Jing-Yao Liu

List of Publications by Year
in descending order

81 papers	1,768 citations	331670 21 h-index	302126 39 g-index
81 all docs	81 docs citations	81 times ranked	2726 citing authors

#	Article	IF	Citations
1	A metallic molybdenum dioxide with high stability for surface enhanced Raman spectroscopy. Nature Communications, 2017, 8, 14903.	12.8	207
2	Rational Design and Functionalization of a Zinc Metalâ€"Organic Framework for Highly Selective Detection of 2,4,6-Trinitrophenol. ACS Applied Materials & Interfaces, 2017, 9, 23828-23835.	8.0	154
3	Adsorption and activation of molecular oxygen over atomic copper(I/II) site on ceria. Nature Communications, 2020, 11, 4008.	12.8	95
4	3,4-Polymerization of Isoprene by Using NSN- and NPN-Ligated Rare Earth Metal Precursors: Switching of Stereo Selectivity and Mechanism. Macromolecules, 2014, 47, 4971-4978.	4.8	70
5	The Uncommon Channelâ€Based Lnâ€MOFs for Highly Selective Fe³⁺ Detection and Superior Rhodamineâ€…B Adsorption. Chemistry - A European Journal, 2016, 22, 16230-16235.	3.3	70
6	Hydrolysis of Sulfur Dioxide in Small Clusters of Sulfuric Acid: Mechanistic and Kinetic Study. Environmental Science & Technology, 2015, 49, 13112-13120.	10.0	66
7	Plasmonic MoO₂ Nanospheres as a Highly Sensitive and Stable Non-Noble Metal Substrate for Multicomponent Surface-Enhanced Raman Analysis. Analytical Chemistry, 2017, 89, 11765-11771.	6.5	65
8	Mechanism of the Gaseous Hydrolysis Reaction of SO₂: Effects of NH₃ versus H₂O. Journal of Physical Chemistry A, 2015, 119, 102-111.	2.5	61
9	Honeycomb Boron Allotropes with Dirac Cones: A True Analogue to Graphene. Journal of Physical Chemistry Letters, 2017, 8, 2647-2653.	4.6	57
10	Direct growth of defect-rich MoO_{3âˆ’x}ultrathin nanobelts for efficiently catalyzed conversion of isopropyl alcohol to propylene under visible light. Journal of Materials Chemistry A, 2016, 4, 1566-1571.	10.3	54
11	Electron Counting and a Large Family of Two-Dimensional Semiconductors. Chemistry of Materials, 2016, 28, 1994-1999.	6.7	52
12	Mechanism of supported Ru₃Sn₇ nanocluster-catalyzed selective hydrogenation of coconut oil to fatty alcohols. Catalysis Science and Technology, 2018, 8, 1322-1332.	4.1	49
13	ZemplÃ©n transesterification: a name reaction that has misled us for 90 years. Green Chemistry, 2015, 17, 1390-1394.	9.0	47
14	Rapid Syndiospecific (Co)Polymerization of Fluorostyrene with High Monomer Conversion. Chemistry - A European Journal, 2017, 23, 18151-18155.	3.3	43
15	Ni anchored C2N monolayers as low-cost and efficient catalysts for hydrogen production from formic acid. Journal of Power Sources, 2019, 413, 399-407.	7.8	40
16	Large-scale synthesis of ultrathin tungsten oxide nanowire networks: an efficient catalyst for aerobic oxidation of toluene to benzaldehyde under visible light. Nanoscale, 2016, 8, 13545-13551.	5.6	38
17	Surface Stabilization of Colloidal Perovskite Nanocrystals via Multi-amine Chelating Ligands. ACS Energy Letters, 2022, 7, 1963-1970.	17.4	34
18	Synthesis and facet-dependent photocatalytic activity of strontium titanate polyhedron nanocrystals. Nano Research, 2016, 9, 1523-1531.	10.4	31

