

# Xin Lu

## List of Publications by Year in descending order

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173  
papers

10,058  
citations

22153

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193  
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193  
docs citations

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times ranked

6701  
citing authors

#	ARTICLE	IF	CITATIONS
1	Carbon Nitride Supported High-Loading Fe Single-Atom Catalyst for Activation of Peroxymonosulfate to Generate $\cdot\text{O}_2$ with 100% Selectivity. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 21751-21755.	13.8	521
2	Curved Pi-Conjugation, Aromaticity, and the Related Chemistry of Small Fullerenes ( $\text{C}_{60}$ ) and Single-Walled Carbon Nanotubes. <i>Chemical Reviews</i> , 2005, 105, 3643-3696.	47.7	517
3	Capturing the Labile Fullerene[50] as $\text{C}_{50}\text{Cl}_{10}$ . <i>Science</i> , 2004, 304, 699-699.	12.6	317
4	Atom-economic generation of gold carbenes: gold-catalyzed formal [3+2] cycloaddition between ynamides and isoxazoles. <i>Chemical Science</i> , 2015, 6, 1265-1271.	7.4	251
5	Generation of $\text{I}^{\pm}$ -Imino Gold Carbenes through Gold-Catalyzed Intermolecular Reaction of Azides with Ynamides. <i>Journal of the American Chemical Society</i> , 2015, 137, 9567-9570.	13.7	245
6	Stabilization of anti-aromatic and strained five-membered rings with a transition metal. <i>Nature Chemistry</i> , 2013, 5, 698-703.	13.6	244
7	Electrochemical $\text{C}^{\sim}\text{H}/\text{N}^{\sim}\text{H}$ Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 9168-9172.	13.8	215
8	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.	13.8	214
9	Isolation and Characterization of $\text{Sc}_2\text{C}_2@C_{68}$ : A Metal-Carbide Endofullerene with a Non-IPR Carbon Cage. <i>Angewandte Chemie - International Edition</i> , 2006, 45, 2107-2111.	13.8	181
10	Planar $\text{M}^{\sim}\text{b}$ aromatic pentalenes incorporating 16 and 18 valence electron osmiums. <i>Nature Communications</i> , 2014, 5, 3265.	12.8	169
11	Electrochemical Synthesis of Imidazo-fused N-heteroaromatic Compounds through a $\text{C}^{\sim}\text{N}$ Bond-Forming Radical Cascade. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 1636-1639.	13.8	155
12	Zinc-Catalyzed Alkyne Oxidation/ $\text{C}^{\sim}\text{H}$ Functionalization: Highly Site-Selective Synthesis of Versatile Isoquinolones and $\text{I}^2$ -Carbolines. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 8245-8249.	13.8	154
13	Open-Shell Singlet Character of Cyclacenes and Short Zigzag Nanotubes. <i>Organic Letters</i> , 2007, 9, 5449-5452.	4.6	147
14	Planar Quinary Cluster inside a Fullerene Cage: Synthesis and Structural Characterizations of $\text{Sc}_3\text{NC}@C_{80}$ . <i>Journal of the American Chemical Society</i> , 2010, 132, 16362-16364.	13.7	147
15	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.	13.8	146
16	Theoretical Predictions of $^{31}\text{P}$ NMR Chemical Shift Threshold of Trimethylphosphine Oxide Absorbed on Solid Acid Catalysts. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4496-4505.	2.6	143
17	Divergent synthesis of N-heterocycles via controllable cyclization of azido-diyne catalyzed by copper and gold. <i>Nature Communications</i> , 2017, 8, 1748.	12.8	139
18	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.	13.7	135

