Anibal J Ramirez-Cuesta

List of Publications by Year
in descending order

224 papers	10,139 citations	31976 53 h-index	42399 92 g-index
232 all docs	232 docs citations	232 times ranked	10496 citing authors

#	Article	IF	Citations
1	Supramolecular binding and separation of hydrocarbons within a functionalized porous metalâ€“organic framework. Nature Chemistry, 2015, 7, 121-129.	13.6	530
2	Selectivity and direct visualization of carbon dioxide and sulfur dioxide in a decorated porous host. Nature Chemistry, 2012, 4, 887-894.	13.6	466
3	Reversible Structural Transition in MIL-53 with Large Temperature Hysteresis. Journal of the American Chemical Society, 2008, 130, 11813-11818.	13.7	402
4	Selective production of arenes via direct lignin upgrading over a niobium-based catalyst. Nature Communications, 2017, 8, 16104.	12.8	346
5	aCLIMAX 4.0.1, The new version of the software for analyzing and interpreting INS spectra. Computer Physics Communications, 2004, 157, 226-238.	7.5	295
6	Selective Adsorption of Sulfur Dioxide in a Robust Metalâ€“Organic Framework Material. Advanced Materials, 2016, 28, 8705-8711.	21.0	214
7	An ultra-tunable platform for molecular engineering of high-performance crystalline porous materials. Nature Communications, 2016, 7, 13645.	12.8	205
8	Confinement of Iodine Molecules into Triple-Helical Chains within Robust Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2017, 139, 16289-16296.	13.7	199
9	l-Cysteine: Neutron spectroscopy, Raman, IR and ab initio study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 2474-2481.	3.9	198
10	Methane hydrate formation in confined nanospace can surpass nature. Nature Communications, 2015, 6, 6432.	12.8	187
11	Control of zeolite pore interior for chemoselective alkyne/olefin separations. Science, 2020, 368, 1002-1006.	12.6	179
12	Reversible coordinative binding and separation of sulfur dioxide in a robust metalâ€“organic framework with open copper sites. Nature Materials, 2019, 18, 1358-1365.	27.5	171
13	Reversible adsorption of nitrogen dioxide within a robust porous metalâ€“organic framework. Nature Materials, 2018, 17, 691-696.	27.5	162
14	Direct Neutron Spectroscopy Observation of Cerium Hydride Species on a Cerium Oxide Catalyst. Journal of the American Chemical Society, 2017, 139, 9721-9727.	13.7	138
15	Hydrogenation of 9-ethylcarbazole as a prototype of a liquid hydrogen carrier. International Journal of Hydrogen Energy, 2010, 35, 11609-11621.	7.1	135
16	Recent and future developments on TOSCA at ISIS. Journal of Physics: Conference Series, 2014, 554, 012003.	0.4	126
17	Hydrogen Spillover on Carbon-Supported Metal Catalysts Studied by Inelastic Neutron Scattering. Surface Vibrational States and Hydrogen Riding Modes. Journal of Physical Chemistry B, 2003, 107, 6838-6845.	2.6	118
18	Capture of nitrogen dioxide and conversion to nitric acid in a porous metalâ€“organic framework. Nature Chemistry, 2019, 11, 1085-1090.	13.6	116

