Xin Lu

List of Publications by Year in descending order

173	10,058	22153 59	39675 94
papers	citations	h-index	g-index

193	193	193	6701
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Insights into the gold(<scp>i</scp>)-catalyzed intermolecular annulations of alkynes with N-allenamides: a mechanistic DFT study. Dalton Transactions, 2022, 51, 3734-3739.	3.3	3
2	Efficient synthesis of tetracyclic Î³-lactamsviagold-catalyzed oxidative cyclization of alkenyl diynes. Organic Chemistry Frontiers, 2022, 9, 2557-2562.	4.5	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.	3.2	5
4	Copperâ€Catalyzed Asymmetric Diyne Cyclization via [1,2]â€Stevensâ€Type Rearrangement for the Synthesis of Chiral Chromeno[3,4â€•c]pyrroles. Angewandte Chemie - International Edition, 2022, 61, e202115554.	13.8	44
5	Copperâ€Catalyzed Asymmetric Diyne Cyclization via [1,2]â€Stevensâ€Type Rearrangement for the Synthesis of Chiral Chromeno[3,4â€•c]pyrroles. Angewandte Chemie, 2022, 134, .	2.0	9
6	Intermolecular 1,2-Difunctionalization of Alkenes Enabled by Fluoroamide-Directed Remote Benzyl C(sp³)â€“H Functionalization. Journal of the American Chemical Society, 2022, 144, 339-348.	13.7	51
7	Catalystâ€Dependent Stereospecific [3,3]â€Sigmatropic Rearrangement of Sulfoxideâ€Ynamides: Divergent Synthesis of Chiral Mediumâ€Sized N,Sâ€Heterocycles. Angewandte Chemie, 2022, 134, .	2.0	6
8	Catalystâ€Dependent Stereospecific [3,3]â€Sigmatropic Rearrangement of Sulfoxideâ€Ynamides: Divergent Synthesis of Chiral Mediumâ€Sized N,Sâ€Heterocycles. Angewandte Chemie - International Edition, 2022, 61, .	13.8	26
9	Copper-catalyzed asymmetric cyclization of alkenyl diynes: method development and new mechanistic insights. Chemical Science, 2021, 12, 9466-9474.	7.4	41
10	Dynamic Effects in Intramolecular Schmidt Reactions: Entropy, Electrostatic Drag, and Selectivity Prediction. ChemPhysChem, 2021, 22, 649-656.	2.1	2
11	Insights into the mechanism of fatty acid photodecarboxylase: A theoretical investigation. Chemical Physics Letters, 2021, 771, 138550.	2.6	2
12	Carbon Nitride Supported Highâ€Loading Fe Singleâ€Atom Catalyst for Activation of Peroxymonosulfate to Generate ¹O₂ with 100â€‰% Selectivity. Angewandte Chemie - International Edition, 2021, 60, 21751-21755.	13.8	521
13	Carbon Nitride Supported Highâ€Loading Fe Singleâ€Atom Catalyst for Activation of Peroxymonosulfate to Generate 1 O 2 with 100â€‰% Selectivity. Angewandte Chemie, 2021, 133, 21919-21923.	2.0	18
14	Atroposelective carbonylation of aryl iodides with amides: facile synthesis of enantioenriched cyclic and acyclic amides. Organic Chemistry Frontiers, 2021, 8, 6067-6073.	4.5	20
15	Synthesis and Spectroscopy of Monodispersed, Quantum-Confined FAPbBr₃ Perovskite Nanocrystals. Chemistry of Materials, 2020, 32, 549-556.	6.7	39
16	Sizeâ€•and Halideâ€Dependent Auger Recombination in Lead Halide Perovskite Nanocrystals. Angewandte Chemie - International Edition, 2020, 59, 14292-14295.	13.8	63
17	Sizeâ€•and Halideâ€Dependent Auger Recombination in Lead Halide Perovskite Nanocrystals. Angewandte Chemie, 2020, 132, 14398-14401.	2.0	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.	13.7	83

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19	Size- and Composition-Dependent Exciton Spin Relaxation in Lead Halide Perovskite Quantum Dots. ACS Energy Letters, 2020, 5, 1701-1708.	17.4	47
