

# Yongqiang Cheng

## List of Publications by Year in descending order

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109  
papers

5,605  
citations

94269

37  
h-index

82410

72  
g-index

115  
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115  
docs citations

115  
times ranked

7908  
citing authors

#	ARTICLE	IF	CITATIONS
1	Structures, Phase Transitions and Tricritical Behavior of the Hybrid Perovskite Methyl Ammonium Lead Iodide. <i>Scientific Reports</i> , 2016, 6, 35685.	1.6	440
2	Soft spots and their structural signature in a metallic glass. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 14052-14056.	3.3	348
3	Selective production of arenes via direct lignin upgrading over a niobium-based catalyst. <i>Nature Communications</i> , 2017, 8, 16104.	5.8	346
4	Guidelines in predicting phase formation of high-entropy alloys. <i>MRS Communications</i> , 2014, 4, 57-62.	0.8	275
5	Aluminum Alloying Effects on Lattice Types, Microstructures, and Mechanical Behavior of High-Entropy Alloys Systems. <i>Jom</i> , 2013, 65, 1848-1858.	0.9	250
6	Selective Adsorption of Sulfur Dioxide in a Robust Metal-Organic Framework Material. <i>Advanced Materials</i> , 2016, 28, 8705-8711.	11.1	214
7	Confinement of Iodine Molecules into Triple-Helical Chains within Robust Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2017, 139, 16289-16296.	6.6	199
8	Control of zeolite pore interior for chemoselective alkyne/olefin separations. <i>Science</i> , 2020, 368, 1002-1006.	6.0	179
9	Reversible coordinative binding and separation of sulfur dioxide in a robust metal-organic framework with open copper sites. <i>Nature Materials</i> , 2019, 18, 1358-1365.	13.3	171
10	Reversible adsorption of nitrogen dioxide within a robust porous metal-organic framework. <i>Nature Materials</i> , 2018, 17, 691-696.	13.3	162
11	Direct Neutron Spectroscopy Observation of Cerium Hydride Species on a Cerium Oxide Catalyst. <i>Journal of the American Chemical Society</i> , 2017, 139, 9721-9727.	6.6	138
12	Capture of nitrogen dioxide and conversion to nitric acid in a porous metal-organic framework. <i>Nature Chemistry</i> , 2019, 11, 1085-1090.	6.6	116
13	First-Order Liquid-Liquid Phase Transition in Cerium. <i>Physical Review Letters</i> , 2013, 110, 125503.	2.9	111
14	Gate-opening effect in ZIF-8: the first experimental proof using inelastic neutron scattering. <i>Chemical Communications</i> , 2016, 52, 3639-3642.	2.2	106
15	Simulation of Inelastic Neutron Scattering Spectra Using OCLIMAX. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1974-1982.	2.3	95
16	Spin-phonon couplings in transition metal complexes with slow magnetic relaxation. <i>Nature Communications</i> , 2018, 9, 2572.	5.8	93
17	Harnessing strong metal-support interactions via a reverse route. <i>Nature Communications</i> , 2020, 11, 3042.	5.8	84
18	Modulating supramolecular binding of carbon dioxide in a redox-active porous metal-organic framework. <i>Nature Communications</i> , 2017, 8, 14212.	5.8	75