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19	Mechanisms of Methane Activation and Transformation on Molybdenum Oxide Based Catalysts. Journal of the American Chemical Society, 2005, 127, 3989-3996.	13.7	134
20	Properties of Fullerene[50] and D <sub>5h</sub> Decachlorofullerene[50]: A Computational Study. Journal of the American Chemical Society, 2004, 126, 14871-14878.	13.7	133
21	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
22	Russian-Doll-Type Metal Carbide Endofullerene: Synthesis, Isolation, and Characterization of Sc <sub>4</sub> C <sub>2</sub> @C <sub>80</sub> . Journal of the American Chemical Society, 2009, 131, 16646-16647.	13.7	118
23	Crystal Structures of Saturn-Like C <sub>50</sub> Cl <sub>10</sub> and Pineapple-Shaped C <sub>64</sub> Cl <sub>4</sub> : Geometric Implications of Double- and Triple-Pentagon-Fused Chlorofullerenes. Angewandte Chemie - International Edition, 2008, 47, 5340-5343.	13.8	116
24	Reactions of some [C, N, O]-containing molecules with Si surfaces: Experimental and theoretical studies. International Reviews in Physical Chemistry, 2002, 21, 137-184.	2.3	114
25	Two Ih-symmetry-breaking C <sub>60</sub> isomers stabilized by chlorination. Nature Materials, 2008, 7, 790-794.	27.5	114
26	Chlorofullerenes featuring triple sequentially fused pentagons. Nature Chemistry, 2010, 2, 269-273.	13.6	107
27	Gold-Catalyzed Intermolecular Ynamide Amination-Initiated Aza-Nazarov Cyclization: Access to Functionalized 2-Aminopyrroles. Organic Letters, 2016, 18, 3254-3257.	4.6	97
28	Dimetalloendofullerene U <sub>2</sub> @C <sub>60</sub> Has a U-U Multiple Bond Consisting of Sixfold One-Electron-Two-Center Bonds. Journal of the American Chemical Society, 2007, 129, 2171-2177.	13.7	95
29	Can the Sidewalls of Single-Wall Carbon Nanotubes Be Ozonized?. Journal of Physical Chemistry B, 2002, 106, 2136-2139.	2.6	94
30	Reversal of Regioselectivity in Catalytic Arene-Ynamide Cyclization: Direct Synthesis of Valuable Azepino[4,5- <i>b</i> ]indoles and 1 <sup>2</sup> -Carbolines and DFT Calculations. ACS Catalysis, 2017, 7, 4004-4010.	11.2	92
31	Dual catalysis for enantioselective convergent synthesis of enantiopure vicinal amino alcohols. Nature Communications, 2018, 9, 410.	12.8	92
32	C <sub>64</sub> H <sub>4</sub> : Production, Isolation, and Structural Characterizations of a Stable Unconventional Fulleride. Journal of the American Chemical Society, 2006, 128, 6605-6610.	13.7	90
33	Assembled molecular face-rotating polyhedra to transfer chirality from two to three dimensions. Nature Communications, 2016, 7, 12469.	12.8	90
34	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
35	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
36	Chemisorption and Decomposition of Thiophene and Furan on the Si(100)-2 × 1 Surface: A Quantum Chemical Study. Journal of Physical Chemistry B, 2001, 105, 10069-10075.	2.6	83

