Xin Liu

List of Publications by Year in descending order

112 papers	3,909 citations	108046 37 h-index	156644 58 g-index
113 all docs	113 docs citations	113 times ranked	5695 citing authors

#	Article	IF	Citations
1	Dual Stimuli-Responsive smart fibrous membranes for efficient Photothermal/Photodynamic/Chemo-Therapy of Drug-Resistant bacterial infection. Chemical Engineering Journal, 2022, 432, 134351.	6.6	26
2	Synthesis and characterization of advanced bio-carbon materials from Kraft lignin with enhanced CO2 capture properties. Journal of Environmental Chemical Engineering, 2022, 10, 107471.	3.3	4
3	Quench-tailored Al-doped V2O5 nanomaterials for efficient aqueous zinc-ion batteries. Journal of Energy Chemistry, 2022, 70, 52-58.	7.1	46
4	Designing Multicomponent Metalâ€“Organic Frameworks with Hierarchical Structure-Mimicking Distribution for High CO₂ Capture Performance. Inorganic Chemistry, 2022, 61, 7663-7670.	1.9	7
5	Pd speciation on black phosphorene in a CO and C₂H₄ atmosphere: a first-principles investigation. Physical Chemistry Chemical Physics, 2022, 24, 14284-14293.	1.3	1
6	Discovery of versatile <scp>batâ€shaped</scp> acceptor materials for <scp>highâ€performance</scp> organic solar cells â€•a <scp>DFT</scp> approach. International Journal of Energy Research, 2022, 46, 13393-13408.	2.2	19
7	Coadsorption Interfered CO Oxidation over Atomically Dispersed Au on h-BN. Molecules, 2022, 27, 3627.	1.7	4
8	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.	0.8	5
9	Efficient tuning of zinc phthalocyanine-based dyes for dye-sensitized solar cells: a detailed DFT study. RSC Advances, 2021, 11, 27570-27582.	1.7	38
10	Recent Advances on Gallium-Modified ZSM-5 for Conversion of Light Hydrocarbons. Molecules, 2021, 26, 2234.	1.7	16
11	A single-molecule van der Waals compass. Nature, 2021, 592, 541-544.	13.7	75
12	Electronic structure engineering through Fe-doping CoP enables hydrogen evolution coupled with electro-Fenton. Nano Energy, 2021, 84, 105943.	8.2	64
13	Supramolecular Catalysis of Acyl Transfer within Zinc Porphyrin-Based Metalâ€“Organic Cages. Inorganic Chemistry, 2021, 60, 8802-8810.	1.9	10
14	Hydrothermal conversion of zeolite omega from magadiite with assistance of seed crystals. Materials Today Chemistry, 2021, 20, 100440.	1.7	4
15	The Promoter Role of Amines in the Condensation of Silicic Acid: A First-Principles Investigation. ACS Omega, 2021, 6, 22811-22819.	1.6	6
16	Titanium carbide/zeolite imidazole framework-8/polylactic acid electrospun membrane for near-infrared regulated photothermal/photodynamic therapy of drug-resistant bacterial infections. Journal of Colloid and Interface Science, 2021, 599, 390-403.	5.0	48
17	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.	1.1	24
18	Layered silicate magadiiteâ€“derived three-dimensional honeycomb-like cobaltâ€“nickel silicates as excellent cathode for hybrid supercapacitors. Materials Today Chemistry, 2021, 22, 100550.	1.7	13