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19	Quantitative production of butenes from biomass-derived $\gamma$ -valerolactone catalysed by hetero-atomic MFI zeolite. <i>Nature Materials</i> , 2020, 19, 86-93.	13.3	74
20	Pore Distortion in a Metal-Organic Framework for Regulated Separation of Propane and Propylene. <i>Journal of the American Chemical Society</i> , 2021, 143, 19300-19305.	6.6	72
21	Discriminating the Role of Surface Hydride and Hydroxyl for Acetylene Semihydrogenation over Ceria through <i>In Situ</i> Neutron and Infrared Spectroscopy. <i>ACS Catalysis</i> , 2020, 10, 5278-5287.	5.5	70
22	High Ammonia Adsorption in MFM-300 Materials: Dynamics and Charge Transfer in Host-Guest Binding. <i>Journal of the American Chemical Society</i> , 2021, 143, 3153-3161.	6.6	67
23	Atomically Dispersed Copper Sites in a Metal-Organic Framework for Reduction of Nitrogen Dioxide. <i>Journal of the American Chemical Society</i> , 2021, 143, 10977-10985.	6.6	66
24	A unique Co@CoO catalyst for hydrogenolysis of biomass-derived 5-hydroxymethylfurfural to 2,5-dimethylfuran. <i>Nature Communications</i> , 2022, 13, .	5.8	66
25	Quest for an Optimal Methane Hydrate Formation in the Pores of Hydrolytically Stable Metal-Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2020, 142, 13391-13397.	6.6	65
26	Post-synthetic modulation of the charge distribution in a metal-organic framework for optimal binding of carbon dioxide and sulfur dioxide. <i>Chemical Science</i> , 2019, 10, 1472-1482.	3.7	62
27	Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 6526-6532.	7.2	62
28	Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copper-Chromium-Iron Oxide Catalyst. <i>Journal of the American Chemical Society</i> , 2019, 141, 7990-7999.	6.6	60
29	Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. <i>Journal of the American Chemical Society</i> , 2020, 142, 7655-7667.	6.6	59
30	Correlating local structure with inhomogeneous elastic deformation in a metallic glass. <i>Applied Physics Letters</i> , 2012, 101, .	1.5	51
31	Purification of Propylene and Ethylene by a Robust Metal-Organic Framework Mediated by Host-Guest Interactions. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 15541-15547.	7.2	51
32	Understanding the breathing phenomena in nano-ZIF-7 upon gas adsorption. <i>Journal of Materials Chemistry A</i> , 2017, 5, 20938-20946.	5.2	50
33	X-ray and Neutron Scattering Study of the Formation of Core-Shell-Type Polyoxometalates. <i>Journal of the American Chemical Society</i> , 2016, 138, 2638-2643.	6.6	49
34	Mesoscopic Framework Enables Facile Ionic Transport in Solid Electrolytes for Li Batteries. <i>Advanced Energy Materials</i> , 2016, 6, 1600053.	10.2	46
35	Uncovering design principles for amorphous-like heat conduction using two-channel lattice dynamics. <i>Materials Today Physics</i> , 2021, 18, 100344.	2.9	42
36	Temperature effects on atomic pair distribution functions of melts. <i>Journal of Chemical Physics</i> , 2014, 140, 064501.	1.2	41

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37	Exceptional Packing Density of Ammonia in a Dual-Functionalized Metal-Organic Framework. <i>Journal of the American Chemical Society</i> , 2021, 143, 6586-6592.	6.6	37
38	Hydrogen adsorption on two catalysts for the ortho- to parahydrogen conversion: Cr-doped silica and ferric oxide gel. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 17281-17293.	1.3	34
39	Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. <i>ChemSusChem</i> , 2019, 12, 93-103.	3.6	29
40	Comparison of two multifunctional catalysts [M/Nb <sub>2</sub> O <sub>5</sub> (M = Pd, Pt)] for one-pot hydrodeoxygenation of lignin. <i>Catalysis Science and Technology</i> , 2018, 8, 6129-6136.	2.1	26
41	Crystal field splitting, local anisotropy, and low-energy excitations in the quantum magnet $\text{YbCl}_3$ . <i>Physical Review B</i> , 2019, 100, .	1.1	26
42	Highly Efficient Proton Conduction in the Metal-Organic Framework Material MFMO-300(Cr)SO <sub>4</sub> (H <sub>3</sub> O) <sub>2</sub> . <i>Journal of the American Chemical Society</i> , 2022, 144, 11969-11974.	6.6	26
43	Inter-Kramers Transitions and Spin-Phonon Couplings in a Lanthanide-Based Single-Molecule Magnet. <i>Inorganic Chemistry</i> , 2020, 59, 5218-5230.	1.9	25
44	Distilling nanoscale heterogeneity of amorphous silicon using tip-enhanced Raman spectroscopy (TERS) via multiresolution manifold learning. <i>Nature Communications</i> , 2021, 12, 578.	5.8	25
45	Guest-Controlled Incommensurate Modulation in a Meta-Rigid Metal-Organic Framework Material. <i>Journal of the American Chemical Society</i> , 2020, 142, 19189-19197.	6.6	24
46	Inelastic neutron scattering evidence for anomalous H-H distances in metal hydrides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 4021-4026.	3.3	24
47	Direct visualization of anionic electrons in an electride reveals inhomogeneities. <i>Science Advances</i> , 2021, 7, .	4.7	24
48	Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. <i>Journal of the American Chemical Society</i> , 2022, 144, 8624-8632.	6.6	24
49	Inherent structure length in metallic glasses: simplicity behind complexity. <i>Scientific Reports</i> , 2015, 5, 12137.	1.6	23
50	An integrated approach for structural characterization of complex solid state electrolytes: the case of lithium lanthanum titanate. <i>Journal of Materials Chemistry A</i> , 2014, 2, 2418.	5.2	22
51	Direct observation of supramolecular binding of light hydrocarbons in vanadium(III) and (IV) metal-organic framework materials. <i>Chemical Science</i> , 2018, 9, 3401-3408.	3.7	22
52	Spectroscopic Studies of the Magnetic Excitation and Spin-Phonon Couplings in a Single-Molecule Magnet. <i>Chemistry - A European Journal</i> , 2019, 25, 15846-15857.	1.7	22
53	Understanding ZIF-8 Performance upon Gas Adsorption by Means of Inelastic Neutron Scattering. <i>ChemistrySelect</i> , 2017, 2, 2750-2753.	0.7	21
54	Lattice-Cell Orientation Disorder in Complex Spinel Oxides. <i>Advanced Energy Materials</i> , 2017, 7, 1601950.	10.2	21

