

Xin Liu

List of Publications by Year in descending order

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112
papers

3,909
citations

94433

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docs citations

113
times ranked

5030
citing authors

#	ARTICLE	IF	CITATIONS
1	Superior Capture of CO ₂ Achieved by Introducing Extra-framework Cations into N-doped Microporous Carbon. <i>Chemistry of Materials</i> , 2012, 24, 4725-4734.	6.7	199
2	Direct Conversion of Cellulose to Glycolic Acid with a Phosphomolybdic Acid Catalyst in a Water Medium. <i>ACS Catalysis</i> , 2012, 2, 1698-1702.	11.2	126
3	Microporous carbonaceous adsorbents for CO ₂ separation via selective adsorption. <i>RSC Advances</i> , 2015, 5, 30310-30330.	3.6	119
4	Light-Induced Self-Assembly of Cubic CsPbBr ₃ Perovskite Nanocrystals into Nanowires. <i>Chemistry of Materials</i> , 2019, 31, 6642-6649.	6.7	119
5	CO oxidation catalyzed by Pt-embedded graphene: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 23584-23593.	2.8	111
6	Role of Electronic Excitation in the Amorphization of Ge-Sb-Te Alloys. <i>Physical Review Letters</i> , 2011, 107, 015501.	7.8	107
7	Coumarin phosphorescence observed with NâN Pt(ii) bisacetylido complex and its applications for luminescent oxygen sensing and triplet-triplet-annihilation based upconversion. <i>Dalton Transactions</i> , 2011, 40, 7834.	3.3	106
8	Palladium Nanoparticles/Defective Graphene Composites as Oxygen Reduction Electrocatalysts: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2012, 116, 2710-2719.	3.1	94
9	Direct Imaging of Tunable Crystal Surface Structures of MOF MIL-101 Using High-Resolution Electron Microscopy. <i>Journal of the American Chemical Society</i> , 2019, 141, 12021-12028.	13.7	93
10	Catalytic oxidative conversion of cellulosic biomass to formic acid and acetic acid with exceptionally high yields. <i>Catalysis Today</i> , 2014, 233, 77-82.	4.4	92
11	Defective Graphene Supported MPd ₁₂ (M = Fe, Co, Ni, Cu, Zn, Pd) Nanoparticles as Potential Oxygen Reduction Electrocatalysts: A First-Principles Study. <i>Journal of Physical Chemistry C</i> , 2013, 117, 1350-1357.	3.1	88
12	Silver Clusters as Robust Nodes and Activation Sites for the Construction of Heterogeneous Catalysts for the Cycloaddition of Propargylamines. <i>ACS Catalysis</i> , 2018, 8, 1384-1391.	11.2	85
13	Atomic Spatial and Temporal Imaging of Local Structures and Light Elements inside Zeolite Frameworks. <i>Advanced Materials</i> , 2020, 32, e1906103.	21.0	81
14	Highly Selective and Complete Conversion of Cellobiose to Gluconic Acid over Au/Cs ₂ HPW ₁₂ O ₄₀ Nanocomposite Catalyst. <i>ChemCatChem</i> , 2011, 3, 1294-1298.	3.7	80
15	Developing hierarchically ultra-micro/mesoporous biocarbons for highly selective carbon dioxide adsorption. <i>Chemical Engineering Journal</i> , 2019, 361, 199-208.	12.7	79
16	Monodisperse Pt atoms anchored on N-doped graphene as efficient catalysts for CO oxidation: a first-principles investigation. <i>Catalysis Science and Technology</i> , 2015, 5, 1658-1667.	4.1	78
17	A single-molecule van der Waals compass. <i>Nature</i> , 2021, 592, 541-544.	27.8	75
18	Efficient tuning of triphenylamine-based donor materials for high-efficiency organic solar cells. <i>Computational and Theoretical Chemistry</i> , 2020, 1191, 113045.	2.5	73