20	Strong Spin-Selective Optical Stark Effect in Lead Halide Perovskite Quantum Dots. Journal of Physical Chemistry Letters, 2020, 11, 3594-3600.	4.6	21
21	Scandium Tetrahedron Supported by H Anion and CN Pentaanion inside Fullerene C₈₀. Inorganic Chemistry, 2020, 59, 8284-8290.	4.0	7
22	Organocatalytic Enantioselective Coniaâ€Eneâ€Type Carbocyclization of Ynamide Cyclohexanones: Regiodivergent Synthesis of Morphans and Normorphans. Angewandte Chemie - International Edition, 2019, 58, 16252-16259.	13.8	72
23	Organocatalytic Enantioselective Coniaâ€Eneâ€Type Carbocyclization of Ynamide Cyclohexanones: Regiodivergent Synthesis of Morphans and Normorphans. Angewandte Chemie, 2019, 131, 16398-16405.	2.0	21
24	Chemoselectivity in Gold(I)-Catalyzed Propargyl Ester Reactions: Insights From DFT Calculations. Frontiers in Chemistry, 2019, 7, 609.	3.6	3
25	Generation of Donor/Donor Copper Carbenes through Copper-Catalyzed Diyne Cyclization: Enantioselective and Divergent Synthesis of Chiral Polycyclic Pyrroles. Journal of the American Chemical Society, 2019, 141, 16961-16970.	13.7	84
26	On the absence of a phonon bottleneck in strongly confined CsPbBr₃ perovskite nanocrystals. Chemical Science, 2019, 10, 5983-5989.	7.4	71
27	Sulfur Moiety as a Double-Edged Sword for Realizing Ultrafine Supported Metal Nanoclusters with a Cationic Nature. ACS Applied Materials & Interfaces, 2019, 11, 11317-11326.	8.0	15
28	Generation of Endocyclic Vinyl Carbene Complexes via Gold-Catalyzed Oxidative Cyclization of Terminal Diynes: Toward Naphthoquinones and Carbazolequinones. ACS Catalysis, 2019, 9, 1019-1025.	11.2	46
29	Biexciton Auger recombination in mono-dispersed, quantum-confined CsPbBr3 perovskite nanocrystals obeys universal volume-scaling. Nano Research, 2019, 12, 619-623.	10.4	63
30	Metalâ€catalyzed alkyne oxidation/C ï£¿ H functionalization: Effects of oxidant, temperature, and metal catalyst on chemoselectivity. Journal of Computational Chemistry, 2019, 40, 1038-1044.	3.3	2
31	Dual catalysis for enantioselective convergent synthesis of enantiopure vicinal amino alcohols. Nature Communications, 2018, 9, 410.	12.8	92
32	Electrochemical Synthesis of Imidazoâ€Fused Nâ€Heteroaromatic Compounds through a Câ^'N Bondâ€Forming Radical Cascade. Angewandte Chemie, 2018, 130, 1652-1655.	2.0	41
33	Electrochemical Synthesis of Imidazoâ€Fused Nâ€Heteroaromatic Compounds through a Câ^'N Bondâ€Forming Radical Cascade. Angewandte Chemie - International Edition, 2018, 57, 1636-1639.	13.8	155
34	Gold-Catalyzed [5+2]- and [5+1]-Annulations between Ynamides and 1,2-Benzisoxazoles with Ligand-Controlled Chemoselectivity. ACS Catalysis, 2018, 8, 9697-9701.	11.2	71
35	Zinc-catalyzed reaction of isoxazoles with thioynol ethers involving an unprecedented 1,2-sulfur migration. Chemical Communications, 2018, 54, 7435-7438.	4.1	28
36	Benign catalysis with zinc: atom-economical and divergent synthesis of nitrogen heterocycles by formal [3 + 2] annulation of isoxazoles with ynol ethers. Green Chemistry, 2018, 20, 4287-4291.	9.0	45

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37	Transition-metal-free oxidative cyclization of N-propargyl ynamides: stereospecific construction of linear polycyclic N-heterocycles. Green Chemistry, 2018, 20, 3271-3278.	9.0	33