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19	Sandwich-Like Sulfur-Doped V2O5/Reduced graphene Oxide/Sulfur-Doped V2O5 Core-shell structure boosts Zinc-Ion storage. Applied Surface Science, 2021, 568, 150919.	3.1	23
20	The formation and evolution of carbonate species in CO oxidation over mono-dispersed Fe on graphene. Physical Chemistry Chemical Physics, 2021, 23, 10509-10517.	1.3	8
21	Atomic Spatial and Temporal Imaging of Local Structures and Light Elements inside Zeolite Frameworks. Advanced Materials, 2020, 32, e1906103.	11.1	81
22	Seed-Assisted Synthesis of Zeolite Beta from Solid-State Conversion of Magadiite and an Investigation on the Crystallization Mechanism. Industrial & Engineering Chemistry Research, 2020, 59, 18824-18834.	1.8	10
23	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. Industrial & Engineering Chemistry Research, 2020, 59, 19574-19583.	1.8	6
24	Efficient tuning of triphenylamine-based donor materials for high-efficiency organic solar cells. Computational and Theoretical Chemistry, 2020, 1191, 113045.	1.1	73
25	Two urea-functionalized pcu metalâ€“organic frameworks based on a pillared-layer strategy for gas adsorption and separation. Inorganic Chemistry Frontiers, 2020, 7, 3500-3508.	3.0	23
26	Adsorption, diffusion and aggregation of Ir atoms on graphdiyne: a first-principles investigation. Physical Chemistry Chemical Physics, 2020, 22, 25841-25847.	1.3	7
27	Superior Catalytic Performance of Atomically Dispersed Palladium on Graphene in CO Oxidation. ACS Catalysis, 2020, 10, 3084-3093.	5.5	44
28	Hydrothermal conversion of kenyaite into zeolite omega in tetramethylammonium cations system. Solid State Sciences, 2020, 103, 106196.	1.5	2
29	Fabrication of vanadium sulfide (VS4) wrapped with carbonaceous materials as an enhanced electrode for symmetric supercapacitors. Journal of Colloid and Interface Science, 2020, 574, 312-323.	5.0	71
30	Direct Imaging of Tunable Crystal Surface Structures of MOF MIL-101 Using High-Resolution Electron Microscopy. Journal of the American Chemical Society, 2019, 141, 12021-12028.	6.6	93
31	Hydrothermal synthesis of VS4/CNTs composite with petal-shape structures performing a high specific capacity in a large potential range for high-performance symmetric supercapacitors. Journal of Colloid and Interface Science, 2019, 554, 191-201.	5.0	57
32	Oligomerization of Silicic Acids in Neutral Aqueous Solution: A First-Principles Investigation. International Journal of Molecular Sciences, 2019, 20, 3037.	1.8	12
33	Self-Assembly of Nanoparticles in a Modular Fashion to Prepare Multifunctional Catalysts for Cascade Reactions: From Simplicity to Complexity. ACS Omega, 2019, 4, 1549-1559.	1.6	6
34	High efficient degradation of levofloxacin by edge-selectively Fe@3D-WS2: Self-renewing behavior and Degradation mechanism study. Applied Catalysis B: Environmental, 2019, 252, 187-197.	10.8	34
35	New lead-free perovskite Rb₇Bi₃Cl₁₆ nanocrystals with blue luminescence and excellent moisture-stability. Nanoscale, 2019, 11, 6719-6726.	2.8	68
36	Light-Induced Self-Assembly of Cubic CsPbBr₃ Perovskite Nanocrystals into Nanowires. Chemistry of Materials, 2019, 31, 6642-6649.	3.2	119