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19	Fabrication of vanadium sulfide (VS ₄) wrapped with carbonaceous materials as an enhanced electrode for symmetric supercapacitors. <i>Journal of Colloid and Interface Science</i> , 2020, 574, 312-323.	9.4	71
20	New lead-free perovskite Rb ₇ Bi ₃ Cl ₁₆ nanocrystals with blue luminescence and excellent moisture-stability. <i>Nanoscale</i> , 2019, 11, 6719-6726.	5.6	68
21	Syngas Segregation Induced by Confinement in Carbon Nanotubes: A Combined First-Principles and Monte Carlo Study. <i>Journal of Physical Chemistry C</i> , 2009, 113, 21687-21692.	3.1	67
22	Fluorescence modulation <i>via</i> photoinduced spin crossover switched energy transfer from fluorophores to Fe ^{II} ions. <i>Chemical Science</i> , 2018, 9, 2892-2897.	7.4	67
23	Electronic structure engineering through Fe-doping CoP enables hydrogen evolution coupled with electro-Fenton. <i>Nano Energy</i> , 2021, 84, 105943.	16.0	64
24	Site-specific growth of Au particles on ZnO nanopramids under ultraviolet illumination. <i>Nanoscale</i> , 2011, 3, 4195.	5.6	61
25	Graphene substrate-mediated catalytic performance enhancement of Ru nanoparticles: a first-principles study. <i>Dalton Transactions</i> , 2012, 41, 1289-1296.	3.3	61
26	Copper atoms embedded in hexagonal boron nitride as potential catalysts for CO oxidation: a first-principles investigation. <i>RSC Advances</i> , 2014, 4, 38750-38760.	3.6	57
27	Hydrothermal synthesis of VS ₄ /CNTs composite with petal-shape structures performing a high specific capacity in a large potential range for high-performance symmetric supercapacitors. <i>Journal of Colloid and Interface Science</i> , 2019, 554, 191-201.	9.4	57
28	Preparation of a Ru Nanoparticles/Defective Graphene Composite as a Highly Efficient Arene Hydrogenation Catalyst. <i>ChemCatChem</i> , 2012, 4, 1938-1942.	3.7	55
29	Pt atoms stabilized on hexagonal boron nitride as efficient single-atom catalysts for CO oxidation: a first-principles investigation. <i>RSC Advances</i> , 2015, 5, 10452-10459.	3.6	54
30	K ₂ Ag ₆ Sn ₃ S ₁₀ : A Quaternary Sulfide Composed of Silver Sulfide Layers Pillared by Zigzag Chains [SnS ₃] ₂ -. <i>Inorganic Chemistry</i> , 2004, 43, 3764-3765.	4.0	48
31	Synthesis of zeolites Na-A and Na-X from tablet compressed and calcinated coal fly ash. <i>Royal Society Open Science</i> , 2017, 4, 170921.	2.4	48
32	Titanium carbide/zeolite imidazole framework-8/poly(lactic acid) electrospun membrane for near-infrared regulated photothermal/photodynamic therapy of drug-resistant bacterial infections. <i>Journal of Colloid and Interface Science</i> , 2021, 599, 390-403.	9.4	48
33	Substrate-mediated enhanced activity of Ru nanoparticles in catalytic hydrogenation of benzene. <i>Nanoscale</i> , 2012, 4, 2288.	5.6	47
34	Regioselectivity control of graphene functionalization by ripples. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 19449.	2.8	46
35	Quench-tailored Al-doped V ₂ O ₅ nanomaterials for efficient aqueous zinc-ion batteries. <i>Journal of Energy Chemistry</i> , 2022, 70, 52-58.	12.9	46
36	Superior Catalytic Performance of Atomically Dispersed Palladium on Graphene in CO Oxidation. <i>ACS Catalysis</i> , 2020, 10, 3084-3093.	11.2	44