38	Highly Site Selective Formal [5+2] and [4+2] Annulations of Isoxazoles with Heterosubstituted Alkynes by Platinum Catalysis: Rapid Access to Functionalized 1,3â€Oxazepines and 2,5â€Dihydropyridines. Angewandte Chemie, 2017, 129, 620-624.	2.0	41
39	Conjugated Microporous Polymer as Heterogeneous Ligand for Highly Selective Oxidative Heck Reaction. Journal of the American Chemical Society, 2017, 139, 3966-3969.	13.7	86
40	Reversal of Regioselectivity in Catalytic Arene-Ynamide Cyclization: Direct Synthesis of Valuable Azepino[4,5-b]indoles and Î²-Carbolines and DFT Calculations. ACS Catalysis, 2017, 7, 4004-4010.	11.2	92
41	Synthesis and Characterization of a Metallacyclic Framework with Three Fused Fiveâ€membered Rings. Angewandte Chemie, 2017, 129, 9195-9199.	2.0	13
42	Highly Site Selective Formal [5+2] and [4+2] Annulations of Isoxazoles with Heterosubstituted Alkynes by Platinum Catalysis: Rapid Access to Functionalized 1,3â€Oxazepines and 2,5â€Dihydropyridines. Angewandte Chemie - International Edition, 2017, 56, 605-609.	13.8	146
43	Divergent synthesis of N-heterocycles via controllable cyclization of azido-diynes catalyzed by copper and gold. Nature Communications, 2017, 8, 1748.	12.8	139
44	Sponge-like quaternary ammonium-based poly(ionic liquid)s for high CO₂ capture and efficient cycloaddition under mild conditions. Journal of Materials Chemistry A, 2017, 5, 25594-25600.	10.3	60
45	Synthesis and Characterization of a Metallacyclic Framework with Three Fused Fiveâ€membered Rings. Angewandte Chemie - International Edition, 2017, 56, 9067-9071.	13.8	45
46	Electrochemical Câ^'H/Nâ^'H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. Angewandte Chemie, 2016, 128, 9314-9318.	2.0	56
47	Electrochemical Câ^'H/Nâ^'H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. Angewandte Chemie - International Edition, 2016, 55, 9168-9172.	13.8	215
48	Electrocatalytic Generation of Amidyl Radicals for Olefin Hydroamidation: Use of Solvent Effects to Enable Anilide Oxidation. Angewandte Chemie - International Edition, 2016, 55, 2226-2229.	13.8	214
49	Catalytic Ynamide Oxidation Strategy for the Preparation of Î±-Functionalized Amides. ACS Catalysis, 2016, 6, 6055-6062.	11.2	68
50	Synthesis of 2-Aza-1,3-butadienes through Gold-Catalyzed Intermolecular Ynamide Amination/Câ€“H Functionalization. Organic Letters, 2016, 18, 4630-4633.	4.6	35
51	Assembled molecular face-rotating polyhedra to transfer chirality from two to three dimensions. Nature Communications, 2016, 7, 12469.	12.8	90
52	CCCCC pentadentate chelates with planar MÃ¶bius aromaticity and unique properties. Science Advances, 2016, 2, e1601031.	10.3	74
53	Electrocatalytic Generation of Amidyl Radicals for Olefin Hydroamidation: Use of Solvent Effects to Enable Anilide Oxidation. Angewandte Chemie, 2016, 128, 2266-2269.	2.0	71
54	Copperâ€Catalyzed Intramolecular Oxidative Amination of Unactivated Internal Alkenes. Chemistry - A European Journal, 2016, 22, 4379-4383.	3.3	52

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55	Gold-Catalyzed Intermolecular Ynamide Amination-Initiated Aza-Nazarov Cyclization: Access to Functionalized 2-Aminopyrroles. Organic Letters, 2016, 18, 3254-3257.	4.6	97
