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 all docs	115 docs citations	115 times ranked	7908 citing authors

#	Article	IF	Citations
1	Neutron vibrational spectroscopic evidence for short Hâ^™â^™â^™H contacts in the RNiInH1.4; 1.6 (R = Ce, La) metal hydride. Journal of Alloys and Compounds, 2022, 894, 162381.	2.8	5
2	Inelastic neutron spectra of polyacrylonitrile-based carbon fibers. Physical Review Materials, 2022, 6, .	0.9	3
3	Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. Physical Chemistry Chemical Physics, 2022, 24, 3586-3597.	1.3	3
4	Role of the third dimension in searching for Majorana fermions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î±</mml:mi><mml:mtext>â^’</mml:mtext><mml:msub>< via phonons. Physical Review Research, 2022, 4, .	1.3	14
5	Influence of Metal Identity on Light-Induced Switchable Adsorption in Azobenzene-Based Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2022, 14, 11192-11199.	4.0	14
6	Neutron Vibrational Spectroscopic Evidence for Short HÂ·Â·Â·H Contacts in the RNiInH_{1.4;1.6} (R = Ce, La) Metal Hydride. Neutron News, 2022, 33, 7-9.	0.1	1
7	High capacity ammonia adsorption in a robust metalâ€“organic framework mediated by reversible hostâ€“guest interactions. Chemical Communications, 2022, 58, 5753-5756.	2.2	6
8	Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. Journal of the American Chemical Society, 2022, 144, 8624-8632.	6.6	24
9	Gapless Dirac magnons in CrCl3. Npj Quantum Materials, 2022, 7, .	1.8	11
10	Structural and Dynamic Analysis of Sulphur Dioxide Adsorption in a Series of Zirconiumâ€Based Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2022, 61, .	7.2	12
11	A unique Co@CoO catalyst for hydrogenolysis of biomass-derived 5-hydroxymethylfurfural to 2,5-dimethylfuran. Nature Communications, 2022, 13, .	5.8	66
12	Highly Efficient Proton Conduction in the Metalâ€“Organic Framework Material MFM-300(Cr)Â·SO₄(H₃O)₂. Journal of the American Chemical Society, 2022, 144, 11969-11974.	6.6	26
13	In situ inelastic neutron scattering of mixed CH4â€“CO2 hydrates. Fuel, 2022, 327, 125197.	3.4	1
14	The ICEMAN, a heterogeneous platform for analysis of neutron scattering data. Neutron News, 2021, 32, 15-16.	0.1	3
15	Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. Angewandte Chemie, 2021, 133, 6600-6606.	1.6	17
16	High Ammonia Adsorption in MFM-300 Materials: Dynamics and Charge Transfer in Hostâ€“Guest Binding. Journal of the American Chemical Society, 2021, 143, 3153-3161.	6.6	67
17	Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. Angewandte Chemie - International Edition, 2021, 60, 6526-6532.	7.2	62
18	Direct visualization of anionic electrons in an electride reveals inhomogeneities. Science Advances, 2021, 7, .	4.7	24

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19	Study of Anharmonicity in Zirconium Hydrides Using Inelastic Neutron Scattering and Ab-Initio Computer Modeling. Inorganics, 2021, 9, 29.	1.2	3
20	Exceptional Packing Density of Ammonia in a Dual-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 6586-6592.	6.6	37
21	On the Structural Transformation of Ni/BaH2 During a N2-H2 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
22	Uncovering design principles for amorphous-like heat conduction using two-channel lattice dynamics. Materials Today Physics, 2021, 18, 100344.	2.9	42
23	Applying Unconventional Spectroscopies to the Singleâ€Molecule Magnets, Co(PPh₃)₂X₂ (X=Cl, Br, I): Unveiling Magnetic Transitions and Spinâ€Phonon Coupling. Chemistry - A European Journal, 2021, 27, 11110-11125.	1.7	21
24	Neutron thermalization in nuclear graphite: A modern story of a classic moderator. Annals of Nuclear Energy, 2021, 161, 108437.	0.9	4
25	Neutron Insights into Sorption Enhanced Methanol Catalysis. Topics in Catalysis, 2021, 64, 638-643.	1.3	3
26	Purification of Propylene and Ethylene by a Robust Metalâ€“Organic Framework Mediated by Hostâ€“Guest Interactions. Angewandte Chemie - International Edition, 2021, 60, 15541-15547.	7.2	51
27	Atomically Dispersed Copper Sites in a Metalâ€“Organic Framework for Reduction of Nitrogen Dioxide. Journal of the American Chemical Society, 2021, 143, 10977-10985.	6.6	66
28	Low rotational barriers for the most dynamically active methyl groups in the proposed antiviral drugs for treatment of SARS-CoV-2, apilimod and tetrandrine. Chemical Physics Letters, 2021, 777, 138727.	1.2	9
29	Distilling nanoscale heterogeneity of amorphous silicon using tip-enhanced Raman spectroscopy (TERS) via multiresolution manifold learning. Nature Communications, 2021, 12, 578.	5.8	25
30	Polymer, Additives, and Processing Effects on N95 Filter Performance. ACS Applied Polymer Materials, 2021, 3, 1022-1031.	2.0	21
31	Catalytic Enhancement of Inductively Heated Fe₃O₄ Nanoparticles by Removal of Surface Ligands. ChemSusChem, 2021, 14, 1122-1130.	3.6	8
32	Pore Distortion in a Metalâ€“Organic Framework for Regulated Separation of Propane and Propylene. Journal of the American Chemical Society, 2021, 143, 19300-19305.	6.6	72
33	Unraveling the structural properties and dynamics of sulfonated solid acid carbon catalysts with neutron vibrational spectroscopy. Catalysis Today, 2020, 358, 387-393.	2.2	6
34	Quantitative production of butenes from biomass-derived Î³-valerolactone catalysed by hetero-atomic MFI zeolite. Nature Materials, 2020, 19, 86-93.	13.3	74
35	Quest for an Optimal Methane Hydrate Formation in the Pores of Hydrolytically Stable Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2020, 142, 13391-13397.	6.6	65
36	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