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37	Defect stabilized gold atoms on graphene as potential catalysts for ethylene epoxidation: a first-principles investigation. <i>Catalysis Science and Technology</i> , 2016, 6, 1632-1641.	4.1	43
38	A Solvothermal Synthesis and the Structure of $K_4Ag_2Sn_3S_9 \cdot 2KOH$. <i>Inorganic Chemistry</i> , 2003, 42, 4248-4249.	4.0	38
39	Efficient tuning of zinc phthalocyanine-based dyes for dye-sensitized solar cells: a detailed DFT study. <i>RSC Advances</i> , 2021, 11, 27570-27582.	3.6	38
40	Potassium and Zeolitic Structure Modified Ultra-microporous Adsorbent Materials from a Renewable Feedstock with Favorable Surface Chemistry for CO_2 Capture. <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 26826-26839.	8.0	36
41	Theoretical Study on the Ground State Structure of Uranofullerene $U@C_{82}$. <i>Journal of Physical Chemistry A</i> , 2012, 116, 11651-11655.	2.5	34
42	High efficient degradation of levofloxacin by edge-selectively Fe@3D-WS ₂ : Self-renewing behavior and Degradation mechanism study. <i>Applied Catalysis B: Environmental</i> , 2019, 252, 187-197.	20.2	34
43	Facile synthesis of high-surface vanadium nitride/vanadium sesquioxide/amorphous carbon composite with porous structures as electrode materials for high performance symmetric supercapacitors. <i>Applied Surface Science</i> , 2019, 471, 842-851.	6.1	33
44	Unique reactivity of Fe nanoparticles@defective graphene composites toward NH_x ($x = 0, 1, 2, 3$) adsorption: a first-principles study. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 15036.	2.8	30
45	High Density and Super Ultra-Microporous Activated Carbon Macrospheres with High Volumetric Capacity for CO_2 Capture. <i>Advanced Sustainable Systems</i> , 2018, 2, 1700115.	5.3	30
46	A solvothermal synthesis of a novel 1D ladder-like $(NH_3CH_2CH_2NH_3)AgAsS_4$ containing $N-H \cdots S$ hydrogen bonding. <i>Inorganic Chemistry Communication</i> , 2003, 6, 1137-1139.	3.9	29
47	Supramolecular Photoinduced Electron Transfer between a Redox-Active Hexanuclear Metal-Organic Cylinder and an Encapsulated Ruthenium(II) Complex. <i>Chemistry - A European Journal</i> , 2016, 22, 5253-5260.	3.3	29
48	High sulfur tolerance of Ni-Si intermetallics as hydrodesulfurization catalysts. <i>RSC Advances</i> , 2013, 3, 1728-1731.	3.6	28
49	$(NH_3CH_2CH_2NH_3)Ag_2SnS_4$: a quaternary sulfide-containing chiral layers. <i>Inorganic Chemistry Communication</i> , 2005, 8, 301-303.	3.9	26
50	Reaction mechanism of tert-butylation of phenol with tert-butyl alcohol over H ⁺ zeolite: An ONIOM study. <i>Catalysis Today</i> , 2011, 165, 120-128.	4.4	26
51	Dual Stimuli-Responsive smart fibrous membranes for efficient Photothermal/Photodynamic/Chemo-Therapy of Drug-Resistant bacterial infection. <i>Chemical Engineering Journal</i> , 2022, 432, 134351.	12.7	26
52	Light-driven hydrogen evolution with a nickel thiosemicarbazone redox catalyst featuring Ni ^{II} -H interactions under basic conditions. <i>New Journal of Chemistry</i> , 2015, 39, 1051-1059.	2.8	25
53	Unique Reactivity of Confined Metal Atoms on a Silicon Substrate. <i>ChemPhysChem</i> , 2008, 9, 975-979.	2.1	24
54	Oxygen-containing coke species in zeolite-catalyzed conversion of methanol to hydrocarbons. <i>Catalysis Science and Technology</i> , 2016, 6, 8157-8165.	4.1	24

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55	Deciphering the role of end-capped acceptor units for amplifying the photovoltaic properties of donor materials for high-performance organic solar cell applications. Computational and Theoretical Chemistry, 2021, 1205, 113454.	2.5	24
56	Two urea-functionalized pcu metal-organic frameworks based on a pillared-layer strategy for gas adsorption and separation. Inorganic Chemistry Frontiers, 2020, 7, 3500-3508.	6.0	23
57	Sandwich-Like Sulfur-Doped V2O5/Reduced graphene Oxide/Sulfur-Doped V2O5 Core-shell structure boosts Zinc-Ion storage. Applied Surface Science, 2021, 568, 150919.	6.1	23
58	SO ₃ H-Functionalized Ionic Liquid Catalyzed Alkylation of Catechol with <i>tert</i> -Butyl Alcohol. Industrial & Engineering Chemistry Research, 2010, 49, 8157-8163.	3.7	22
59	Tuning the reactivity of Ru nanoparticles by defect engineering of the reduced graphene oxide support. RSC Advances, 2014, 4, 22230-22240.	3.6	20
60	Molecular dynamics study on superheating of Pd at high heating rates. Phase Transitions, 2006, 79, 249-259.	1.3	19
61	Selective and efficient adsorption of boron (III) from water by 3D porous CQDs/LDHs with oxygen-rich functional groups. Journal of the Taiwan Institute of Chemical Engineers, 2018, 83, 192-203.	5.3	19
62	Melting and Superheating of Ag at High Heating Rate. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2004, 20, 280-284.	4.9	19
63	Discovery of versatile bat -shaped acceptor materials for high -performance organic solar cells a DFT approach. International Journal of Energy Research, 2022, 46, 13393-13408.	4.5	19
64	A solvothermal synthesis and structure of K ₂ Ag ₂ GeS ₄ with the simplest helical chains. Inorganic Chemistry Communication, 2004, 7, 114-116.	3.9	18
65	Wavevector-dependent quantum-size effect in electron decay length at Pb thin film surfaces. Applied Physics Letters, 2008, 93, 093105.	3.3	18
66	Unique Reactivity of Transition Metal Atoms Embedded in Graphene to CO, NO, O ₂ and O Adsorption: A First-Principles Investigation. Molecules, 2015, 20, 19540-19553.	3.8	17
67	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. Physical Review B, 2012, 85, .	3.2	16
68	Synthesis of Zeolite Omega by the Magadiite Conversion Method and Insight into the Changes of Medium-Range Structure during Crystallization. Crystal Growth and Design, 2017, 17, 3940-3947.	3.0	16
69	Recent Advances on Gallium-Modified ZSM-5 for Conversion of Light Hydrocarbons. Molecules, 2021, 26, 2234.	3.8	16
70	Oxygen Adsorption and Diffusion on NiTi Alloy (100) Surface: A Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 21771-21779.	3.1	15
71	Study on the synthesis of MFI and FER in the presence of n-butylamine and the property of n-butylamine in a confined region of zeolites. RSC Advances, 2016, 6, 114808-114817.	3.6	15
72	A Solvothermal Synthesis and the Structure of (NH ₄) ₂ Ag ₆ Sn ₃ S ₁₀ . Bulletin of the Chemical Society of Japan, 2005, 78, 1283-1284.	3.2	14