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55	Chemical Bonding and Transport Properties in Clathrates-I with Cu <sup>2+</sup> Zn <sup>2+</sup> P Frameworks. Chemistry of Materials, 2018, 30, 3419-3428.	3.2	21
56	Applying Unconventional Spectroscopies to the Single-Molecule Magnets, Co(PPH <sub>3</sub> ) <sub>2</sub> X <sub>2</sub> (X=Cl, Br, I): Unveiling Magnetic Transitions and Spin-Phonon Coupling. Chemistry - A European Journal, 2021, 27, 11110-11125.	1.7	21
57	Polymer, Additives, and Processing Effects on N95 Filter Performance. ACS Applied Polymer Materials, 2021, 3, 1022-1031.	2.0	21
58	On the origin of elastic strain limit of bulk metallic glasses. Applied Physics Letters, 2014, 104, .	1.5	20
59	Neutron Spectroscopic and Thermochemical Characterization of Lithium-Aluminum-Layered Double Hydroxide Chloride: Implications for Lithium Recovery. Journal of Physical Chemistry C, 2019, 123, 20723-20729.	1.5	20
60	<i>In situ</i> quasi-elastic neutron scattering study on the water dynamics and reaction mechanisms in alkali-activated slags. Physical Chemistry Chemical Physics, 2019, 21, 10277-10292.	1.3	20
61	Insight into the Selectivity of Isopropanol Conversion at Strontium Titanate (100) Surfaces: A Combination Kinetic and Spectroscopic Study. ACS Catalysis, 2017, 7, 8118-8129.	5.5	19
62	Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. Angewandte Chemie, 2021, 133, 6600-6606.	1.6	17
63	Charge transfer and atomic-level pressure in metallic glasses. Applied Physics Letters, 2014, 104, 051903.	1.5	16
64	New insights into the breathing phenomenon in ZIF-4. Journal of Materials Chemistry A, 2019, 7, 14552-14558.	5.2	15
65	Probing Magnetic Excitations in Co <sup>II</sup> Single-Molecule Magnets by Inelastic Neutron Scattering. European Journal of Inorganic Chemistry, 2019, 2019, 1119-1127.	1.0	14
66	Calculation of the Thermal Neutron Scattering Cross-Section of Solids Using OCLIMAX. Journal of Chemical Theory and Computation, 2020, 16, 5212-5217.	2.3	14
67	Simulation of Inelastic Neutron Scattering Spectra Directly from Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2020, 16, 7702-7708.	2.3	14
68	Role of the third dimension in searching for Majorana fermions in $\text{Co}_2\text{V}_2\text{O}_7$ via phonons. Physical Review Research, 2022, 4, .		
69	Influence of Metal Identity on Light-Induced Switchable Adsorption in Azobenzene-Based Metal-Organic Frameworks. ACS Applied Materials & Interfaces, 2022, 14, 11192-11199.	4.0	14
70	Vacancy-driven variations in the phonon density of states of fast neutron irradiated nuclear graphite. Carbon, 2020, 168, 42-54.	5.4	13
71	Structural and Dynamic Analysis of Sulphur Dioxide Adsorption in a Series of Zirconium-Based Metal-Organic Frameworks. Angewandte Chemie - International Edition, 2022, 61, .	7.2	12
72	On the Structural Transformation of Ni/BaH <sub>2</sub> During a N <sub>2</sub> -H <sub>2</sub> Chemical Looping Process for Ammonia Synthesis: A Joint In Situ Inelastic Neutron Scattering and First-Principles Simulation Study. Topics in Catalysis, 2021, 64, 685-692.	1.3	11