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37	Guest-Controlled Incommensurate Modulation in a Meta-Rigid Metalâ€“Organic Framework Material. Journal of the American Chemical Society, 2020, 142, 19189-19197.	6.6	24
38	Effect of Hydration on the Molecular Dynamics of Hydroxychloroquine Sulfate. ACS Omega, 2020, 5, 21231-21240.	1.6	8
39	Clathrate BaNi₂P₄: An Interplay of Heat and Charge Transport Due to Strong Hostâ€“Guest Interactions. Chemistry of Materials, 2020, 32, 7932-7940.	3.2	9
40	Phonon Spectroscopy in Antimony and Tellurium Oxides. Journal of Physical Chemistry A, 2020, 124, 7869-7880.	1.1	6
41	Hydration-Induced Disorder Lowers the Energy Barriers for Methyl Rotation in Drug Molecules. Journal of Physical Chemistry Letters, 2020, 11, 10256-10261.	2.1	7
42	Simulation of Inelastic Neutron Scattering Spectra Directly from Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2020, 16, 7702-7708.	2.3	14
43	Control of zeolite pore interior for chemoselective alkyne/olefin separations. Science, 2020, 368, 1002-1006.	6.0	179
44	Harnessing strong metalâ€“support interactions via a reverse route. Nature Communications, 2020, 11, 3042.	5.8	84
45	Inter-Kramers Transitions and Spinâ€“Phonon Couplings in a Lanthanide-Based Single-Molecule Magnet. Inorganic Chemistry, 2020, 59, 5218-5230.	1.9	25
46	Vacancy-driven variations in the phonon density of states of fast neutron irradiated nuclear graphite. Carbon, 2020, 168, 42-54.	5.4	13
47	Inelastic neutron scattering evidence for anomalous Hâ€“H distances in metal hydrides. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 4021-4026.	3.3	24
48	Discriminating the Role of Surface Hydride and Hydroxyl for Acetylene Semihydrogenation over Ceria through In Situ Neutron and Infrared Spectroscopy. ACS Catalysis, 2020, 10, 5278-5287.	5.5	70
49	Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. Journal of the American Chemical Society, 2020, 142, 7655-7667.	6.6	59
50	Substrate Binding Stiffens Aspartate Aminotransferase by Altering the Enzyme Picosecond Vibrational Dynamics. ACS Omega, 2020, 5, 18787-18797.	1.6	7
51	Studying Materials and Processes with VISION, VirtuES and ICEMAN ï¼•Modeling INS Data with DFT Methods. Hamon, 2020, 30, 154-159.	0.0	5
52	Neutron Spectroscopic and Thermochemical Characterization of Lithiumâ€“Aluminum-Layered Double Hydroxide Chloride: Implications for Lithium Recovery. Journal of Physical Chemistry C, 2019, 123, 20723-20729.	1.5	20
53	Vibrational properties of uranium fluorides. Physica B: Condensed Matter, 2019, 570, 194-205.	1.3	5
54	Large-Scale Phonon Calculations Using the Real-Space Multigrid Method. Journal of Chemical Theory and Computation, 2019, 15, 6859-6864.	2.3	9