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73	A solvothermal synthesis and characterization of a new open-framework K ₄ Ag ₂ Ce ₃ S ₉ ·H ₂ O. <i>Journal of Solid State Chemistry</i> , 2004, 177, 2506-2510.	2.9	13
74	Brønsted acid-catalyzed tert-butylation of phenol, o-cresol and catechol: A comparative computational study. <i>Journal of Molecular Catalysis A</i> , 2010, 332, 145-151.	4.8	13
75	Fe atoms trapped on graphene as a potential efficient catalyst for room-temperature complete oxidation of formaldehyde: a first-principles investigation. <i>Catalysis Science and Technology</i> , 2017, 7, 2012-2021.	4.1	13
76	Layered silicate magadiite-derived three-dimensional honeycomb-like cobalt-nickel silicates as excellent cathode for hybrid supercapacitors. <i>Materials Today Chemistry</i> , 2021, 22, 100550.	3.5	13
77	Mechanical Properties and Defective Effects of 316LN Stainless Steel by First-Principles Simulations. <i>Journal of Materials Science and Technology</i> , 2011, 27, 1029-1033.	10.7	12
78	Oligomerization of Silicic Acids in Neutral Aqueous Solution: A First-Principles Investigation. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3037.	4.1	12
79	OSDA-free synthesis of zeolite beta by magadiite hydrothermal conversion method and an insight into the changes of medium-range structure during crystallization. <i>Microporous and Mesoporous Materials</i> , 2019, 278, 81-90.	4.4	12
80	Seed-Assisted Synthesis of Zeolite Beta from Solid-State Conversion of Magadiite and an Investigation on the Crystallization Mechanism. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 18824-18834.	3.7	10
81	Supramolecular Catalysis of Acyl Transfer within Zinc Porphyrin-Based Metal-Organic Cages. <i>Inorganic Chemistry</i> , 2021, 60, 8802-8810.	4.0	10
82	The formation and evolution of carbonate species in CO oxidation over mono-dispersed Fe on graphene. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10509-10517.	2.8	8
83	Morphology-controlled assembly and enhanced emission of fluorescence in organic nanospheres and microrods based on 1,2-diphenyl-4-(4-dibenzothienyl)phenyl-1,3-cyclopentadiene. <i>CrystEngComm</i> , 2015, 17, 9311-9317.	2.6	7
84	Adsorption, diffusion and aggregation of Ir atoms on graphdiyne: a first-principles investigation. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25841-25847.	2.8	7
85	Designing Multicomponent Metal-Organic Frameworks with Hierarchical Structure-Mimicking Distribution for High CO ₂ Capture Performance. <i>Inorganic Chemistry</i> , 2022, 61, 7663-7670.	4.0	7
86	Self-Assembly of Nanoparticles in a Modular Fashion to Prepare Multifunctional Catalysts for Cascade Reactions: From Simplicity to Complexity. <i>ACS Omega</i> , 2019, 4, 1549-1559.	3.5	6
87	Solid-State and Organic Template-Free Synthesis of Zeolite Omega by Conversion of Magadiite in the Presence of Seed Crystals and Investigation of Conversion Mechanism. <i>Industrial & Engineering Chemistry Research</i> , 2020, 59, 19574-19583.	3.7	6
88	The Promoter Role of Amines in the Condensation of Silicic Acid: A First-Principles Investigation. <i>ACS Omega</i> , 2021, 6, 22811-22819.	3.5	6
89	Interfacial-Bonding-Regulated CO Oxidation over Pt Atoms Immobilized on Gas-Exfoliated Hexagonal Boron Nitride. <i>ChemistrySelect</i> , 2017, 2, 9412-9419.	1.5	5
90	Solid-state transformation of TMA-magadiite into zeolite omega and detailed insights into the crystallization process. <i>Dalton Transactions</i> , 2019, 48, 16974-16985.	3.3	5