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73	Gapless Dirac magnons in CrCl <sub>3</sub> . <i>Npj Quantum Materials</i> , 2022, 7, .	1.8	11
74	Effect of magnetic fields on the methyl rotation in a paramagnetic cobalt( <sup>ii</sup> ) complex. Quasielastic neutron scattering studies. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 21119-21126.	1.3	10
75	Ab Initio Molecular Dynamics Simulation of the Amorphous Structure of Ca-Mg-Cu and Ca-Mg-Zn Alloys. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2013, 44, 1980-1989.	1.1	9
76	The influence of the local structure on proton transport in a solid oxide proton conductor La <sub>0.8</sub> Ba <sub>1.2</sub> GaO <sub>3.9</sub> . <i>Journal of Materials Chemistry A</i> , 2017, 5, 15507-15511.	5.2	9
77	Thermal scattering law of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll" \rangle \langle \text{mml:mrow} \langle \text{mml:msub} \langle \text{mml:mrow} \langle \text{mml:mfenced open="("} \rangle \text{Tj ETQq1 1 0.784314 rgBT /Overl$ . <i>Annals of Nuclear Energy</i> , 2018, 120, 778-787.	0.9	9
78	Large-Scale Phonon Calculations Using the Real-Space Multigrid Method. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6859-6864.	2.3	9
79	Clathrate BaNi <sub>2</sub> P <sub>4</sub> : An Interplay of Heat and Charge Transport Due to Strong Host-Guest Interactions. <i>Chemistry of Materials</i> , 2020, 32, 7932-7940.	3.2	9
80	Low rotational barriers for the most dynamically active methyl groups in the proposed antiviral drugs for treatment of SARS-CoV-2, apilimod and tetrandrine. <i>Chemical Physics Letters</i> , 2021, 777, 138727.	1.2	9
81	Effect of Hydration on the Molecular Dynamics of Hydroxychloroquine Sulfate. <i>ACS Omega</i> , 2020, 5, 21231-21240.	1.6	8
82	Catalytic Enhancement of Inductively Heated Fe <sub>3</sub> O <sub>4</sub> Nanoparticles by Removal of Surface Ligands. <i>ChemSusChem</i> , 2021, 14, 1122-1130.	3.6	8
83	Low-temperature vibrational dynamics of fused silica and binary silicate glasses. <i>Physical Review B</i> , 2018, 97, .	1.1	7
84	Hydration-Induced Disorder Lowers the Energy Barriers for Methyl Rotation in Drug Molecules. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 10256-10261.	2.1	7
85	Substrate Binding Stiffens Aspartate Aminotransferase by Altering the Enzyme Picosecond Vibrational Dynamics. <i>ACS Omega</i> , 2020, 5, 18787-18797.	1.6	7
86	Nanoconfinement Inside Molecular Metal Oxide Clusters: Dynamics and Modified Encapsulation Behavior. <i>Chemistry - A European Journal</i> , 2016, 22, 14131-14136.	1.7	6
87	Design of a facility for the <i>in situ</i> measurement of catalytic reaction by neutron scattering spectroscopy. <i>Review of Scientific Instruments</i> , 2018, 89, 014101.	0.6	6
88	Unraveling the structural properties and dynamics of sulfonated solid acid carbon catalysts with neutron vibrational spectroscopy. <i>Catalysis Today</i> , 2020, 358, 387-393.	2.2	6
89	Phonon Spectroscopy in Antimony and Tellurium Oxides. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7869-7880.	1.1	6
90	High capacity ammonia adsorption in a robust metal-organic framework mediated by reversible host-guest interactions. <i>Chemical Communications</i> , 2022, 58, 5753-5756.	2.2	6