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55	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. Journal of Physical Chemistry A, 2019, 123, 10079-10085.	1.1	1
56	Spectroscopic Studies of the Magnetic Excitation and Spinâ€Phonon Couplings in a Singleâ€Molecule Magnet. Chemistry - A European Journal, 2019, 25, 15846-15857.	1.7	22
57	Post-synthetic modulation of the charge distribution in a metalâ€“organic framework for optimal binding of carbon dioxide and sulfur dioxide. Chemical Science, 2019, 10, 1472-1482.	3.7	62
58	New insights into the breathing phenomenon in ZIF-4. Journal of Materials Chemistry A, 2019, 7, 14552-14558.	5.2	15
59	In situ 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
60	Elucidation of the Reaction Mechanism for High-Temperature Water Gas Shift over an Industrial-Type Copperâ€“Chromiumâ€“Iron Oxide Catalyst. Journal of the American Chemical Society, 2019, 141, 7990-7999.	6.6	60
61	Probing Magnetic Excitations in CoII Single-Molecule Magnets by Inelastic Neutron Scattering. European Journal of Inorganic Chemistry, 2019, 2019, 1055-1055.	1.0	0
62	Simulation of Inelastic Neutron Scattering Spectra Using OCLIMAX. Journal of Chemical Theory and Computation, 2019, 15, 1974-1982.	2.3	95
63	Capture of nitrogen dioxide and conversion to nitric acid in a porous metalâ€“organic framework. Nature Chemistry, 2019, 11, 1085-1090.	6.6	116
64	Crystal field splitting, local anisotropy, and low-energy excitations in the quantum magnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YbCl</mml:mi><mml:mn>3</mml:mn></mml:msub></mm Physical Review B, 2019, 100, .	1.1	26
65	Reversible coordinative binding and separation of sulfur dioxide in a robust metalâ€“organic framework with open copper sites. Nature Materials, 2019, 18, 1358-1365.	13.3	171
66	Probing Magnetic Excitations in Co^{II} Singleâ€Molecule Magnets by Inelastic Neutron Scattering. European Journal of Inorganic Chemistry, 2019, 2019, 1119-1127.	1.0	14
67	Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. ChemSusChem, 2019, 12, 5-5.	3.6	0
68	Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. ChemSusChem, 2019, 12, 93-103.	3.6	29
69	Direct observation of supramolecular binding of light hydrocarbons in vanadium(<scp>iii</scp>) and (<scp>iv</scp>) metalâ€“organic framework materials. Chemical Science, 2018, 9, 3401-3408.	3.7	22
70	Low-temperature vibrational dynamics of fused silica and binary silicate glasses. Physical Review B, 2018, 97, .	1.1	7
71	Chemical Bonding and Transport Properties in Clathrates-I with Cuâ€“Znâ€“P Frameworks. Chemistry of Materials, 2018, 30, 3419-3428.	3.2	21
72	Design of a facility for the in situ measurement of catalytic reaction by neutron scattering spectroscopy. Review of Scientific Instruments, 2018, 89, 014101.	0.6	6

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73	Comparison of two multifunctional catalysts [M/Nb₂O₅ (M = Pd, Pt)] for one-pot hydrodeoxygenation of lignin. Catalysis Science and Technology, 2018, 8, 6129-6136.	2.1	26
74	Thermal scattering law of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:msub><mml:mrow><mml:mfenced open="(") Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Annals of Nuclear Energy, 2018, 120, 778-787.	0.9	9
75	Spinâ€“phonon couplings in transition metal complexes with slow magnetic relaxation. Nature Communications, 2018, 9, 2572.	5.8	93
76	Effect of magnetic fields on the methyl rotation in a paramagnetic cobalt(<scp>ii</scp>) complex. Quasielastic neutron scattering studies. Physical Chemistry Chemical Physics, 2018, 20, 21119-21126.	1.3	10
77	Exposing Key Vibrational Contributions to Properties of Organic Molecular Solids with High Signal, Low Frequency Neutron Spectroscopy and Ab Initio Simulations. Crystal Growth and Design, 2018, 18, 4815-4821.	1.4	5
78	Reversible adsorption of nitrogen dioxide within a robust porous metalâ€“organic framework. Nature Materials, 2018, 17, 691-696.	13.3	162
79	Energy Storage: Latticeâ€Cell Orientation Disorder in Complex Spinel Oxides (Adv. Energy Mater. 4/2017). Advanced Energy Materials, 2017, 7, .	10.2	0
80	Modulating supramolecular binding of carbon dioxide in a redox-active porous metal-organic framework. Nature Communications, 2017, 8, 14212.	5.8	75
81	Understanding ZIFâ€8 Performance upon Gas Adsorption by Means of Inelastic Neutron Scattering. ChemistrySelect, 2017, 2, 2750-2753.	0.7	21
82	Confinement of Iodine Molecules into Triple-Helical Chains within Robust Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 16289-16296.	6.6	199
83	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
84	Understanding the breathing phenomena in nano-ZIF-7 upon gas adsorption. Journal of Materials Chemistry A, 2017, 5, 20938-20946.	5.2	50
85	The influence of the local structure on proton transport in a solid oxide proton conductor La_{0.8}Ba_{1.2}GaO_{3.9}. Journal of Materials Chemistry A, 2017, 5, 15507-15511.	5.2	9
86	Selective production of arenes via direct lignin upgrading over a niobium-based catalyst. Nature Communications, 2017, 8, 16104.	5.8	346
87	Direct Neutron Spectroscopy Observation of Cerium Hydride Species on a Cerium Oxide Catalyst. Journal of the American Chemical Society, 2017, 139, 9721-9727.	6.6	138
88	Latticeâ€Cell Orientation Disorder in Complex Spinel Oxides. Advanced Energy Materials, 2017, 7, 1601950.	10.2	21
89	Hydrogen adsorption on two catalysts for the ortho- to parahydrogen conversion: Cr-doped silica and ferric oxide gel. Physical Chemistry Chemical Physics, 2016, 18, 17281-17293.	1.3	34
90	Nanoconfinement Inside Molecular Metal Oxide Clusters: Dynamics and Modified Encapsulation Behavior. Chemistry - A European Journal, 2016, 22, 14073-14073.	1.7	3