#	Article	IF	Citations
19	Gate-opening effect in ZIF-8: the first experimental proof using inelastic neutron scattering. Chemical Communications, 2016, 52, 3639-3642.	4.1	106
20	Capture of heavy hydrogen isotopes in a metal-organic framework with active Cu(I) sites. Nature Communications, 2017, 8, 14496.	12.8	98
21	Study of Catalytic Sites on Ruthenium For Hydrogenation of N-ethylcarbazole: Implications of Hydrogen Storage via Reversible Catalytic Hydrogenation. Journal of Physical Chemistry C, 2010, 114, 9720-9730.	3.1	97
22	Simulation of Inelastic Neutron Scattering Spectra Using OCLIMAX. Journal of Chemical Theory and Computation, 2019, 15, 1974-1982.	5.3	95
23	Spinâ€“phonon couplings in transition metal complexes with slow magnetic relaxation. Nature Communications, 2018, 9, 2572.	12.8	93
24	Integration of mesopores and crystal defects in metal-organic frameworks via templated electrosynthesis. Nature Communications, 2019, 10, 4466.	12.8	90
25	Negative Thermal Expansion in LnCo(CN)₆ (Ln=La, Pr, Sm, Ho, Lu, Y): Mechanisms and Compositional Trends. Angewandte Chemie - International Edition, 2013, 52, 5266-5270.	13.8	88
26	Local Vibrational Mechanism for Negative Thermal Expansion: A Combined Neutron Scattering and Firstâ€Principles Study. Angewandte Chemie - International Edition, 2010, 49, 585-588.	13.8	87
27	Quantum rattling of molecular hydrogen in clathrate hydrate nanocavities. Physical Review B, 2007, 76, .	3.2	82
28	Evidence for CO2 reactive adsorption on nanoporous S- and N-doped carbon at ambient conditions. Carbon, 2016, 96, 856-863.	10.3	79
29	Hydrogen adsorption in the metalâ€“organic frameworks Fe2(dobdc) and Fe2(O2)(dobdc). Dalton Transactions, 2012, 41, 4180.	3.3	78
30	Direct photo-oxidation of methane to methanol over a mono-iron hydroxyl site. Nature Materials, 2022, 21, 932-938.	27.5	77
31	Modulating supramolecular binding of carbon dioxide in a redox-active porous metal-organic framework. Nature Communications, 2017, 8, 14212.	12.8	75
32	Quantitative production of butenes from biomass-derived Î³-valerolactone catalysed by hetero-atomic MFI zeolite. Nature Materials, 2020, 19, 86-93.	27.5	74
33	Some New Insights into the Sensing Mechanism of Palladium Promoted Tin (IV) Oxide Sensor. Journal of Physical Chemistry B, 2001, 105, 5737-5742.	2.6	73
34	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.	11.2	70
35	Dynamical properties and temperature induced molecular disordering of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiBH</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiBD</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 78, .	3.2	69
36	Hydrogenâ€“deuterium exchange experiments to probe the decomposition reaction of sodium alanate. Physical Chemistry Chemical Physics, 2008, 10, 4045.	2.8	67

#	Article	IF	Citations
37	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.	13.7	67
38	Atomically Dispersed Copper Sites in a Metalâ€“Organic Framework for Reduction of Nitrogen Dioxide. Journal of the American Chemical Society, 2021, 143, 10977-10985.	13.7	66
39	A unique Co@CoO catalyst for hydrogenolysis of biomass-derived 5-hydroxymethylfurfural to 2,5-dimethylfuran. Nature Communications, 2022, 13, .	12.8	66
40	Structural information on ball milled magnesium hydride from vibrational spectroscopy and ab-initio calculations. Journal of Alloys and Compounds, 2005, 393, 1-4.	5.5	65
41	Hydrogen adsorption strength and sites in the metal organic framework MOF5: Comparing experiment and model calculations. Chemical Physics, 2008, 351, 72-76.	1.9	65
42	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.	13.7	65
43	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.	7.4	62
44	Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. Angewandte Chemie - International Edition, 2021, 60, 6526-6532.	13.8	62
45	The rotational and translational dynamics of molecular hydrogen physisorbed in activated carbon: A direct probe of microporosity and hydrogen storage performance. Carbon, 2006, 44, 2724-2738.	10.3	61
46	Refinement of pore size at sub-angstrom precision in robust metalâ€“organic frameworks for separation of xylenes. Nature Communications, 2020, 11, 4280.	12.8	61
47	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.	13.7	60
48	Scrutinizing negative thermal expansion in MOF-5 by scattering techniques and ab initio calculations. Dalton Transactions, 2013, 42, 1996-2007.	3.3	59
49	Nature of Reactive Hydrogen for Ammonia Synthesis over a Ru/C12A7 Electride Catalyst. Journal of the American Chemical Society, 2020, 142, 7655-7667.	13.7	59
50	Molecular Aluminum Hydrides Identified by Inelastic Neutron Scattering during H2Regeneration of Catalyst-Doped NaAlH4. Journal of Physical Chemistry B, 2006, 110, 711-715.	2.6	58
51	Direct Evidence for Solid-like Hydrogen in a Nanoporous Carbon Hydrogen Storage Material at Supercritical Temperatures. ACS Nano, 2015, 9, 8249-8254.	14.6	57
52	Enhancement of Proton Conductivity in Nonporous Metalâ€“Organic Frameworks: The Role of Framework Proton Density and Humidity. Chemistry of Materials, 2018, 30, 7593-7602.	6.7	55
53	A combined neutron scattering and simulation study on bioprotectant systems. Chemical Physics, 2005, 317, 258-266.	1.9	52
54	Identifying Atomic Scale Structure in Undoped/Doped Semicrystalline P3HT Using Inelastic Neutron Scattering. Macromolecules, 2017, 50, 2424-2435.	4.8	52

