Chris J Pickard

List of Publications by Year
in descending order

302 papers	45,762 citations	5558 82 h-index	1851 209 g-index
309 all docs	309 docs citations	309 times ranked	27524 citing authors

#	Article	IF	Citations
1	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
2	First-principles simulation: ideas, illustrations and the CASTEP code. Journal of Physics Condensed Matter, 2002, 14, 2717-2744.	0.7	8,382
3	Electronic structure, properties, and phase stability of inorganic crystals: A pseudopotential plane-wave study. International Journal of Quantum Chemistry, 2000, 77, 895-910.	1.0	1,566
4	All-electron magnetic response with pseudopotentials: NMR chemical shifts. Physical Review B, 2001, 63, .	1.1	1,502
5	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
6	Population analysis of plane-wave electronic structure calculations of bulk materials. Physical Review B, 1996, 54, 16317-16320.	1.1	1,075
7	Ab initiorandom structure searching. Journal of Physics Condensed Matter, 2011, 23, 053201.	0.7	832
8	Calculation of NMR chemical shifts for extended systems using ultrasoft pseudopotentials. Physical Review B, 2007, 76, .	1.1	794
9	Structure of phase III of solid hydrogen. Nature Physics, 2007, 3, 473-476.	6.5	593
10	Hydrogen Clathrate Structures in Rare Earth Hydrides at High Pressures: Possible Route to Room-Temperature Superconductivity. Physical Review Letters, 2017, 119, 107001.	2.9	591
11	High-Pressure Phases of Silane. Physical Review Letters, 2006, 97, 045504.	2.9	576
12	Mechanism for linear and nonlinear optical effects inÎ²â˜BaB2O4crystals. Physical Review B, 1999, 60, 13380-13389.	1.1	465
13	First-Principles Calculation of NMR Parameters Using the Gauge Including Projector Augmented Wave Method: A Chemistâ€™s Point of View. Chemical Reviews, 2012, 112, 5733-5779.	23.0	446
14	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
15	Structure prediction drives materials discovery. Nature Reviews Materials, 2019, 4, 331-348.	23.3	402
16	Accurate First Principles Prediction of17O NMR Parameters in SiO2:Â Assignment of the Zeolite Ferrierite Spectrum. Journal of the American Chemical Society, 2003, 125, 541-548.	6.6	389
17	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	2.9	377
18	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. Nature Chemistry, 2014, 6, 644-648.	6.6	369

#	Article	IF	Citations
19	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
20	Population analysis in plane wave electronic structure calculations. Molecular Physics, 1996, 89, 571-577.	0.8	277
21	Theoretical Strength and Cleavage of Diamond. Physical Review Letters, 2000, 84, 5160-5163.	2.9	267
22	The role of the interlayer state in the electronic structure of superconducting graphite intercalated compounds. Nature Physics, 2005, 1, 42-45.	6.5	255
23	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
24	Citrate bridges between mineral platelets in bone. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E1354-63.	3.3	234
25	High-Pressure Phases of Nitrogen. Physical Review Letters, 2009, 102, 125702.	2.9	226
26	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	13.7	222
27	Single-Layered Hittorfâ€™s Phosphorus: A Wide-Bandgap High Mobility 2D Material. Nano Letters, 2016, 16, 2975-2980.	4.5	219
28	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
29	Aluminium at terapascal pressures. Nature Materials, 2010, 9, 624-627.	13.3	202
30	Powder Crystallography by Combined Crystal Structure Prediction and High-Resolution ¹H Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2010, 132, 2564-2566.	6.6	201
31	Chemical shift computations on a crystallographic basis: some reflections and comments. Magnetic Resonance in Chemistry, 2007, 45, S174-S186.	1.1	197
32	An Investigation of Weak CHÂ·Â·Â·O Hydrogen Bonds in Maltose Anomers by a Combination of Calculation and Experimental Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2005, 127, 10216-10220.	6.6	185
33	Ab Initio Study of Phosphorus Anodes for Lithium- and Sodium-Ion Batteries. Chemistry of Materials, 2016, 28, 2011-2021.	3.2	182
34	Powder NMR crystallography of thymol. Physical Chemistry Chemical Physics, 2009, 11, 2610.	1.3	180
35	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	2.9	176
36	First-Principles Calculation of 17O, 29Si, and 23Na NMR Spectra of Sodium Silicate Crystals and Glasses. Journal of Physical Chemistry B, 2004, 108, 4147-4161.	1.2	174