#	Article	IF	Citations
19	Dual-level direct dynamics studies for the reactions of CH3OCH3 and CF3OCH3 with the OH radical. Journal of Chemical Physics, 2003, 118, 10986-10995.	3.0	30
20	Advanced Li₂S/Si Full Battery Enabled by TiN Polysulfide Immobilizer. Small, 2019, 15, e1902377.	10.0	29
21	Band gap engineering of graphenylene by hydrogenation and halogenation: a density functional theory study. RSC Advances, 2015, 5, 70766-70771.	3.6	26
22	Enhanced Basicity of Ag₂O by Coordination to Soft Anions. ChemCatChem, 2015, 7, 761-765.	3.7	23
23	Building egg-tray-shaped graphenes that have superior mechanical strength and band gap. Npj Computational Materials, 2019, 5, .	8.7	19
24	Microporosity as a new property control factor in graphene-like 2D allotropes. Journal of Materials Chemistry A, 2018, 6, 10348-10353.	10.3	18
25	Macrocycles inserted in graphene: from coordination chemistry on graphene to graphitic carbon oxide. Nanoscale, 2016, 8, 17976-17983.	5.6	16
26	Theoretical study of the oxidation reactions of sulfurous acid/sulfite with ozone to produce sulfuric acid/sulfate with atmospheric implications. RSC Advances, 2018, 8, 7988-7996.	3.6	15
27	Bubble-wrap carbon: an integration of graphene and fullerenes. Nanoscale, 2018, 10, 11328-11334.	5.6	15
28	Reduction of NO with CO on the Co₃O₄(110)-B and CoO(110) Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2019, 123, 1770-1778.	3.1	15
29	Transition metal single atom anchored C3N for highly efficient formic acid dehydrogenation: A DFT study. Applied Surface Science, 2021, 562, 150186.	6.1	15
30	Defect-engineered Mn3O4/CNTs composites enhancing reaction kinetics for zinc-ions storage performance. Journal of Energy Chemistry, 2022, 68, 538-547.	12.9	15
31	Theoretical study and rate constant calculation of the CH2O+CH3 reaction. Journal of Chemical Physics, 2003, 119, 7214-7221.	3.0	14
32	Computational Studies on the Mechanisms and Dynamics of OH Reactions with CHF2CHFOCF3 and CHF2CH2OCF3. Journal of Chemical Theory and Computation, 2008, 4, 1073-1082.	5.3	14
33	Effect of Subsurface Oxygen on Selective Catalytic Reduction of NO by H₂ on Pt(100): A First-Principles Study. Journal of Physical Chemistry C, 2015, 119, 24819-24826.	3.1	14
34	DFT Study on the Mechanism of Palladium(0)-Catalyzed Reaction of Aryl Iodides, Norbornene, and Di-tert-butyldiaziridinone. Organometallics, 2019, 38, 2189-2198.	2.3	14
35	A novel two-dimensional material B₂S₃and its structural implication to new carbon and boron nitride allotropes. Journal of Materials Chemistry C, 2015, 3, 9921-9927.	5.5	13
36	A CNH monolayer: a direct gap 2D semiconductor with anisotropic electronic and optical properties. Journal of Materials Chemistry C, 2017, 5, 8498-8503.	5.5	13