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37	Organic Functionalization of the Sidewalls of Carbon Nanotubes by Diels-Alder Reactions: A Theoretical Prediction. <i>Organic Letters</i> , 2002, 4, 4313-4315.	4.6	83
38	Copper-Catalyzed Asymmetric Reaction of Alkenyl Dienes 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. <i>Journal of the American Chemical Society</i> , 2020, 142, 7618-7626.	13.7	83
39	Adsorption of methanol, formaldehyde and formic acid on the Si(100)-2 $\times$ 1 surface: A computational study. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 2156-2161.	2.8	81
40	Comparative Spectroscopic and Reactivity Studies of Sc <sub>3-x</sub> C <sub>x</sub> N@C <sub>80</sub> (0 $\leq$ x $\leq$ 3). <i>Journal of Physical Chemistry C</i> , 2007, 111, 11823-11828.	3.1	81
41	Size Effect of Encaged Clusters on the Exohedral Chemistry of Endohedral Fullerenes: A Case Study on the Pyrrolidino Reaction of Sc <sub>x</sub> Gd <sub>3-x</sub> N@C <sub>80</sub> (x = 0-3). <i>Organic Letters</i> , 2007, 9, 2011-2013.	4.6	80
42	CCCCC pentadentate chelates with planar M $\pi$ aromaticity and unique properties. <i>Science Advances</i> , 2016, 2, e1601031.	10.3	74
43	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.	13.8	72
44	Electrocatalytic Generation of Amidyl Radicals for Olefin Hydroamidation: Use of Solvent Effects to Enable Anilide Oxidation. <i>Angewandte Chemie</i> , 2016, 128, 2266-2269.	2.0	71
45	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.	11.2	71
46	On the absence of a phonon bottleneck in strongly confined CsPbBr <sub>3</sub> perovskite nanocrystals. <i>Chemical Science</i> , 2019, 10, 5983-5989.	7.4	71
47	An Entrant of Smaller Fullerene: C <sub>56</sub> Captured by Chlorines and Aligned in Linear Chains. <i>Journal of the American Chemical Society</i> , 2008, 130, 15240-15241.	13.7	69
48	Carbon arc production of heptagon-containing fullerene [68]. <i>Nature Communications</i> , 2011, 2, 420.	12.8	69
49	Ti <sub>2</sub> C <sub>80</sub> is more likely a titanium carbide endohedral metallofullerene (Ti <sub>2</sub> C <sub>2</sub> )@C <sub>78</sub> . <i>Chemical Communications</i> , 2005, , 4444.	4.1	68
50	Catalytic Ynamide Oxidation Strategy for the Preparation of $\beta$ -Functionalized Amides. <i>ACS Catalysis</i> , 2016, 6, 6055-6062.	11.2	68
51	Diradical Mechanism for the [2 + 2] Cycloaddition of Ethylene on Si(100) Surface. <i>Journal of the American Chemical Society</i> , 2003, 125, 6384-6385.	13.7	66
52	Spin Divergence Induced by Exohedral Modification: ESR Study of Sc <sub>3</sub> C <sub>2</sub> @C <sub>80</sub> Fulleropyrrolidine. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 1786-1789.	13.8	65
53	Design, synthesis and discovery of 5-hydroxyaurone derivatives as growth inhibitors against HUVEC and some cancer cell lines. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 5950-5957.	5.5	65
54	Mechanisms of Initial Propane Activation on Molybdenum Oxides: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 6416-6421.	2.6	63

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55	Biexciton Auger recombination in mono-dispersed, quantum-confined CsPbBr <sub>3</sub> perovskite nanocrystals obeys universal volume-scaling. <i>Nano Research</i> , 2019, 12, 619-623.	10.4	63
56	Size- and Halide-Dependent Auger Recombination in Lead Halide Perovskite Nanocrystals. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 14292-14295.	13.8	63
57	Electronic Structure and Redox Properties of the Open-Shell Metal-Carbide Endofullerene Sc <sub>3</sub> C <sub>2</sub> @C <sub>80</sub> : A Density Functional Theory Investigation. <i>Journal of Physical Chemistry A</i> , 2006, 110, 1171-1176.	2.5	62
58	Diradical Mechanisms for the Cycloaddition Reactions of 1,3-Butadiene, Benzene, Thiophene, Ethylene, and Acetylene on a Si(111)-7 $\times$ 7 Surface. <i>Journal of the American Chemical Society</i> , 2003, 125, 7923-7929.	13.7	61
59	Sponge-like quaternary ammonium-based poly(ionic liquid)s for high CO <sub>2</sub> capture and efficient cycloaddition under mild conditions. <i>Journal of Materials Chemistry A</i> , 2017, 5, 25594-25600.	10.3	60
60	Is C <sub>60</sub> buckminsterfullerene aromatic?. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14886.	2.8	58
61	La <sub>2</sub> @C <sub>72</sub> and Sc <sub>2</sub> @C <sub>72</sub> : Computational Characterizations. <i>Journal of Physical Chemistry A</i> , 2006, 110, 2231-2234.	2.5	57
62	Electrochemical C-H/N-H Functionalization for the Synthesis of Highly Functionalized (Aza)indoles. <i>Angewandte Chemie</i> , 2016, 128, 9314-9318.	2.0	56
63	Cluster modeling of metal oxides: how to cut out a cluster?. <i>Chemical Physics Letters</i> , 1998, 291, 445-452.	2.6	54
64	The [2+1] Cycloadditions of Dichlorocarbene, Silylene, Germylene, and Oxycarbonylnitrene onto the Sidewall of Armchair (5,5) Single-Wall Carbon Nanotube. <i>Journal of Physical Chemistry B</i> , 2003, 107, 8388-8391.	2.6	54
65	Copper-Catalyzed Intramolecular Oxidative Amination of Unactivated Internal Alkenes. <i>Chemistry - A European Journal</i> , 2016, 22, 4379-4383.	3.3	52
66	Intermolecular 1,2-Difunctionalization of Alkenes Enabled by Fluoroamide-Directed Remote Benzyl C(sp <sup>3</sup> )-H Functionalization. <i>Journal of the American Chemical Society</i> , 2022, 144, 339-348.	13.7	51
67	Unprecedented 1/4-C <sub>26</sub> -Anion in Sc <sub>4</sub> C <sub>2</sub> @C <sub>80</sub> . <i>Journal of Physical Chemistry B</i> , 2006, 110, 11098-11102.	2.6	48
68	Size- and Composition-Dependent Exciton Spin Relaxation in Lead Halide Perovskite Quantum Dots. <i>ACS Energy Letters</i> , 2020, 5, 1701-1708.	17.4	47
69	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.	11.2	46
70	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.	9.0	45
71	Synthesis and Characterization of a Metallacyclic Framework with Three Fused Five-membered Rings. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 9067-9071.	13.8	45
72	Copper-Catalyzed Asymmetric Diyne Cyclization via [1,2]-Stevens-Type Rearrangement for the Synthesis of Chiral Chromeno[3,4- <i>cd</i> ]pyrroles. <i>Angewandte Chemie - International Edition</i> , 2022, 61, e202115554.	13.8	44