#	Article	IF	Citations
55	Hydrogen in the Metalâ"Organic Framework Cr MIL-53. Journal of Physical Chemistry C, 2010, 114, 10648-10655.	3.1	51
56	Hydrogen Dynamics in Nanoconfined Lithiumborohydride. Journal of Physical Chemistry C, 2013, 117, 3789-3798.	3.1	51
57	Purification of Propylene and Ethylene by a Robust Metalâ€"Organic Framework Mediated by Hostâ€"Guest Interactions. Angewandte Chemie - International Edition, 2021, 60, 15541-15547.	13.8	51
58	In situ inelastic neutron scattering studies of the rotational and translational dynamics of molecular hydrogen adsorbed in single-wall carbon nanotubes (SWNTs). Carbon, 2005, 43, 895-906.	10.3	50
59	LDA or GGA? A combined experimental inelastic neutron scattering and ab initio lattice dynamics study of alkali metal hydrides. Chemical Physics, 2005, 317, 119-129.	1.9	50
60	Neutron scattering and hydrogen storage. Materials Today, 2009, 12, 54-61.	14.2	50
61	Understanding the breathing phenomena in nano-ZIF-7 upon gas adsorption. Journal of Materials Chemistry A, 2017, 5, 20938-20946.	10.3	50
62	Characteristic features of water dynamics in restricted geometries investigated with quasi-elastic neutron scattering. Chemical Physics, 2016, 465-466, 1-8.	1.9	49
63	X-ray and Neutron Scattering Study of the Formation of Coreâ€"Shell-Type Polyoxometalates. Journal of the American Chemical Society, 2016, 138, 2638-2643.	13.7	49
64	Pore with gate: modulating hydrogen storage in metal-organic framework materials via cation exchange. Faraday Discussions, 2011, 151, 19.	3.2	48
65	Inelastic Incoherent Neutron Scattering Measurements of Intact Cells and Tissues and Detection of Interfacial Water. Journal of the American Chemical Society, 2004, 126, 4682-4688.	13.7	47
66	Hostâ€"guest selectivity in a series of isoreticular metalâ€"organic frameworks: observation of acetylene-to-alkyne and carbon dioxide-to-amide interactions. Chemical Science, 2019, 10, 1098-1106.	7.4	47
67	Inelastic neutron scattering study on bioprotectant systems. Journal of the Royal Society Interface, 2005, 2, 527-532.	3.4	45
68	The Vibrational Spectrum and Ultimate Modulus of Polyethylene. Macromolecules, 2006, 39, 2683-2690.	4.8	44
69	Inelastic Neutron Scattering and Raman Spectroscopies and Periodic DFT Studies of Rb2PtH6and Rb2PtD6. Journal of the American Chemical Society, 2003, 125, 11656-11661.	13.7	43
70	The vibrational spectrum of magnesium hydride from inelastic neutron scattering and density functional theory. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2004, 108, 38-41.	3.5	41
71	Direct Observation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Binding to a Metal Oxide Surface. Physical Review Letters, 2008, 101, 165302.	7.8	39
72	Pure Monte Carlo Simulation of Model Heterogeneous Substrates:â€‰ From Random Surfaces to Many-Site Correlations. Langmuir, 1997, 13, 1064-1072.	3.5	38

#	Article	IF	Citations
73	Evidence for hydrogen transport in deuterated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiBH</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> low-temperature Raman-scattering measurements and first-principles calculations. Physical Review B, 2009, 80, .	3.2	37
74	Exceptional Packing Density of Ammonia in a Dual-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2021, 143, 6586-6592.	13.7	37
75	Hydrogen adsorption in a copper ZSM5 zeoliteAn inelastic neutron scattering study. Catalysis Today, 2007, 120, 368-373.	4.4	35
76	Impurity Gas Analysis of the Decomposition of Complex Hydrides. Journal of Physical Chemistry C, 2011, 115, 17220-17226.	3.1	35
77	In consideration of precursor states, spillover and Boudartâ€™s â€˜collection zoneâ€™ and of their role in catalytic processes. Journal of Molecular Catalysis A, 2000, 163, 221-232.	4.8	34
78	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.	2.8	34
79	Dihydrogen in cation-substituted zeolites Xâ€”an inelastic neutron scattering study. Journal of Materials Chemistry, 2007, 17, 2533-2539.	6.7	33
80	Vibrational Dynamics of LiBH₄ by Infrared Pumpâ€’Probe and 2D Spectroscopy. Journal of Physical Chemistry A, 2009, 113, 12838-12846.	2.5	33
81	The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite. Physics and Chemistry of Minerals, 2010, 37, 571-579.	0.8	33
82	Inelastic neutron scattering in spectroscopic studies of hydrogen on carbon-supported catalysts-experimental spectra and computed spectra of model systems. Journal of Molecular Structure, 2003, 651-653, 781-785.	3.6	32
83	Inelastic neutron scattering from hydrogen clathrate hydrates. Journal of Physics Condensed Matter, 2008, 20, 104242.	1.8	32
84	Optimal Binding of Acetylene to a Nitro-Decorated Metalâ€“Organic Framework. Journal of the American Chemical Society, 2018, 140, 16006-16009.	13.7	31
85	Neutron Instruments for Research in Coordination Chemistry. European Journal of Inorganic Chemistry, 2019, 2019, 1065-1089.	2.0	29
86	Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. ChemSusChem, 2019, 12, 93-103.	6.8	29
87	High Resolution Raman and Neutron Investigation of Mg(BH₄)₂ in an Extensive Temperature Range. Journal of Physical Chemistry A, 2010, 114, 2788-2793.	2.5	28
88	Structure of Spontaneously Formed Solid-Electrolyte Interphase on Lithiated Graphite Determined Using Small-Angle Neutron Scattering. Journal of Physical Chemistry C, 2015, 119, 9816-9823.	3.1	28
89	Observation of binding of carbon dioxide to nitro-decorated metalâ€“organic frameworks. Chemical Science, 2020, 11, 5339-5346.	7.4	28
90	Hydrogen self-dynamics in orthorhombic alkaline earth hydrides through incoherent inelastic neutron scattering. Journal of Alloys and Compounds, 2007, 427, 18-24.	5.5	27