56	Zincâ€Catalyzed Alkyne Oxidation/Cï£¿H Functionalization: Highly Siteâ€Selective Synthesis of Versatile Isoquinolones and Î²â€Carbolines. Angewandte Chemie, 2015, 127, 8363-8367.	2.0	35
57	Zincâ€Catalyzed Alkyne Oxidation/Cï£¿H Functionalization: Highly Siteâ€Selective Synthesis of Versatile Isoquinolones and Î²â€Carbolines. Angewandte Chemie - International Edition, 2015, 54, 8245-8249.	13.8	154
58	Pristine graphene dispersion in solvents and its application as a catalyst support: a combined theoretical and experimental study. Journal of Materials Chemistry A, 2015, 3, 6282-6285.	10.3	26
59	Generation of Î±-Imino Gold Carbenes through Gold-Catalyzed Intermolecular Reaction of Azides with Ynamides. Journal of the American Chemical Society, 2015, 137, 9567-9570.	13.7	245
60	Atom-economic generation of gold carbenes: gold-catalyzed formal [3+2] cycloaddition between ynamides and isoxazoles. Chemical Science, 2015, 6, 1265-1271.	7.4	251
61	Practical, Modular, and General Synthesis of 3â€Coumaranones through Goldâ€Catalyzed Intermolecular Alkyne Oxidation Strategy. Chemistry - an Asian Journal, 2015, 10, 91-95.	3.3	39
62	Planar MÃ¶bius aromatic pentalenes incorporating 16 and 18 valence electron osmiums. Nature Communications, 2014, 5, 3265.	12.8	169
63	Mechanism of Lewis-acid-catalyzed intramolecular coupling of sp³Câ€“H bond and alkene: A theoretical investigation. Journal of Theoretical and Computational Chemistry, 2014, 13, 1450015.	1.8	0
64	Hydrogen bonding in microsolvation: photoelectron imaging and theoretical studies on Auxâ¯â€“(H2O)n and Auxâ¯â€“(CH3OH)n (x = 1, 2; n = 1, 2) complexes. Physical Chemistry Chemical Physics, 2014, 16, 4771.	2.8	11
65	Real-time analysis of self-assembled nucleobases by Venturi easy ambient sonic-spray ionization mass spectrometry. Talanta, 2014, 128, 366-372.	5.5	15
66	Control of the Charge Distribution and Modulation of the Class IIâ€“III Transition in Weakly Coupled Mo2â€“Mo2 Systems. Inorganic Chemistry, 2013, 52, 12624-12633.	4.0	37
67	Exohedrally stabilized C70 isomer with adjacent pentagons characterized by crystallography. Chemical Science, 2013, 4, 2967.	7.4	22
68	Stabilization of anti-aromatic and strained five-membered rings with a transition metal. Nature Chemistry, 2013, 5, 698-703.	13.6	244
69	Vibrationally resolved photoelectron imaging of platinum carbonyl anion Pt(CO)nâ¯ (n =) Tj ETQq1 1 0.784314 rgBT /O	3.0	9
70	CHAMELEON GROUND STATE AND EXCITED STATES OF EDT-TTF-IM-F4TCNQ RADICAL DYAD IN DIFFERENT ENVIRONMENTS. Journal of Theoretical and Computational Chemistry, 2012, 11, 505-525.	1.8	6
71	INSIGHTS INTO THE SOLVATO-/THERMO-PROMOTED INTRAMOLECULAR ELECTRON TRANSFER IN A TTF-Ïƒ-TCNQ DYAD WITH AN EXTREMELY LOW HOMOâ€“LUMO GAP. Journal of Theoretical and Computational Chemistry, 2012, 11, 599-609.	1.8	5
72	Is C60 buckminsterfullerene aromatic?. Physical Chemistry Chemical Physics, 2012, 14, 14886.	2.8	58

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73	Identification of the Most Stable Sc₂C₈₀ Isomers: Structure, Electronic Property, and Molecular Spectra Investigations. Chinese Journal of Chemistry, 2012, 30, 765-770.	4.9	5
74	Combustion Synthesis and Electrochemical Properties of the Small Hydrofullerene C₅₀H₁₀. Chemistry - A European Journal, 2012, 18, 3408-3415.	3.3	15