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91	Exposing Key Vibrational Contributions to Properties of Organic Molecular Solids with High Signal, Low Frequency Neutron Spectroscopy and Ab Initio Simulations. <i>Crystal Growth and Design</i> , 2018, 18, 4815-4821.	1.4	5
92	Vibrational properties of uranium fluorides. <i>Physica B: Condensed Matter</i> , 2019, 570, 194-205.	1.3	5
93	Neutron vibrational spectroscopic evidence for short H <sup>δ</sup> -M <sup>δ</sup> -H contacts in the RNi <sub>2</sub> NH <sub>1.4</sub> ; 1.6 (R = Ce, La) metal hydride. <i>Journal of Alloys and Compounds</i> , 2022, 894, 162381.	2.8	5
94	Studying Materials and Processes with VISION, VirtuES and ICEMAN – Modeling INS Data with DFT Methods. <i>Hamon</i> , 2020, 30, 154-159.	0.0	5
95	Neutron thermalization in nuclear graphite: A modern story of a classic moderator. <i>Annals of Nuclear Energy</i> , 2021, 161, 108437.	0.9	4
96	Nanoconfinement Inside Molecular Metal Oxide Clusters: Dynamics and Modified Encapsulation Behavior. <i>Chemistry - A European Journal</i> , 2016, 22, 14073-14073.	1.7	3
97	The ICEMAN, a heterogeneous platform for analysis of neutron scattering data. <i>Neutron News</i> , 2021, 32, 15-16.	0.1	3
98	Study of Anharmonicity in Zirconium Hydrides Using Inelastic Neutron Scattering and Ab-Initio Computer Modeling. <i>Inorganics</i> , 2021, 9, 29.	1.2	3
99	Neutron Insights into Sorption Enhanced Methanol Catalysis. <i>Topics in Catalysis</i> , 2021, 64, 638-643.	1.3	3
100	Inelastic neutron spectra of polyacrylonitrile-based carbon fibers. <i>Physical Review Materials</i> , 2022, 6, .	0.9	3
101	Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3586-3597.	1.3	3
102	Theoretical Study of Alkali-Metal Hydrides at High Pressures: A Case of NaH Supported by Inelastic Neutron Scattering (INS) Experiments at 1 and 2 GPa. <i>Journal of Physical Chemistry A</i> , 2019, 123, 10079-10085.	1.1	1
103	Neutron Vibrational Spectroscopic Evidence for Short H <sup>δ</sup> -M <sup>δ</sup> -H Contacts in the RNi <sub>2</sub> NH <sub>1.4</sub> ; 1.6 (R = Ce, La) Metal Hydride. <i>Neutron News</i> , 2022, 33, 7-9.	0.1	1
104	In situ inelastic neutron scattering of mixed CH <sub>4</sub> -CO <sub>2</sub> hydrates. <i>Fuel</i> , 2022, 327, 125197.	3.4	1
105	A “Hidden” Mesoscopic Feature Revealed By Electron Microscopy Could Facilitate Ion Transport In Solid Electrolytes. <i>Microscopy and Microanalysis</i> , 2016, 22, 1308-1309.	0.2	0
106	Energy Storage: Lattice Cell Orientation Disorder in Complex Spinel Oxides ( <i>Adv. Energy Mater.</i> 4/2017). <i>Advanced Energy Materials</i> , 2017, 7, .	10.2	0
107	Probing Magnetic Excitations in Coll Single-Molecule Magnets by Inelastic Neutron Scattering. <i>European Journal of Inorganic Chemistry</i> , 2019, 2019, 1055-1055.	1.0	0
108	Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. <i>ChemSusChem</i> , 2019, 12, 5-5.	3.6	0

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109	Structural and dynamic analysis of adsorption of sulphur dioxide in a series of Zr-based metal-organic frameworks. <i>Angewandte Chemie</i> , 0, , .	1.6	0