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37	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.	3.0	2
38	Solid-state transformation of TMA-magadiite into zeolite omega and detailed insights into the crystallization process. Dalton Transactions, 2019, 48, 16974-16985.	1.6	5
39	Developing hierarchically ultra-micro/mesoporous biocarbons for highly selective carbon dioxide adsorption. Chemical Engineering Journal, 2019, 361, 199-208.	6.6	79
40	OSDA-free synthesis of zeolite beta by magadiite hydrothermal conversion method and an insight into the changes of medium-range structure during crystallization. Microporous and Mesoporous Materials, 2019, 278, 81-90.	2.2	12
41	Facile synthesis of high-surface vanadium nitride/vanadium sesquioxide/amorphous carbon composite with porous structures as electrode materials for high performance symmetric supercapacitors. Applied Surface Science, 2019, 471, 842-851.	3.1	33
42	Fluorescence modulation via photoinduced spin crossover switched energy transfer from fluorophores to Fe^{II} ions. Chemical Science, 2018, 9, 2892-2897.	3.7	67
43	High Density and Super Ultraâ€Microporousâ€Activated Carbon Macrospheres with High Volumetric Capacity for CO₂ Capture. Advanced Sustainable Systems, 2018, 2, 1700115.	2.7	30
44	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.	2.7	19
45	Silver Clusters as Robust Nodes and Ï€â€“Activation Sites for the Construction of Heterogeneous Catalysts for the Cycloaddition of Propargylamines. ACS Catalysis, 2018, 8, 1384-1391.	5.5	85
46	Fe atoms trapped on graphene as a potential efficient catalyst for room-temperature complete oxidation of formaldehyde: a first-principles investigation. Catalysis Science and Technology, 2017, 7, 2012-2021.	2.1	13
47	Interfacial-Bonding-Regulated CO Oxidation over Pt Atoms Immobilized on Gas-Exfoliated Hexagonal Boron Nitride. ChemistrySelect, 2017, 2, 9412-9419.	0.7	5
48	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.	1.4	16
49	Synthesis of zeolites Na-A and Na-X from tablet compressed and calcinated coal fly ash. Royal Society Open Science, 2017, 4, 170921.	1.1	48
50	Potassium and Zeolitic Structure Modified Ultra-microporous Adsorbent Materials from a Renewable Feedstock with Favorable Surface Chemistry for CO₂ Capture. ACS Applied Materials & Interfaces, 2017, 9, 26826-26839.	4.0	36
51	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.	1.7	15
52	Oxygen-containing coke species in zeolite-catalyzed conversion of methanol to hydrocarbons. Catalysis Science and Technology, 2016, 6, 8157-8165.	2.1	24
53	Supramolecular Photoinduced Electron Transfer between a Redoxâ€Active Hexanuclear Metalâ€“Organic Cylinder and an Encapsulated Ruthenium(II) Complex. Chemistry - A European Journal, 2016, 22, 5253-5260.	1.7	29
54	Defect stabilized gold atoms on graphene as potential catalysts for ethylene epoxidation: a first-principles investigation. Catalysis Science and Technology, 2016, 6, 1632-1641.	2.1	43

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55	Unique Reactivity of Transition Metal Atoms Embedded in Graphene to CO, NO, O2 and O Adsorption: A First-Principles Investigation. Molecules, 2015, 20, 19540-19553.	1.7	17
56	Understanding the Enhanced Catalytic Performance of Ultrafine Transition Metal Nanoparticlesâ€“Graphene Composites. Journal of Molecular and Engineering Materials, 2015, 03, 1540002.	0.9	3
57	Pt atoms stabilized on hexagonal boron nitride as efficient single-atom catalysts for CO oxidation: a first-principles investigation. RSC Advances, 2015, 5, 10452-10459.	1.7	54
58	Light-driven hydrogen evolution with a nickel thiosemicarbazone redox catalyst featuring Niâ‹¯H interactions under basic conditions. New Journal of Chemistry, 2015, 39, 1051-1059.	1.4	25
59	Microporous carbonaceous adsorbents for CO₂separation via selective adsorption. RSC Advances, 2015, 5, 30310-30330.	1.7	119
60	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. CrystEngComm, 2015, 17, 9311-9317.	1.3	7
61	Monodisperse Pt atoms anchored on N-doped graphene as efficient catalysts for CO oxidation: a first-principles investigation. Catalysis Science and Technology, 2015, 5, 1658-1667.	2.1	78
62	Catalytic oxidative conversion of cellulosic biomass to formic acid and acetic acid with exceptionally high yields. Catalysis Today, 2014, 233, 77-82.	2.2	92
63	Copper atoms embedded in hexagonal boron nitride as potential catalysts for CO oxidation: a first-principles investigation. RSC Advances, 2014, 4, 38750-38760.	1.7	57
64	CO oxidation catalyzed by Pt-embedded graphene: a first-principles investigation. Physical Chemistry Chemical Physics, 2014, 16, 23584-23593.	1.3	111
65	Tuning the reactivity of Ru nanoparticles by defect engineering of the reduced graphene oxide support. RSC Advances, 2014, 4, 22230-22240.	1.7	20
66	Modulation of the Band Gap Increase in Nanocrystals by Surface Passivation. Journal of Physical Chemistry C, 2014, 118, 14026-14030.	1.5	2
67	Defective Graphene Supported MPd₁₂ (M = Fe, Co, Ni, Cu, Zn, Pd) Nanoparticles as Potential Oxygen Reduction Electrocatalysts: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 1350-1357.	1.5	88
68	High sulfur tolerance of Niâ€“Si intermetallics as hydrodesulfurization catalysts. RSC Advances, 2013, 3, 1728-1731.	1.7	28
69	Phase diagram of graphene nanoribbons and band-gap bifurcation of Dirac fermions under quantum confinement. Physical Review B, 2012, 85, .	1.1	16
70	Preparation of a Ruâ€Nanoparticles/Defectiveâ€Graphene Composite as a Highly Efficient Areneâ€Hydrogenation Catalyst. ChemCatChem, 2012, 4, 1938-1942.	1.8	55
71	Graphene substrate-mediated catalytic performance enhancement of Runanoparticles: a first-principles study. Dalton Transactions, 2012, 41, 1289-1296.	1.6	61
72	Oxygen Adsorption and Diffusion on NiTi Alloy (100) Surface: A Theoretical Study. Journal of Physical Chemistry C, 2012, 116, 21771-21779.	1.5	15