#	Article	IF	Citations
91	Structure and Dynamics of Octamethyl-POSS Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 5579-5592.	3.1	27
92	Comparison of two multifunctional catalysts [M/Nb₂O₅ (M = Pd, Pt)] for one-pot hydrodeoxygenation of lignin. Catalysis Science and Technology, 2018, 8, 6129-6136.	4.1	26
93	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.	13.7	26
94	Hydrogen site occupancies in single-walled carbon nanotubes studied by inelastic neutron scattering. Journal of Physics Condensed Matter, 2004, 16, L73-L78.	1.8	25
95	Mobility and dynamics in the complex hydrides LiAlH4 and LiBH4. Faraday Discussions, 2011, 151, 213.	3.2	25
96	Inter-Kramers Transitions and Spinâ€“Phonon Couplings in a Lanthanide-Based Single-Molecule Magnet. Inorganic Chemistry, 2020, 59, 5218-5230.	4.0	25
97	Infrared, Raman, and Inelastic Neutron Scattering Spectra of Dodecahedrane:Â anIhMolecule inThSite Symmetry. Journal of Physical Chemistry A, 2005, 109, 3418-3424.	2.5	24
98	Experimental evidence of librational vibrations determining the stability of calcium borohydride. Physical Review B, 2011, 83, .	3.2	24
99	Interaction of methanol with the flexible metal-organic framework MIL-53(Fe) observed by inelastic neutron scattering. Chemical Physics, 2013, 427, 30-37.	1.9	24
100	Penicillin's catalytic mechanism revealed by inelastic neutrons and quantum chemical theory. Physical Chemistry Chemical Physics, 2013, 15, 20447-20455.	2.8	24
101	Guest-Controlled Incommensurate Modulation in a Meta-Rigid Metalâ€“Organic Framework Material. Journal of the American Chemical Society, 2020, 142, 19189-19197.	13.7	24
102	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.	7.1	24
103	Direct Observation of Ammonia Storage in UiO-66 Incorporating Cu(II) Binding Sites. Journal of the American Chemical Society, 2022, 144, 8624-8632.	13.7	24
104	Structure and spectroscopy of hydrogen adsorbed in a nickel metalâ€“organic framework. Chemical Physics, 2013, 427, 3-8.	1.9	23
105	Control of zeolite microenvironment for propene synthesis from methanol. Nature Communications, 2021, 12, 822.	12.8	23
106	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.	7.4	22
107	Vibrational spectroscopy with neutrons: Recent developments. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 190, 518-523.	3.9	22
108	Spectroscopic Studies of the Magnetic Excitation and Spinâ€Phonon Couplings in a Singleâ€Molecule Magnet. Chemistry - A European Journal, 2019, 25, 15846-15857.	3.3	22