75	Separation and Characterization of C₇₀(C₁₄H₁₀) and C₇₀(C₅H₆) from an Acetyleneâ€“Benzeneâ€“Oxygen Flame. Journal of Physical Chemistry C, 2011, 115, 11016-11022.	3.1	7
76	Photoelectron Imaging and Theoretical Studies of Silver Monohalides AgX^{â€“} (X = Cl, Br, I) and AuCl^{â€“}. Journal of Physical Chemistry A, 2011, 115, 6321-6326.	2.5	8
77	The Dinitrogenâ€Ligated Triaurum Cation, Aurodiazenylium, Auronitrenium, Auroammonia, and Auroammonium. Angewandte Chemie - International Edition, 2011, 50, 2166-2170.	13.8	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.	3.3	21
79	Carbon arc production of heptagon-containing fullerene[68]. Nature Communications, 2011, 2, 420.	12.8	69
80	Mononuclear Bis(imino)arylcopper(I) Nâ€Heterocyclic Carbene Complex: Synthesis, Structure, and Reaction with Organic Azide. European Journal of Inorganic Chemistry, 2010, 2010, 4506-4512.	2.0	12
81	Addition of Carbene to the Equator of C₇₀ To Produce the Most Stable C₇₁H₂ Isomer: 2â€‰aHâ€2(12)aâ€Homo(C₇₀â€D_{5h(6)})[5,6]fullerene. Angewandte Chemie - International Edition, 2010, 49, 962-966.	13.8	25
82	Spin Divergence Induced by Exohedral Modification: ESR Study of Sc₃C₂@C₈₀ Fulleropyrrolidine. Angewandte Chemie - International Edition, 2010, 49, 1786-1789.	13.8	65
83	The oddâ€“even alternation of heteroatom-doped carbon clusters AuCnâ^ (nâ©½12): Experimental observations and density functional studies. Journal of Molecular Structure, 2010, 967, 153-158.	3.6	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.	5.5	65
85	Chlorofullerenes featuring triple sequentially fused pentagons. Nature Chemistry, 2010, 2, 269-273.	13.6	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.	4.0	16
87	Pentagon-Fused Hollow Fullerene in C78Family Retrieved by Chlorination. Journal of the American Chemical Society, 2010, 132, 12648-12652.	13.7	37
88	Simple Combustion Production and Characterization of Octahydro[60]fullerene with a Non-IPR C₆₀ Cage. Journal of the American Chemical Society, 2010, 132, 15093-15095.	13.7	32
89	NC unit trapped by fullerenes: a density functional theory study on Sc3NC@C2n (2n = 68, 78 and 80). Physical Chemistry Chemical Physics, 2010, 12, 12442.	2.8	35
90	Planar Quinary Cluster inside a Fullerene Cage: Synthesis and Structural Characterizations of Sc₃NC@C₈₀-I_h. Journal of the American Chemical Society, 2010, 132, 16362-16364.	13.7	147

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91	Russian-Doll-Type Metal Carbide Endofullerene: Synthesis, Isolation, and Characterization of Sc₄C₂@C₈₀. Journal of the American Chemical Society, 2009, 131, 16646-16647.	13.7	118
92	Homoconjugation/Homoaromaticity in Main Group Inorganic Molecules. Journal of the American Chemical Society, 2009, 131, 9789-9799.	13.7	36
93	Crystal Structures of Saturnâ€Like C₅₀Cl₁₀ and Pineappleâ€Shaped C₆₄Cl₄: Geometric Implications of Doubleâ€and Tripleâ€Pentagonâ€Fused Chlorofullerenes. Angewandte Chemie - International Edition, 2008, 47, 5340-5343.	13.8	116
94	Two Ih-symmetry-breaking C60 isomers stabilized by chlorination. Nature Materials, 2008, 7, 790-794.	27.5	114
95	An Entrant of Smaller Fullerene: C56 Captured by Chlorines and Aligned in Linear Chains. Journal of the American Chemical Society, 2008, 130, 15240-15241.	13.7	69