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73	Unique reactivity of Fe nanoparticlesâ€“defective graphene composites toward NHx (x = 0, 1, 2, 3) adsorption: a first-principles study. Physical Chemistry Chemical Physics, 2012, 14, 15036.	1.3	30
74	Substrate-mediated enhanced activity of Ru nanoparticles in catalytic hydrogenation of benzene. Nanoscale, 2012, 4, 2288.	2.8	47
75	Theoretical Study on the Ground State Structure of Uranofullerene U@C₈₂. Journal of Physical Chemistry A, 2012, 116, 11651-11655.	1.1	34
76	Palladium Nanoparticles/Defective Graphene Composites as Oxygen Reduction Electrocatalysts: A First-Principles Study. Journal of Physical Chemistry C, 2012, 116, 2710-2719.	1.5	94
77	Superior Capture of CO₂ Achieved by Introducing Extra-framework Cations into N-doped Microporous Carbon. Chemistry of Materials, 2012, 24, 4725-4734.	3.2	199
78	Direct Conversion of Cellulose to Glycolic Acid with a Phosphomolybdic Acid Catalyst in a Water Medium. ACS Catalysis, 2012, 2, 1698-1702.	5.5	126
79	Coumarin phosphorescence observed with NâN Pt(ii) bisacetylide complex and its applications for luminescent oxygen sensing and tripletâ€“triplet-annihilation based upconversion. Dalton Transactions, 2011, 40, 7834.	1.6	106
80	Site-specific growth of Au particles on ZnO nanopyramids under ultraviolet illumination. Nanoscale, 2011, 3, 4195.	2.8	61
81	Regioselectivity control of graphene functionalization by ripples. Physical Chemistry Chemical Physics, 2011, 13, 19449.	1.3	46
82	Mechanical Properties and Defective Effects of 316LN Stainless Steel by First-Principles Simulations. Journal of Materials Science and Technology, 2011, 27, 1029-1033.	5.6	12
83	First-Principles Study on Alloying Effect on the Migration Barrier of He in Titanium Ditritide. Journal of Computational and Theoretical Nanoscience, 2011, 8, 858-861.	0.4	3
84	Highly Selective and Complete Conversion of Cellobiose to Gluconic Acid over Au/Cs₂HPW₁₂O₄₀ Nanocomposite Catalyst. ChemCatChem, 2011, 3, 1294-1298.	1.8	80
85	Reaction mechanism of tert-butylation of phenol with tert-butyl alcohol over H-Î² zeolite: An ONIOM study. Catalysis Today, 2011, 165, 120-128.	2.2	26
86	Role of Electronic Excitation in the Amorphization of Ge-Sb-Te Alloys. Physical Review Letters, 2011, 107, 015501.	2.9	107
87	Electronic Excitation Induced Solid-State Amorphization in Ge-Sb-Te Alloy. Materials Research Society Symposia Proceedings, 2011, 1370, 77.	0.1	0
88	BrÃ¸nsted acid-catalyzed tert-butylation of phenol, o-cresol and catechol: A comparative computational study. Journal of Molecular Catalysis A, 2010, 332, 145-151.	4.8	13
89	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.	0.6	1
90	Melting of Bulk Gold During Continuous Heating: A Molecular Dynamics Study. , 2010, , .		1