#	Article	IF	Citations
109	Simple analytical model for fitting QENS data from liquids. Physica B: Condensed Matter, 2019, 566, 50-54.	2.7	22
110	Hydrogen dynamics in heavy alkali metal hydrides obtained through inelastic neutron scattering. Journal of Physics Condensed Matter, 2004, 16, 5731-5743.	1.8	21
111	Neutron Vibrational Spectroscopy Gives New Insights into the Structure of Poly(p-phenylene) Tj ETQq1 1 0.784314 rgBT /Overlock 10	13.7	21
112	Properties of immobile hydrogen confined in microporous carbon. Carbon, 2017, 117, 383-392.	10.3	21
113	Understanding ZIFâ€8 Performance upon Gas Adsorption by Means of Inelastic Neutron Scattering. ChemistrySelect, 2017, 2, 2750-2753.	1.5	21
114	Chemical Bonding and Transport Properties in Clathrates-I with Cuâ€“Znâ€“P Frameworks. Chemistry of Materials, 2018, 30, 3419-3428.	6.7	21
115	Wide-angle diamond cell for neutron scattering. High Pressure Research, 2017, 37, 495-506.	1.2	20
116	Diborane release and structure distortion in borohydrides. Dalton Transactions, 2013, 42, 719-725.	3.3	19
117	The Role of Ti in Alanates and Borohydrides: Catalysis and Metathesis. Journal of Physical Chemistry C, 2014, 118, 77-84.	3.1	19
118	Simulation of benzene formation from acetylene on palladium and oxygen-covered palladium surfaces. Surface Science, 1995, 340, 109-118.	1.9	18
119	An inelastic neutron scattering study of the interaction of dihydrogen with the cobalt site of a cobalt aluminophosphate catalyst. Journal of Molecular Catalysis A, 2001, 167, 217-224.	4.8	18
120	Efficient Separation of Acetylene and Carbon Dioxide in a Decorated Zeolite. Angewandte Chemie, 2021, 133, 6600-6606.	2.0	17
121	Phonon density of states in different clathrate hydrates measured by inelastic neutron scattering. Journal of Physics: Conference Series, 2012, 340, 012051.	0.4	16
122	The characterisation of commercial 2D carbons: graphene, graphene oxide and reduced graphene oxide. Materials Advances, 2022, 3, 2810-2826.	5.4	16
123	Structure and Dynamics of Maleic Anhydride. Journal of Physical Chemistry A, 2001, 105, 3064-3070.	2.5	15
124	Hydrogen Dynamics in Lightweight Tetrahydroborates. Zeitschrift Fur Physikalische Chemie, 2010, 224, 263-278.	2.8	15
125	The Combined Inelastic Neutron Scattering (INS) and Solid-State DFT Study of Hydrogen-Atoms Dynamics in Kaolinite-dimethylsulfoxide Intercalate. Clays and Clay Minerals, 2010, 58, 52-61.	1.3	15
126	Low energy structural dynamics and constrained libration of Li(NH₃)₄, the lowest melting point metal. Chemical Communications, 2014, 50, 10778-10781.	4.1	15

#	Article	IF	Citations
127	New insights into the breathing phenomenon in ZIF-4. Journal of Materials Chemistry A, 2019, 7, 14552-14558.	10.3	15
128	STM investigation and Monte-Carlo modelling of spillover in a supported metal catalyst. Journal of Molecular Catalysis A, 2001, 167, 171-179.	4.8	14
129	Extraction of the density of phonon states in LiH and NaH. Physica B: Condensed Matter, 2004, 350, E983-E986.	2.7	14
130	Dihydrogen in zeolite CaXâ€"An inelastic neutron scattering study. Journal of Alloys and Compounds, 2007, 446-447, 393-396.	5.5	14
131	Changes in vibrational modes of water and bioprotectants in solution. Biophysical Chemistry, 2007, 125, 138-142.	2.8	14
132	Neutron Compton scattering investigation of sodium hydride: From bulk material to encapsulated nanoparticulates in amorphous silica gel. Journal of Chemical Physics, 2011, 134, 114511.	3.0	14
133	High-resolution inelastic neutron scattering and neutron powder diffraction study of the adsorption of dihydrogen by the Cu(II) metalâ€"organic framework material HKUST-1. Chemical Physics, 2013, 427, 9-17.	1.9	14
134	Rapid Diffusion and Nanosegregation of Hydrogen in Magnesium Alloys from Exposure to Water. ACS Applied Materials & Interfaces, 2017, 9, 38125-38134.	8.0	14
135	Probing Magnetic Excitations in Co^{II} Singleâ€Molecule Magnets by Inelastic Neutron Scattering. European Journal of Inorganic Chemistry, 2019, 2019, 1119-1127.	2.0	14
136	Calculation of the Thermal Neutron Scattering Cross-Section of Solids Using OCLIMAX. Journal of Chemical Theory and Computation, 2020, 16, 5212-5217.	5.3	14
137	Simulation of Inelastic Neutron Scattering Spectra Directly from Molecular Dynamics Trajectories. Journal of Chemical Theory and Computation, 2020, 16, 7702-7708.	5.3	14
138	Direct observation of molecular hydrogen binding to magnesium oxide (100) surfaces. Physica B: Condensed Matter, 2006, 385-386, 144-146.	2.7	13
139	Hydrogen-storage materials dispersed into nanoporous substrates studied through incoherent inelastic neutron scattering. Journal of Alloys and Compounds, 2012, 538, 91-99.	5.5	13
140	Local probes show that framework modification in zeolites occurs on ammonium exchange without calcination. Journal of Materials Chemistry A, 2013, 1, 7415.	10.3	13
141	Raman scattering study of Î±-MgH2 and Î³-MgH2. Solid State Communications, 2013, 154, 77-80.	1.9	13
142	Alternative view of oxygen reduction on porous carbon electrocatalysts: The substance of complex oxygen-surface interactions. IScience, 2021, 24, 102216.	4.1	13
143	Concentration dependence of vibrational properties of bioprotectant/water mixtures by inelastic neutron scattering. Journal of the Royal Society Interface, 2007, 4, 167-173.	3.4	12
144	Coupled Multimodal Dynamics of Hydrogen-Containing Ion Networks in Water-Deficient, Sodium Hydroxide-Aluminate Solutions. Journal of Physical Chemistry B, 2018, 122, 12097-12106.	2.6	12