96	Theoretical Predictions of ³¹P NMR Chemical Shift Threshold of Trimethylphosphine Oxide Absorbed on Solid Acid Catalysts. Journal of Physical Chemistry B, 2008, 112, 4496-4505.	2.6	143
97	Synthesis of a Dy@C₈₂ Derivative Bearing a Single Phosphorus Substituent via a Zwitterion Approach. Journal of the American Chemical Society, 2007, 129, 10636-10637.	13.7	36
98	Dimetalloendofullerene U2@C60Has a Uâ”U Multiple Bond Consisting of Sixfold One-Electron-Two-Center Bonds. Journal of the American Chemical Society, 2007, 129, 2171-2177.	13.7	95
99	Comparative Spectroscopic and Reactivity Studies of Sc₃₋_xY_xN@C₈₀ (x = 0â”3). Journal of Physical Chemistry C, 2007, 111, 11823-11828.	3.1	81
100	Open-Shell Singlet Character of Cyclacenes and Short Zigzag Nanotubes. Organic Letters, 2007, 9, 5449-5452.	4.6	147
101	Size Effect of Encaged Clusters on the Exohedral Chemistry of Endohedral Fullerenes:Â A Case Study on the Pyrrolidino Reaction of ScxGd3-xN@C80(x= 0â”3). Organic Letters, 2007, 9, 2011-2013.	4.6	80
102	Mechanism for the Regioselective Asymmetric Addition of Grignard Reagents to Malimides:Â A Computational Explorationâ€–. Journal of Organic Chemistry, 2007, 72, 35-42.	3.2	30
103	High Activity of Amine-Doped H-ZSM-5 Zeolite in Ethene Protonation: Revealed by Embedding Calculations. ChemPhysChem, 2007, 8, 231-234.	2.1	17
104	Structures and Electronic Properties of M2C2 @C78(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)-2Ã—1 Surfaces (X = C,) Tj ETQq1 1 0.784314 rgBT 10461-10466.	2.6	3
106	Unprecedented Î¼4-C26-Anion in Sc4C2@C80. Journal of Physical Chemistry B, 2006, 110, 11098-11102.	2.6	48
107	Pericyclic Transition-State-Like Aromaticity in the Inorganic Ions Se2I42+and S2O42-. Inorganic Chemistry, 2006, 45, 2457-2460.	4.0	8
108	Electronic Structure and Redox Properties of the Open-Shell Metalâ”Carbide Endofullerene Sc3C2@C80:Â A Density Functional Theory Investigation. Journal of Physical Chemistry A, 2006, 110, 1171-1176.	2.5	62

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109	C64H4:Â Production, Isolation, and Structural Characterizations of a Stable Unconventional Fulleride. Journal of the American Chemical Society, 2006, 128, 6605-6610.	13.7	90
110	La2@C72and Sc2@C72:Â Computational Characterizations. Journal of Physical Chemistry A, 2006, 110, 2231-2234.	2.5	57
111	Highly Efficient Amination of Benzene to Aniline Mediated by Bromine with Metal Oxide as Cataloreactant. Chemistry Letters, 2006, 35, 1358-1359.	1.3	9
112	Curved Pi-Conjugation, Aromaticity, and the Related Chemistry of Small Fullerenes (<C60) and Single-Walled Carbon Nanotubes. ChemInform, 2006, 37, no.	0.0	0
113	Isolation and Characterization of Sc2C2@C68: A Metal-Carbide Endofullerene with a Non-IPR Carbon Cage. Angewandte Chemie - International Edition, 2006, 45, 2107-2111.	13.8	181
114	Ti2C80 is more likely a titanium carbide endohedral metallofullerene (Ti2C2)@C78. Chemical Communications, 2005, , 4444.	4.1	68
115	Mechanisms of Methane Activation and Transformation on Molybdenum Oxide Based Catalysts. Journal of the American Chemical Society, 2005, 127, 3989-3996.	13.7	134
116	Mechanisms of Initial Propane Activation on Molybdenum Oxides:â€‰ A Density Functional Theory Study. Journal of Physical Chemistry B, 2005, 109, 6416-6421.	2.6	63