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91	Deep eutectic solvent for curing of phthalonitrile resin: Lower the curing temperature but improve the properties of thermosetting. High Performance Polymers, 2021, 33, 538-545.	1.8	5
92	Locally Enhanced Sampling Study of Dioxygen Diffusion Pathways in Homoprotocatechuate 2,3-Dioxygenase. Journal of Physical Chemistry B, 2009, 113, 13596-13603.	2.6	4
93	Hydrothermal conversion of zeolite omega from magadiite with assistance of seed crystals. Materials Today Chemistry, 2021, 20, 100440.	3.5	4
94	Synthesis and characterization of advanced bio-carbon materials from Kraft lignin with enhanced CO ₂ capture properties. Journal of Environmental Chemical Engineering, 2022, 10, 107471.	6.7	4
95	Coadsorption Interfered CO Oxidation over Atomically Dispersed Au on h-BN. Molecules, 2022, 27, 3627.	3.8	4
96	First-Principles Study on Alloying Effect on the Migration Barrier of He in Titanium Dinitride. Journal of Computational and Theoretical Nanoscience, 2011, 8, 858-861.	0.4	3
97	Understanding the Enhanced Catalytic Performance of Ultrafine Transition Metal Nanoparticles in Graphene Composites. Journal of Molecular and Engineering Materials, 2015, 03, 1540002.	1.8	3
98	Heating Rate Induced Melting and Superheating of Pb. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2003, 19, 681-685.	4.9	3
99	Molecular Dynamics Study on Superheating of Ni at High Heating Rates. , 2009, , .		2
100	TiO ₂ Film Formation on NiTi Alloy (100) Surface: Density Functional Theory Investigation. Materials Science Forum, 0, 675-677, 353-356.	0.3	2
101	Modulation of the Band Gap Increase in Nanocrystals by Surface Passivation. Journal of Physical Chemistry C, 2014, 118, 14026-14030.	3.1	2
102	Conversion of magadiite to pure-silica-Nu-1 and an insight into the changes in its medium-range structure during crystallization. Inorganic Chemistry Frontiers, 2019, 6, 837-847.	6.0	2
103	Hydrothermal conversion of kenyaite into zeolite omega in tetramethylammonium cations system. Solid State Sciences, 2020, 103, 106196.	3.2	2
104	Design and Implementation of HPC-Based Research-Oriented Learning Environment for Structural Chemistry. , 2009, , .		1
105	Synthesis, Crystal Structures, and Characterization of Two 3d-3d Heterometallic Coordination Frameworks: [ZnCo(Hcit)Cl] and [ZnCo(Hcit)Br]. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2010, 637, n/a-n/a.	1.2	1
106	Melting of Bulk Gold During Continuous Heating: A Molecular Dynamics Study. , 2010, , .		1
107	Pd speciation on black phosphorene in a CO and C ₂ H ₄ atmosphere: a first-principles investigation. Physical Chemistry Chemical Physics, 2022, 24, 14284-14293.	2.8	1
108	A Solvothermal Synthesis and the Structure of K ₄ Ag ₂ Sn ₃ S ₉ ·2KOH.. ChemInform, 2003, 34, no.	0.0	0

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109	K ₂ Ag ₆ Sn ₃ S ₁₀ : A Quaternary Sulfide Composed of Silver Sulfide Layers Pillared by Zigzag Chains [SnS ₃] ²⁻ . ChemInform, 2004, 35, no.	0.0	0
110	A Solvothermal Synthesis and the Structure of (NH ₄) ₂ Ag ₆ Sn ₃ S ₁₀ . ChemInform, 2005, 36, no.	0.0	0
111	Detection of Phenolate with a Solvent Polymeric Membrane Electrode. , 2009, , .		0
112	Electronic Excitation Induced Solid-State Amorphization in Ge-Sb-Te Alloy. Materials Research Society Symposia Proceedings, 2011, 1370, 77.	0.1	0