#	Article	IF	Citations
145	Structural and Dynamic Analysis of Sulphur Dioxide Adsorption in a Series of Zirconiumâ€Based Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2022, 61, .	13.8	12
146	On Modeling, Simulation and Statistical Properties of Realistic Three Dimensional Porous Networks. Journal of Porous Materials, 2001, 8, 61-76.	2.6	11
147	A combined experimental inelastic neutron scattering, Raman and ab initio lattice dynamics study of Î±-lithium amidoborane. Physical Chemistry Chemical Physics, 2011, 13, 12249.	2.8	11
148	Evidence of Intermediate Hydrogen States in the Formation of a Complex Hydride. Inorganic Chemistry, 2018, 57, 867-872.	4.0	11
149	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.	2.8	11
150	Purification of Propylene and Ethylene by a Robust Metalâ€“Organic Framework Mediated by Hostâ€“Guest Interactions. Angewandte Chemie, 2021, 133, 15669-15675.	2.0	11
151	Templateâ€“framework interactions in chiral AlPOs. Journal of the Chemical Society, Faraday Transactions, 1998, 94, 2249-2255.	1.7	10
152	Experimental Observations of Waterâ^'Framework Interactions in a Hydrated Microporous Aluminum Phosphate. Journal of Physical Chemistry B, 2005, 109, 4464-4469.	2.6	10
153	Raman and Inelastic Neutron Scattering Study on a Melt-Infiltrated Composite of NaAlH₄ and Nanoporous Carbon. Journal of Physical Chemistry A, 2011, 115, 7503-7510.	2.5	10
154	Understanding Vibrational Anharmonicity and Phonon Dispersion in Solid Ammonia Borane. Journal of Physical Chemistry C, 2012, 116, 5926-5931.	3.1	10
155	The use of direct geometry spectrometers in molecular spectroscopy. Journal of Physics: Conference Series, 2014, 554, 012004.	0.4	10
156	Inelastic neutron scattering study of binding of para-hydrogen in an ultra-microporous metalâ€“organic framework. Chemical Physics, 2014, 428, 111-116.	1.9	10
157	Hydrogen release reactions of Al-based complex hydrides enhanced by vibrational dynamics and valences of metal cations. Chemical Communications, 2016, 52, 11807-11810.	4.1	10
158	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.	2.8	10
159	Probing the internal structure of a cobalt aluminophosphate catalyst. An inelastic neutron scattering study of sorbed dihydrogen molecules behaving as one- and two-dimensional rotors. Chemical Communications, 2000, , 1257-1258.	4.1	9
160	Neutron Compton scattering as a molecular characterization technique: A study onNaHF2. Physical Review B, 2007, 76, .	3.2	9
161	Inelastic neutron scattering and DFT study of 1,6-anhydro-Î²-d-glucopyranose (levoglucosan). Journal of Molecular Structure, 2008, 874, 108-120.	3.6	9
162	Large-Scale Phonon Calculations Using the Real-Space Multigrid Method. Journal of Chemical Theory and Computation, 2019, 15, 6859-6864.	5.3	9