117	Curved Pi-Conjugation, Aromaticity, and the Related Chemistry of Small Fullerenes (<C60) and Single-Walled Carbon Nanotubes. Chemical Reviews, 2005, 105, 3643-3696.	47.7	517
118	Are Stoneâ˜Wales Defect Sites Always More Reactive Than Perfect Sites in the Sidewalls of Single-Wall Carbon Nanotubes?. Journal of the American Chemical Society, 2005, 127, 20-21.	13.7	135
119	Prediction of the 13C NMR chemical shifts of organic species adsorbed on H-ZSM-5 zeolite by the ONIOM-GIAO method. Chemical Communications, 2005, , 2474.	4.1	28
120	Capturing the Labile Fullerene[50] as C50Cl10. Science, 2004, 304, 699-699.	12.6	317
121	Can the Nitroso Ene Reaction Proceed Concertedly?. Organic Letters, 2004, 6, 2813-2815.	4.6	22
122	Adsorbate lone-pair-electron stimulated charge transfer between surface dangling bonds: methanol chemisorption on Si(111)-7Ã—7. Chemical Physics Letters, 2004, 388, 190-194.	2.6	10
123	Beyond the intradimer [2 + 2] cycloaddition chemistry of ethylene on Si(1 0 0): theoretical evidence on the occurrence of interdimer reaction. Chemical Physics Letters, 2004, 393, 124-127.	2.6	24
124	The formation of an enynic-like intermediate in diacetylene binding on Si(100)-2Ã—1. Chemical Physics Letters, 2004, 398, 11-14.	2.6	11
125	Producing Reactive Species on Si(100), Ge(100), and Si(111) Surfaces by Attachments of Diacetylenes. Journal of Physical Chemistry B, 2004, 108, 4478-4484.	2.6	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	2.6	26

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127	Properties of Fullerene[50] andD5hDecachlorofullerene[50]:Â A Computational Study. Journal of the American Chemical Society, 2004, 126, 14871-14878.	13.7	133
128	Computer simulation of Pr(III) speciation in human interstitial fluid. Chemical Speciation and Bioavailability, 2004, 16, 153-158.	2.0	2
129	A Theoretical Exploration of the 1,3-Dipolar Cycloadditions onto the Sidewalls of (n,n) Armchair Single-Wall Carbon Nanotubes. Journal of the American Chemical Society, 2003, 125, 10459-10464.	13.7	119
130	Hydroboration of C(100) Surface, Fullerene, and the Sidewalls of Single-Wall Carbon Nanotubes with Borane.. ChemInform, 2003, 34, no.	0.0	0
131	The chemistry of HN3 on Ge(100)-2Ã—1: a theoretical study. Chemical Physics Letters, 2003, 371, 172-177.	2.6	7
132	The chemisorption of NO on Si(111)-7Ã—7 surface: a DFT study. Chemical Physics Letters, 2003, 375, 106-112.	2.6	15
133	Diradical Mechanisms for the Cycloaddition Reactions of 1,3-Butadiene, Benzene, Thiophene, Ethylene, and Acetylene on a Si(111)-7Ã—7 Surface. Journal of the American Chemical Society, 2003, 125, 7923-7929.	13.7	61
134	Hydroboration of C(100) Surface, Fullerene, and the Sidewalls of Single-Wall Carbon Nanotubes with Borane. Journal of Organic Chemistry, 2003, 68, 4495-4498.	3.2	29
135	The [2+1] Cycloadditions of Dichlorocarbene, Silylene, Germylene, and Oxycarbonylnitrene onto the Sidewall of Armchair (5,5) Single-Wall Carbon Nanotube. Journal of Physical Chemistry B, 2003, 107, 8388-8391.	2.6	54
136	Sidewall Epoxidation of Single-Walled Carbon Nanotubes:â€‰ A Theoretical Prediction. Organic Letters, 2003, 5, 3527-3530.	4.6	25
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