C ₂ @C ₈₀ . Journal of the American Chemical Society, 2009, 131, 16646-16647.	6.6	118
92	Homoconjugation/Homoaromaticity in Main Group Inorganic Molecules. Journal of the American Chemical Society, 2009, 131, 9789-9799.	6.6	36
93	Crystal Structures of Saturn-Like C ₅₀ Cl ₁₀ and Pineapple-Shaped C ₆₄ Cl ₄ : Geometric Implications of Double- and Triple-Pentagon-Fused Chlorofullerenes. Angewandte Chemie - International Edition, 2008, 47, 5340-5343.	7.2	116
94	Two Ih-symmetry-breaking C ₆₀ isomers stabilized by chlorination. Nature Materials, 2008, 7, 790-794.	13.3	114
95	An Entrant of Smaller Fullerene: C ₅₆ Captured by Chlorines and Aligned in Linear Chains. Journal of the American Chemical Society, 2008, 130, 15240-15241.	6.6	69
96	Theoretical Predictions of ³¹ P NMR Chemical Shift Threshold of Trimethylphosphine Oxide Adsorbed on Solid Acid Catalysts. Journal of Physical Chemistry B, 2008, 112, 4496-4505.	1.2	143
97	Synthesis of a Dy@C ₈₂ Derivative Bearing a Single Phosphorus Substituent via a Zwitterion Approach. Journal of the American Chemical Society, 2007, 129, 10636-10637.	6.6	36
98	Dimetalloendofullerene U ₂ @C ₆₀ Has a U-U Multiple Bond Consisting of Sixfold One-Electron-Two-Center Bonds. Journal of the American Chemical Society, 2007, 129, 2171-2177.	6.6	95
99	Comparative Spectroscopic and Reactivity Studies of Sc ₃ Y _x N@C ₈₀ (x = 0-3). Journal of Physical Chemistry C, 2007, 111, 11823-11828.	1.5	81
100	Open-Shell Singlet Character of Cyclacenes and Short Zigzag Nanotubes. Organic Letters, 2007, 9, 5449-5452.	2.4	147
101	Size Effect of Encaged Clusters on the Exohedral Chemistry of Endohedral Fullerenes: A Case Study on the Pyrrolidino Reaction of Sc _x Gd _{3-x} N@C ₈₀ (x = 0-3). Organic Letters, 2007, 9, 2011-2013.	2.4	80
102	Mechanism for the Regioselective Asymmetric Addition of Grignard Reagents to Malimides: A Computational Exploration. Journal of Organic Chemistry, 2007, 72, 35-42.	1.7	30
103	High Activity of Amine-Doped H-ZSM-5 Zeolite in Ethene Protonation: Revealed by Embedding Calculations. ChemPhysChem, 2007, 8, 231-234.	1.0	17
104	Structures and Electronic Properties of M ₂ C ₂ @C ₇₈ (M = Ti, Zr, Hf): A Density Functional Theory Study. Journal of Nanoscience and Nanotechnology, 2007, 7, 1346-1352.	0.9	8
105	Mechanism and Regioselectivity for the Reactions of Propylene Oxide with X(100)-2 $\bar{1}$ Surfaces (X = C, Tl). Journal of Physical Chemistry B, 2006, 110, 10461-10466.	1.2	3
106	Unprecedented $\frac{1}{4}$ -C ₂₆ -Anion in Sc ₄ C ₂ @C ₈₀ . Journal of Physical Chemistry B, 2006, 110, 11098-11102.	1.2	48
107	Pericyclic Transition-State-Like Aromaticity in the Inorganic Ions Se ²⁺ and S ₂ O ₄ ²⁻ . Inorganic Chemistry, 2006, 45, 2457-2460.	1.9	8
108	Electronic Structure and Redox Properties of the Open-Shell Metal Carbide Endofullerene Sc ₃ C ₂ @C ₈₀ : A Density Functional Theory Investigation. Journal of Physical Chemistry A, 2006, 110, 1171-1176.	1.1	62

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109	C ₆₄ H ₄ : Production, Isolation, and Structural Characterizations of a Stable Unconventional Fullerene. <i>Journal of the American Chemical Society</i> , 2006, 128, 6605-6610.	6.6	90