#	Article	IF	Citations
163	Clathrate BaNi₂P₄: An Interplay of Heat and Charge Transport Due to Strong Hostâ€“Guest Interactions. Chemistry of Materials, 2020, 32, 7932-7940.	6.7	9
164	Volatile Hydrogen Intermediates of CO2 Methanation by Inelastic Neutron Scattering. Catalysts, 2020, 10, 433.	3.5	9
165	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.	2.6	9
166	Dynamics of water and template molecules in the interlayer space of a layered aluminophosphate. Experimental inelastic neutron scattering spectra and molecular dynamics simulated spectra. Physical Chemistry Chemical Physics, 1999, 1, 5711-5715.	2.8	8
167	Textural Characterisation of Iron-Promoted Raney Nickel Catalysts Synthesised by Mechanical Alloying. Adsorption Science and Technology, 2001, 19, 871-885.	3.2	8
168	On the effect of thermal treatment and hydrogen vibrational dynamics in sodium alanates: An inelastic neutron scattering study. Journal of Alloys and Compounds, 2012, 523, 108-113.	5.5	8
169	Understanding compositionâ€“property relationships in Tiâ€“Crâ€“Vâ€“Mo alloys for optimisation of hydrogen storage in pressurised tanks. Physical Chemistry Chemical Physics, 2014, 16, 16563-16572.	2.8	8
170	Heterolytic Scission of Hydrogen Within a Crystalline Frustrated Lewis Pair. Inorganic Chemistry, 2020, 59, 15295-15301.	4.0	8
171	Effect of Hydration on the Molecular Dynamics of Hydroxychloroquine Sulfate. ACS Omega, 2020, 5, 21231-21240.	3.5	8
172	Lattice vibrations of para-hydrogen impurities in a solid deuterium matrix: An inelastic neutron scattering study. Physical Review B, 2007, 76, .	3.2	7
173	Kosmotrope character of maltose in water mixtures. Journal of Molecular Structure, 2007, 830, 167-170.	3.6	7
174	Formation of Crystalline Sodium Hydride Nanoparticles Encapsulated Within an Amorphous Framework. Journal of Cluster Science, 2010, 21, 543-549.	3.3	7
175	Vibrational Properties of CaAlH₅ and Î±-AlH₃ with Different AlH₆ Networks Studied by Inelastic Neutron Scattering. Inorganic Chemistry, 2011, 50, 8007-8011.	4.0	7
176	Hydrogen gas sample environment for TOSCA. Journal of Physics: Conference Series, 2014, 554, 012006.	0.4	7
177	Quantum Dynamics of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">H</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml Trapped within Organic Clathrate Cages. Physical Review Letters, 2018, 120, 120402.	7.8	7
178	Hydration-Induced Disorder Lowers the Energy Barriers for Methyl Rotation in Drug Molecules. Journal of Physical Chemistry Letters, 2020, 11, 10256-10261.	4.6	7
179	The structure and vibrational spectroscopy of cryolite, Na₃AlF₆. RSC Advances, 2020, 10, 25856-25863.	3.6	7
180	Kinetics and energetics of adsorption for the CO/K/Ni(110) system. Surface Science, 1992, 275, L636-L639.	1.9	6

#	Article	IF	Citations
181	Nonmonotonical behavior in correlated site-bond percolation. Physical Review E, 1998, 57, 735-738.	2.1	6
182	Origin of the large anharmonicity in the phonon modes of LiBH4. Chemical Physics, 2013, 427, 22-29.	1.9	6
183	The free-energy barrier to hydride transfer across a dipalladium complex. Faraday Discussions, 2015, 177, 99-109.	3.2	6
184	Nanoconfinement Inside Molecular Metal Oxide Clusters: Dynamics and Modified Encapsulation Behavior. Chemistry - A European Journal, 2016, 22, 14131-14136.	3.3	6
185	Phonon Spectroscopy in Antimony and Tellurium Oxides. Journal of Physical Chemistry A, 2020, 124, 7869-7880.	2.5	6
186	Hydrogen in tungsten trioxide by membrane photoemission and density functional theory modeling. Physical Review B, 2021, 103, .	3.2	6
187	Thermal neutron scattering measurements and modeling of yttrium-hydrides for high temperature moderator applications. Annals of Nuclear Energy, 2021, 157, 108224.	1.8	6
188	High capacity ammonia adsorption in a robust metalâ€“organic framework mediated by reversible hostâ€“guest interactions. Chemical Communications, 2022, 58, 5753-5756.	4.1	6
189	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.	3.0	5
190	Hydrogenâ€Release Reaction of a Complex Transition Metal Hydride with Covalently Bound Hydrogen and Hydride Ions. ChemPhysChem, 2019, 20, 1392-1397.	2.1	5
191	Neutron vibrational spectroscopic evidence for short Hâ˜™â˜™H contacts in the RNiInH1.4; 1.6 (R = Ce, La) metal hydride. Journal of Alloys and Compounds, 2022, 894, 162381.	5.5	5
192	Studying Materials and Processes with VISION, VirtuES and ICEMAN ï¼•Modeling INS Data with DFT Methods. Hamon, 2020, 30, 154-159.	0.0	5
193	Dynamics of water molecules in a templated aluminophosphate: molecular dynamics simulation of inelastic neutron scattering spectra. Chemical Communications, 1998, , 2653-2654.	4.1	4
194	Lattice dynamics and molecular rotations in solid hydrogen deuteride: Inelastic neutron scattering study. Physical Review B, 2009, 79, .	3.2	4
195	Inelastic neutron scattering of Na-zeolite A with in situ ammoniation: an examination of initial coordination. Physical Chemistry Chemical Physics, 2010, 12, 9661.	2.8	4
196	Proton vibrational dynamics in lithium imide investigated through incoherent inelastic and Compton neutron scattering. Journal of Chemical Physics, 2012, 137, 204309.	3.0	4
197	Desorption of benzene from Pd(111): a simulation study. Journal of Physics Condensed Matter, 1993, 5, A239-A240.	1.8	3
198	Neutron scattering measurements of intact cells show changes after heat shock consistent with an increase in molecular crowding. Journal of Molecular Recognition, 2004, 17, 505-511.	2.1	3