#	Article	IF	Citations
37	A highly sensitive and stable SERS substrate using hybrid tungsten dioxide/carbon ultrathin nanowire beams. Journal of Materials Chemistry C, 2018, 6, 3200-3205.	5.5	13
38	Direct Dynamics Study on the Hydrogen Abstraction Reaction PH3 + H âť’ PH2 + H2. Journal of Physical Chemistry A, 1999, 103, 6402-6405.	2.5	12
39	Mechanism of Nitric Oxide Reduction by Hydrogen on Ni(110) and Ir/Ni(110): First Principles and Microkinetic Modeling. Journal of Physical Chemistry C, 2019, 123, 4825-4836.	3.1	12
40	Rational design of highly efficient electrocatalytic single-atom catalysts for nitrogen reduction on nitrogen-doped graphene and g-C2N supports. Journal of Power Sources, 2022, 535, 231449.	7.8	12
41	Computational study of the rate constants and kinetic isotope effects for the CH3+HBrâť’CH4+Br reaction. Journal of Chemical Physics, 2003, 119, 10585-10590.	3.0	10
42	Mechanism of ammonia decomposition and oxidation on Ir(110): A first-principles study. Journal of Chemical Physics, 2013, 138, 144703.	3.0	10
43	Metallic carbide nanoparticles as stable and reusable substrates for sensitive surface-enhanced Raman spectroscopy. Chemical Communications, 2018, 54, 10843-10846.	4.1	10
44	Theoretical study on the reaction of (Z)-CF₃CHï£¾CHCF₃with OH radicals. International Journal of Quantum Chemistry, 2014, 114, 176-182.	2.0	9
45	Direct Dynamics Studies on the Hydrogen Abstraction Reactions of an F Atom with CH₃X (X = F, Cl, and Br). Journal of Chemical Theory and Computation, 2005, 1, 201-207.	5.3	8
46	On Close Parallels between the Zintl-Based Superatom Ge₉Be and Chalcogen Elements. Inorganic Chemistry, 2021, 60, 3196-3206.	4.0	8
47	On the kinetic mechanism of reactions of hydroxyl radical with CHF2CH3Ââ^'Ân F n (n = 1â€"3). Theoretical Chemistry Accounts, 2007, 118, 315-323.	1.4	7
48	Formaldehyde Decomposition and Coupling on V(100): A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 10639-10648.	3.1	7
49	Stereoelectronic control of cleavage of dioxolane five-membered ring on carbohydrates. Chemical Research in Chinese Universities, 2013, 29, 551-555.	2.6	7
50	DFT studies on the mechanism of palladium catalyzed arylthiolation of unactive arene to diaryl sulfide. RSC Advances, 2016, 6, 18300-18307.	3.6	7
51	Unveiling the potential of superalkali cation Li₃⁺for capturing nitrogen. Physical Chemistry Chemical Physics, 2020, 22, 26536-26543.	2.8	6
52	First-Principles Study of NO Reduction by CO on Cu₂O(110) and Pd₁/Cu₂O(110) Surfaces. Journal of Physical Chemistry C, 2021, 125, 20309-20319.	3.1	6
53	Carbon-wrapped Feâ€"Ni bimetallic nanoparticle-catalyzed Friedelâ€"Crafts acylation for green synthesis of aromatic ketones. Catalysis Science and Technology, 0, , .	4.1	6
54	Ab initio direct dynamics studies on the reactions of H atoms with CH3Cl and CH3Br. Journal of Chemical Physics, 2003, 118, 4920-4928.	3.0	5