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91	Selective Adsorption of Sulfur Dioxide in a Robust Metalâ€“Organic Framework Material. Advanced Materials, 2016, 28, 8705-8711.	11.1	214
92	Structures, Phase Transitions and Tricritical Behavior of the Hybrid Perovskite Methyl Ammonium Lead Iodide. Scientific Reports, 2016, 6, 35685.	1.6	440
93	Nanoconfinement Inside Molecular Metal Oxide Clusters: Dynamics and Modified Encapsulation Behavior. Chemistry - A European Journal, 2016, 22, 14131-14136.	1.7	6
94	A â€œHiddenâ€•Mesoscopic Feature Revealed By Electron Microscopy Could Facilitate Ion Transport In Solid Electrolytes. Microscopy and Microanalysis, 2016, 22, 1308-1309.	0.2	0
95	Mesoscopic Framework Enables Facile Ionic Transport in Solid Electrolytes for Li Batteries. Advanced Energy Materials, 2016, 6, 1600053.	10.2	46
96	Gate-opening effect in ZIF-8: the first experimental proof using inelastic neutron scattering. Chemical Communications, 2016, 52, 3639-3642.	2.2	106
97	X-ray and Neutron Scattering Study of the Formation of Coreâ€“Shell-Type Polyoxometalates. Journal of the American Chemical Society, 2016, 138, 2638-2643.	6.6	49
98	Inherent structure length in metallic glasses: simplicity behind complexity. Scientific Reports, 2015, 5, 12137.	1.6	23
99	Guidelines in predicting phase formation of high-entropy alloys. MRS Communications, 2014, 4, 57-62.	0.8	275
100	Temperature effects on atomic pair distribution functions of melts. Journal of Chemical Physics, 2014, 140, 064501.	1.2	41
101	On the origin of elastic strain limit of bulk metallic glasses. Applied Physics Letters, 2014, 104, .	1.5	20
102	Charge transfer and atomic-level pressure in metallic glasses. Applied Physics Letters, 2014, 104, 051903.	1.5	16
103	An integrated approach for structural characterization of complex solid state electrolytes: the case of lithium lanthanum titanate. Journal of Materials Chemistry A, 2014, 2, 2418.	5.2	22
104	Soft spots and their structural signature in a metallic glass. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 14052-14056.	3.3	348
105	Aluminum Alloying Effects on Lattice Types, Microstructures, and Mechanical Behavior of High-Entropy Alloys Systems. Jom, 2013, 65, 1848-1858.	0.9	250
106	First-Order Liquid-Liquid Phase Transition in Cerium. Physical Review Letters, 2013, 110, 125503.	2.9	111
107	Ab Initio Molecular Dynamics Simulation of the Amorphous Structure of Ca-Mg-Cu and Ca-Mg-Zn Alloys. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2013, 44, 1980-1989.	1.1	9
108	Correlating local structure with inhomogeneous elastic deformation in a metallic glass. Applied Physics Letters, 2012, 101, .	1.5	51

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109	Structural and dynamic analysis of adsorption of sulphur dioxide in a series of Zrâ€based metalâ€organic frameworks. Angewandte Chemie, 0, , .	1.6	0