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73	Chemisorption of acetonitrile, pyridine and pyrazine on the Si(100)-2x1 surface: theoretical predictions. <i>New Journal of Chemistry</i> , 2002, 26, 160-164.	2.8	41
74	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.	2.0	41
75	Electrochemical Synthesis of Imidazo-Fused N-Heteroaromatic Compounds through a C-N Bond-Forming Radical Cascade. <i>Angewandte Chemie</i> , 2018, 130, 1652-1655.	2.0	41
76	Copper-catalyzed asymmetric cyclization of alkenyl diynes: method development and new mechanistic insights. <i>Chemical Science</i> , 2021, 12, 9466-9474.	7.4	41
77	Sidewall Oxidation and Complexation of Carbon Nanotubes by Base-Catalyzed Cycloaddition of Transition Metal Oxide: A Theoretical Prediction. <i>Nano Letters</i> , 2002, 2, 1325-1327.	9.1	40
78	Practical, Modular, and General Synthesis of 3-Coumaranones through Gold-Catalyzed Intermolecular Alkyne Oxidation Strategy. <i>Chemistry - an Asian Journal</i> , 2015, 10, 91-95.	3.3	39
79	Synthesis and Spectroscopy of Monodispersed, Quantum-Confined FAPbBr <sub>3</sub> Perovskite Nanocrystals. <i>Chemistry of Materials</i> , 2020, 32, 549-556.	6.7	39
80	Bonding of NO <sub>2</sub> to the Au Atom and Au(111) Surface: A Quantum Chemical Study. <i>Journal of Physical Chemistry A</i> , 1999, 103, 10969-10974.	2.5	38
81	Pentagon-Fused Hollow Fullerene in C <sub>78</sub> Family Retrieved by Chlorination. <i>Journal of the American Chemical Society</i> , 2010, 132, 12648-12652.	13.7	37
82	Control of the Charge Distribution and Modulation of the Class II-III Transition in Weakly Coupled Mo <sub>2</sub> -Mo <sub>2</sub> Systems. <i>Inorganic Chemistry</i> , 2013, 52, 12624-12633.	4.0	37
83	Dissociation mechanism of methanol on a Si(111)-(7x7) surface studied by scanning tunneling microscopy. <i>Physical Review B</i> , 2002, 66, .	3.2	36
84	Synthesis of a Dy@C <sub>82</sub> Derivative Bearing a Single Phosphorus Substituent via a Zwitterion Approach. <i>Journal of the American Chemical Society</i> , 2007, 129, 10636-10637.	13.7	36
85	Homoconjugation/Homoaromaticity in Main Group Inorganic Molecules. <i>Journal of the American Chemical Society</i> , 2009, 131, 9789-9799.	13.7	36
86	NC unit trapped by fullerenes: a density functional theory study on Sc <sub>3</sub> NC@C <sub>2n</sub> (2n = 68, 78 and 80). <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12442.	2.8	35
87	Zinc-Catalyzed Alkyne Oxidation/C-H Functionalization: Highly Site-Selective Synthesis of Versatile Isoquinolones and 1-Carbolines. <i>Angewandte Chemie</i> , 2015, 127, 8363-8367.	2.0	35
88	Synthesis of 2-Aza-1,3-butadienes through Gold-Catalyzed Intermolecular Ynamide Amination/C-H Functionalization. <i>Organic Letters</i> , 2016, 18, 4630-4633.	4.6	35
89	N <sub>2</sub> O Decomposition on MgO and Li/MgO Catalysts: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 1999, 103, 3373-3379.	2.6	34
90	Transition-metal-free oxidative cyclization of N-propargyl ynamides: stereospecific construction of linear polycyclic N-heterocycles. <i>Green Chemistry</i> , 2018, 20, 3271-3278.	9.0	33