110	La ₂ @C ₇₂ and Sc ₂ @C ₇₂ : Computational Characterizations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2231-2234.	1.1	57
111	Highly Efficient Amination of Benzene to Aniline Mediated by Bromine with Metal Oxide as Cataloreactant. <i>Chemistry Letters</i> , 2006, 35, 1358-1359.	0.7	9
112	Curved Pi-Conjugation, Aromaticity, and the Related Chemistry of Small Fullerenes (<C ₆₀) and Single-Walled Carbon Nanotubes. <i>ChemInform</i> , 2006, 37, no.	0.1	0
113	Isolation and Characterization of Sc ₂ C ₂ @C ₆₈ : A Metal-Carbide Endofullerene with a Non-IPR Carbon Cage. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 2107-2111.	7.2	181
114	Ti ₂ C ₈₀ is more likely a titanium carbide endohedral metallofullerene (Ti ₂ C ₂)@C ₇₈ . <i>Chemical Communications</i> , 2005, , 4444.	2.2	68
115	Mechanisms of Methane Activation and Transformation on Molybdenum Oxide Based Catalysts. <i>Journal of the American Chemical Society</i> , 2005, 127, 3989-3996.	6.6	134
116	Mechanisms of Initial Propane Activation on Molybdenum Oxides: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6416-6421.	1.2	63
117	Curved Pi-Conjugation, Aromaticity, and the Related Chemistry of Small Fullerenes (<C ₆₀) and Single-Walled Carbon Nanotubes. <i>Chemical Reviews</i> , 2005, 105, 3643-3696.	23.0	517
118	Are Stone-Wales Defect Sites Always More Reactive Than Perfect Sites in the Sidewalls of Single-Wall Carbon Nanotubes?. <i>Journal of the American Chemical Society</i> , 2005, 127, 20-21.	6.6	135
119	Prediction of the ¹³ C NMR chemical shifts of organic species adsorbed on H-ZSM-5 zeolite by the ONIOM-GIAO method. <i>Chemical Communications</i> , 2005, , 2474.	2.2	28
120	Capturing the Labile Fullerene[50] as C ₅₀ Cl ₁₀ . <i>Science</i> , 2004, 304, 699-699.	6.0	317
121	Can the Nitroso Ene Reaction Proceed Concertedly?. <i>Organic Letters</i> , 2004, 6, 2813-2815.	2.4	22
122	Adsorbate lone-pair-electron stimulated charge transfer between surface dangling bonds: methanol chemisorption on Si(111)-7x7. <i>Chemical Physics Letters</i> , 2004, 388, 190-194.	1.2	10
123	Beyond the intradimer [2 + 2] cycloaddition chemistry of ethylene on Si(1 0 0): theoretical evidence on the occurrence of interdimer reaction. <i>Chemical Physics Letters</i> , 2004, 393, 124-127.	1.2	24
124	The formation of an enynic-like intermediate in diacetylene binding on Si(100)-2x1. <i>Chemical Physics Letters</i> , 2004, 398, 11-14.	1.2	11
125	Producing Reactive Species on Si(100), Ge(100), and Si(111) Surfaces by Attachments of Diacetylenes. <i>Journal of Physical Chemistry B</i> , 2004, 108, 4478-4484.	1.2	24
126	Diradical Mechanisms for the Cycloaddition Chemistry of Ethylene on X(100) Surfaces (X = C, Si, and Tj ETQq0 0 0,rgBT /Overlock 10 TF	1.2	26

#	ARTICLE	IF	CITATIONS
127	Properties of Fullerene[50] and D5h Decachlorofullerene[50]: A Computational Study. <i>Journal of the American Chemical Society</i> , 2004, 126, 14871-14878.	6.6	133
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