#	Article	IF	Citations
55	Hydrogen abstraction from CF3CF2CFH2 and CF3CFHCF2H by OH radicals and Cl atoms: theoretical enthalpies and rate constants. Theoretical Chemistry Accounts, 2009, 124, 59-70.	1.4	5
56	Theoretical study on the reaction mechanism of â€œligandlessâ€•Ni-catalyzed hydrodesulfurization of aryl sulfide. RSC Advances, 2017, 7, 51475-51484.	3.6	5
57	Theoretical study of the hydrogen abstraction by chlorine atoms for CH2BrCl and CHBrCl2. Physical Chemistry Chemical Physics, 2002, 4, 46-50.	2.8	4
58	Radicalâ€"molecule reaction CH2Cl + NO2: a mechanistic study. Theoretical Chemistry Accounts, 2007, 117, 579-586.	1.4	4
59	Theoretical studies on the reactions of hydroxyl radicals with trimethylsilane and tetramethylsilane. Theoretical Chemistry Accounts, 2008, 119, 319-327.	1.4	4
60	Theoretical studies on the reactions of acetone with chlorine atom and methyl radical. Theoretical Chemistry Accounts, 2008, 119, 445-451.	1.4	4
61	Insight into the Reaction Mechanism of the Reduction of NO by H₂ on the Singly Dispersed Bimetallic Pt(Rh)Co₄/Co₃O₄ Catalysts: A First-Principles Study. Journal of Physical Chemistry C, 2020, 124, 9908-9916.	3.1	4
62	Catalytic Activity of the Transition-Metal Atom Doped Platinum Surface for NO Reduction by CO. Journal of Physical Chemistry C, 2021, 125, 9703-9714.	3.1	4
63	Direct ab initio dynamics calculations of the reaction rates for the hydrogen abstraction reaction Clâ€‰+â€‰HC(O)Fâ€‰â†'â€‰HClâ€‰+â€‰CFO. Physical Chemistry Chemical Physics, 2002, 4, 2927-2931.	2.8	3
64	Direct ab initio dynamics calculations on the rate constants for the hydrogen-abstraction reaction of C 2 H 5 F with O (3 P). Theoretical Chemistry Accounts, 2002, 108, 179-186.	1.4	3
65	Theoretical Study of the Hydrogen-Abstraction Reactions for CH3CX3 + Cl â†' CH2CX3 + HCl (X = Cl and) Tj ETQq1 1 0.784314 rgBT /O	2.5	3
66	Dual-level direct dynamics studies on the reactions of tetramethylsilane with chlorine and bromine atoms. Theoretical Chemistry Accounts, 2010, 125, 75-82.	1.4	3
67	Theoretical studies and rate constants calculation for the reactions of acetone with fluorine and bromine atoms. Theoretical Chemistry Accounts, 2011, 128, 317-325.	1.4	2
68	Mechanistic study and kinetic properties of the CF3CHO + Cl reaction. Science China Chemistry, 2012, 55, 2197-2201.	8.2	2
69	Asymmetric passivation of edges: a route to make magnetic graphene nanoribbons. RSC Advances, 2017, 7, 27932-27937.	3.6	2
70	DFT study on the mechanism of palladium(II)-catalyzed reaction of allyl-substituted 3,4-dienoate, alkyne and carbon monoxide. Molecular Catalysis, 2020, 492, 111028.	2.0	2
71	High electron affinity triggered by lithium coordination: quasi-chalcogen properties of Li₂Sn₈Be. Physical Chemistry Chemical Physics, 2022, 24, 10611-10621.	2.8	2
72	Direct ab initio dynamics calculations of the rate constants for the reaction of CHF2CF2OCH3 with Cl. International Journal of Chemical Kinetics, 2007, 39, 221-230.	1.6	1

#	Article	IF	Citations
73	Theoretical studies on the reactions OHÂ+ÂCH3COCCl2 X (XÂ=ÂF, Cl, Br). Theoretical Chemistry Accounts, 2009, 122, 107-114.	1.4	1
74	Theoretical Mechanism Study on the Reaction of FOO Radical with NO. Journal of Chemistry, 2016, 2016, 1-6.	1.9	1
75	On single-electron magnesium bonding formation and the effect of methyl substitution. RSC Advances, 2020, 10, 34413-34420.	3.6	1
76	DFT study on the mechanism of bimetallic Pdâ€"Zn-catalyzed cycloaddition of alkynyl aryl ethers with internal alkynes. Dalton Transactions, 2020, 49, 2914-2923.	3.3	1
77	DFT study on the mechanism of palladium(0)-catalyzed reaction of o-iodoanilines, CO2, and CO. Molecular Catalysis, 2021, 501, 111344.	2.0	1
78	Dual-level direct dynamics study on the reactions of SH (SD) with F2. International Journal of Chemical Kinetics, 2005, 37, 710-716.	1.6	0
79	Theoretical study on the reactions of trimethylsilane with chlorine and bromine atoms. Theoretical Chemistry Accounts, 2011, 130, 115-125.	1.4	0
80	Theoretical study for the CH3OCF2CF2OCHOÂ+ÂCl reaction. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	0
81	Hydrocarbon chain growth and hydrogenation on V(100): a density functional theory study. RSC Advances, 2015, 5, 4909-4917.	3.6	0