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91	Simple Combustion Production and Characterization of Octahydro[60]fullerene with a Non-IPR C <sub>60</sub> Cage. <i>Journal of the American Chemical Society</i> , 2010, 132, 15093-15095.	13.7	32
92	Mechanism for the Regioselective Asymmetric Addition of Grignard Reagents to Malimides: A Computational Exploration. <i>Journal of Organic Chemistry</i> , 2007, 72, 35-42.	3.2	30
93	Hydroboration of C(100) Surface, Fullerene, and the Sidewalls of Single-Wall Carbon Nanotubes with Borane. <i>Journal of Organic Chemistry</i> , 2003, 68, 4495-4498.	3.2	29
94	Prediction of the <sup>13</sup> C NMR chemical shifts of organic species adsorbed on H-ZSM-5 zeolite by the ONIOM-GIAO method. <i>Chemical Communications</i> , 2005, , 2474.	4.1	28
95	Zinc-catalyzed reaction of isoxazoles with thioynol ethers involving an unprecedented 1,2-sulfur migration. <i>Chemical Communications</i> , 2018, 54, 7435-7438.	4.1	28
96	Adsorption, Isomerization, and Decomposition of HCN on Si(100)2 Å–1: A Computational Study with a Double-Dimer Cluster Model. <i>Journal of Physical Chemistry B</i> , 2001, 105, 4368-4373.	2.6	27
97	Bonding configurations of acetylene adsorbed on the Si(100)-2 Å–1 surface predicted by density functional cluster model calculations. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 4213-4217.	2.8	26
98	Diradical Mechanisms for the Cycloaddition Chemistry of Ethylene on X(100) Surfaces (X = C, Si, and Tj ETQq0 0 0,rgBT /Overlock 10 TF	2.8	26
99	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.	10.3	26
100	Catalyst-Dependent Stereospecific [3,3]-Sigmatropic Rearrangement of Sulfoxide- <i>N</i> -amides: Divergent Synthesis of Chiral Medium-Sized <i>N</i> , <i>S</i> -Heterocycles. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	26
101	Sidewall Epoxidation of Single-Walled Carbon Nanotubes: A Theoretical Prediction. <i>Organic Letters</i> , 2003, 5, 3527-3530.	4.6	25
102	Addition of Carbene to the Equator of C <sub>70</sub> To Produce the Most Stable C <sub>71</sub> H <sub>2</sub> Isomer: A Homocyclic C <sub>70</sub> -D <sub>5h</sub> (6)[5,6]fullerene. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 962-966.	13.8	25
103	Gas-Phase Reactions of HONO with HNO and NH <sub>3</sub> : An Ab Initio MO/TST Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 5141-5148.	2.5	24
104	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.	2.6	24
105	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.	2.6	24
106	Gas Phase Reactions of HONO with NO <sub>2</sub> , O <sub>3</sub> , and HCl: An Ab Initio and TST Study. <i>Journal of Physical Chemistry A</i> , 2000, 104, 8730-8738.	2.5	23
107	A DFT Study of the 1,3-Dipolar Cycloadditions on the C(100)-2 Å–1 Surface. <i>Journal of Organic Chemistry</i> , 2002, 67, 515-520.	3.2	23
108	Adsorption and Decomposition of NO on Magnesium Oxide: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 1999, 103, 5657-5664.	2.6	22