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91	SO₃H-Functionalized Ionic Liquid Catalyzed Alkylation of Catechol with tert-Butyl Alcohol. Industrial & Engineering Chemistry Research, 2010, 49, 8157-8163.	1.8	22
92	Detection of Phenolate with a Solvent Polymeric Membrane Electrode. , 2009, , .		0
93	Molecular Dynamics Study on Superheating of Ni at High Heating Rates. , 2009, , .		2
94	Syngas Segregation Induced by Confinement in Carbon Nanotubes: A Combined First-Principles and Monte Carlo Study. Journal of Physical Chemistry C, 2009, 113, 21687-21692.	1.5	67
95	Locally Enhanced Sampling Study of Dioxygen Diffusion Pathways in Homoprotocatechuate 2,3-Dioxygenase. Journal of Physical Chemistry B, 2009, 113, 13596-13603.	1.2	4
96	Design and Implementation of HPC-Based Research-Oriented Learning Environment for Structural Chemistry. , 2009, , .		1
97	Unique Reactivity of Confined Metal Atoms on a Silicon Substrate. ChemPhysChem, 2008, 9, 975-979.	1.0	24
98	Wavevector-dependent quantum-size effect in electron decay length at Pb thin film surfaces. Applied Physics Letters, 2008, 93, 093105.	1.5	18
99	Molecular dynamics study on superheating of Pd at high heating rates. Phase Transitions, 2006, 79, 249-259.	0.6	19
100	A Solvothermal Synthesis and the Structure of (NH4)2Ag6Sn3S10. Bulletin of the Chemical Society of Japan, 2005, 78, 1283-1284.	2.0	14
101	(NH3CH2CH2NH3)Ag2SnS4: a quaternary sulfide-containing chiral layers. Inorganic Chemistry Communication, 2005, 8, 301-303.	1.8	26
102	A Solvothermal Synthesis and the Structure of (NH4)2Ag6Sn3S10.. ChemInform, 2005, 36, no.	0.1	0
103	K2Ag6Sn3S10: A Quaternary Sulfide Composed of Silver Sulfide Layers Pillared by Zigzag Chains1âˆž[SnS3]2-.. ChemInform, 2004, 35, no.	0.1	0
104	A solvothermal synthesis and characterization of a new open-framework K4Ag2Ge3S9Â·H2O. Journal of Solid State Chemistry, 2004, 177, 2506-2510.	1.4	13
105	A solvothermal synthesis and structure of K2Ag2GeS4 with the simplest helical chains. Inorganic Chemistry Communication, 2004, 7, 114-116.	1.8	18
106	K2Ag6Sn3S10:Â A Quaternary Sulfide Composed of Silver Sulfide Layers Pillared by Zigzag Chains [SnS3]2-. Inorganic Chemistry, 2004, 43, 3764-3765.	1.9	48
107	Melting and Superheating of Ag at High Heating Rate. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2004, 20, 280-284.	2.2	19
108	A Solvothermal Synthesis and the Structure of K4Ag2Sn3S9Ã—2KOH.. ChemInform, 2003, 34, no.	0.1	0

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109	A solvothermal synthesis of a novel 1D ladder-like (NH3CH2CH2NH3)AgAsS4 containing Nâ€“Hâ‹¯S hydrogen bonding. Inorganic Chemistry Communication, 2003, 6, 1137-1139.	1.8	29
110	A Solvothermal Synthesis and the Structure of K4Ag2Sn3S9Â·2KOH. Inorganic Chemistry, 2003, 42, 4248-4249.	1.9	38
111	Heating Rate Induced Melting and Superheating of Pb. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2003, 19, 681-685.	2.2	3
112	TiO_x Film Formation on NiTi Alloy (100) Surface: Density Functional Theory Investigation. Materials Science Forum, 0, 675-677, 353-356.	0.3	2