#	Article	IF	Citations
199	Catalyst-free synthesis of sodium amide nanoparticles encapsulated in silica gel. Chemical Physics, 2013, 427, 61-65.	1.9	3
200	Nanoconfinement Inside Molecular Metal Oxide Clusters: Dynamics and Modified Encapsulation Behavior. Chemistry - A European Journal, 2016, 22, 14073-14073.	3.3	3
201	The ICEMAN, a heterogeneous platform for analysis of neutron scattering data. Neutron News, 2021, 32, 15-16.	0.2	3
202	Study of Anharmonicity in Zirconium Hydrides Using Inelastic Neutron Scattering and Ab-Initio Computer Modeling. Inorganics, 2021, 9, 29.	2.7	3
203	Neutron Insights into Sorption Enhanced Methanol Catalysis. Topics in Catalysis, 2021, 64, 638-643.	2.8	3
204	Simulation and study of the percolation effect in the magnetic susceptibility of high-temperature superconducting composites. Physical Review B, 2000, 61, 9176-9180.	3.2	2
205	Breakdown of the Gaussian approximation in semi-quantum liquids. Physica B: Condensed Matter, 2004, 350, E1083-E1086.	2.7	2
206	Microscopic self dynamics in liquid hydrogen and in its mixtures with deuterium and neon: a neutron scattering study. Journal of Low Temperature Physics, 2005, 138, 887-892.	1.4	2
207	Chemical spectroscopy using neutrons. Chemical Physics, 2013, 427, 1-2.	1.9	2
208	Future directions for spectroscopy at the Spallation Neutron Source. Physica B: Condensed Matter, 2019, 564, 5-9.	2.7	2
209	Catalytic activity of a Langmuir-Hinshelwood reaction with surface reconstruction. Journal of Physics Condensed Matter, 1993, 5, A235-A236.	1.8	1
210	Statistics of reactive ensembles on regular surfaces: application to benzene from acetylene on Pd(111). Journal of Physics Condensed Matter, 1996, 8, 1359-1366.	1.8	1
211	Inelastic neutron scattering and raman light scattering from hydrogen-filled clathrates hydrates. Journal of Physics: Conference Series, 2008, 121, 042018.	0.4	1
212	Cryogenic sample environment on TOSCA. Journal of Physics: Conference Series, 2014, 554, 012007.	0.4	1
213	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.	2.5	1
214	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.	0.2	1
215	Vibrational Spectroscopy of Hexahalo Complexes. Inorganic Chemistry, 2022, , .	4.0	1
216	Acetylene to benzene conversion on Pd(111). A simulation study. AIP Conference Proceedings, 1996, , .	0.4	0

#	Article	IF	Citations
217	Molecular dynamics simulation of inelastic neutron scattering spectra of librational modes of water molecules in a layered aluminophosphate. , 1999, , .		0
218	A statistical model for flash thermal desorption of carbon dioxide from polycrystalline molybdenum. Journal of Molecular Catalysis A, 2001, 167, 157-163.	4.8	0
219	Inelastic Neutron Scattering and Raman Spectroscopies and Periodic DFT Studies of Rb2PtH6 and Rb2PtD6.. ChemInform, 2003, 34, no.	0.0	0
220	Molecular Vibrations as the Origin of Solid State Effects in Borohydrides. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	0
221	Time and Frequency Resolved Hydrogen Dynamics in deuterated LiBH₄. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	0
222	Probing Magnetic Excitations in CoII Single-Molecule Magnets by Inelastic Neutron Scattering. European Journal of Inorganic Chemistry, 2019, 2019, 1055-1055.	2.0	0
223	Neutron Scattering Investigations of Hydride Species in Heterogeneous Catalysis. ChemSusChem, 2019, 12, 5-5.	6.8	0
224	Structural and dynamic analysis of adsorption of sulphur dioxide in a series of Zrâ€based metalâ€organic frameworks. Angewandte Chemie, 0, , .	2.0	0