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109	High charge flexibility of the surface dangling bonds on the Si(111)-7 $\times$ 7 surface and NH <sub>3</sub> chemisorption: a DFT study. <i>Chemical Physics Letters</i> , 2002, 355, 365-370.	2.6	22
110	Can the Nitroso Ene Reaction Proceed Concertedly?. <i>Organic Letters</i> , 2004, 6, 2813-2815.	4.6	22
111	Exohedrally stabilized C <sub>70</sub> isomer with adjacent pentagons characterized by crystallography. <i>Chemical Science</i> , 2013, 4, 2967.	7.4	22
112	Experimental and Theoretical Evidence of Aromatic Behavior in Heterobenzene-Like Molecules with Metal-Metal Multiple Bonds. <i>Chemistry - A European Journal</i> , 2011, 17, 10288-10296.	3.3	21
113	Organocatalytic Enantioselective Conia $\alpha$ -Type Carbocyclization of Ynamide Cyclohexanones: Regiodivergent Synthesis of Morphans and Normorphans. <i>Angewandte Chemie</i> , 2019, 131, 16398-16405.	2.0	21
114	Strong Spin-Selective Optical Stark Effect in Lead Halide Perovskite Quantum Dots. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 3594-3600.	4.6	21
115	Atroposelective carbonylation of aryl iodides with amides: facile synthesis of enantioenriched cyclic and acyclic amides. <i>Organic Chemistry Frontiers</i> , 2021, 8, 6067-6073.	4.5	20
116	A quantum chemical study of the NO/MgO chemisorption system: hybrid B3LYP calculations on NO/(MgO) (n=4,6,8) model systems. <i>Chemical Physics Letters</i> , 1999, 300, 109-117.	2.6	19
117	Carbon Nitride Supported High $\alpha$ -Loading Fe Single $\alpha$ -Atom Catalyst for Activation of Peroxymonosulfate to Generate 1 O <sub>2</sub> with 100 $\alpha$ % Selectivity. <i>Angewandte Chemie</i> , 2021, 133, 21919-21923.	2.0	18
118	A theoretical study of HN <sub>3</sub> reaction with the C(1 0 0)-2 $\times$ 1 surface. <i>Chemical Physics Letters</i> , 2001, 343, 212-218.	2.6	17
119	Theoretical studies of XC <sub>n</sub> X (X=O, S, Se; n=1 $\alpha$ 8): structures, spectroscopic properties, and dissociation energies. <i>Computational and Theoretical Chemistry</i> , 2002, 593, 187-197.	1.5	17
120	High Activity of Amine-Doped H-ZSM-5 Zeolite in Ethene Protonation: Revealed by Embedding Calculations. <i>ChemPhysChem</i> , 2007, 8, 231-234.	2.1	17
121	Functionalization of the C(100) 2 $\times$ 1 Surface by 1,3-Dipolar Cycloadditions: A Theoretical Prediction. <i>Journal of Physical Chemistry B</i> , 2002, 106, 5972-5974.	2.6	16
122	Synthesis, Properties, and Bishomoaromaticity of the First Tetrahalogenated Derivative of a 1, 5-Diphosphadithiatetrazocine: A Combined Experimental and Computational Investigation. <i>Inorganic Chemistry</i> , 2010, 49, 3810-3815.	4.0	16
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