#	Article	IF	Citations
37	Combined First-Principles Computational and Experimental Multinuclear Solid-State NMR Investigation of Amino Acids. Journal of Physical Chemistry A, 2005, 109, 6960-6969.	1.1	169
38	Two Dimensional Ice from First Principles: Structures and Phase Transitions. Physical Review Letters, 2016, 116, 025501.	2.9	167
39	Highly compressed ammonia forms an ionic crystal. Nature Materials, 2008, 7, 775-779.	13.3	166
40	Data-Driven Learning of Total and Local Energies in Elemental Boron. Physical Review Letters, 2018, 120, 156001.	2.9	150
41	Superconducting Hydrides Under Pressure. Annual Review of Condensed Matter Physics, 2020, 11, 57-76.	5.2	149
42	Atomic Structure of IcosahedralB4CBoron Carbide from a First Principles Analysis of NMR Spectra. Physical Review Letters, 2001, 87, 085506.	2.9	145
43	Assigning carbon-13 NMR spectra to crystal structures by the INADEQUATE pulse sequence and first principles computation: a case study of two forms of testosterone. Physical Chemistry Chemical Physics, 2006, 8, 137-143.	1.3	142
44	First-Principles Theory of the EPRgTensor in Solids: Defects in Quartz. Physical Review Letters, 2002, 88, 086403.	2.9	139
45	A combined first principles computational and solid-state NMR study of a molecular crystal: flurbiprofen. Physical Chemistry Chemical Physics, 2005, 7, 1402.	1.3	136
46	Density functional theory study of phase IV of solid hydrogen. Physical Review B, 2012, 85, .	1.1	134
47	OptaDOS: A tool for obtaining density of states, core-level and optical spectra from electronic structure codes. Computer Physics Communications, 2014, 185, 1477-1485.	3.0	124
48	Experimental evidence of new tetragonal polymorphs of silicon formed through ultrafast laser-induced confined microexplosion. Nature Communications, 2015, 6, 7555.	5.8	122
49	Investigating Sodium Storage Mechanisms in Tin Anodes: A Combined Pair Distribution Function Analysis, Density Functional Theory, and Solid-State NMR Approach. Journal of the American Chemical Society, 2017, 139, 7273-7286.	6.6	121
50	Resolving Structures from Powders by NMR Crystallography Using Combined Proton Spin Diffusion and Plane Wave DFT Calculations. Journal of the American Chemical Society, 2007, 129, 8932-8933.	6.6	120
51	Crystal Structures of Dense Lithium: A Metal-Semiconductor-Metal Transition. Physical Review Letters, 2011, 106, 095502.	2.9	120
52	Dissociation products and structures of solid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">S</mml:mi></mml:math>at strong compression. Physical Review B, 2016, 93, .	1.1	119
53	Structural Studies of the Polymorphs of Carbamazepine, Its Dihydrate, and Two Solvates. Organic Process Research and Development, 2005, 9, 902-910.	1.3	117
54	Metallization of aluminum hydride at high pressures: A first-principles study. Physical Review B, 2007, 76, .	1.1	116

#	Article	IF	Citations
55	Perspective: Role of structure prediction in materials discovery and design. APL Materials, 2016, 4, 053210.	2.2	114
56	Stochastic generation of complex crystal structures combining group and graph theory with application to carbon. Physical Review B, 2018, 97, .	1.1	114
57	Quantifying Weak Hydrogen Bonding in Uracil and 4-Cyano-4â€˜-ethynylbiphenyl:â€‰ A Combined Computational and Experimental Investigation of NMR Chemical Shifts in the Solid State. Journal of the American Chemical Society, 2008, 130, 945-954.	6.6	112
58	Revisiting metal fluorides as lithium-ion battery cathodes. Nature Materials, 2021, 20, 841-850.	13.3	109
59	Population analysis in plane wave electronic structure calculations. Molecular Physics, 1996, 89, 571-577.	0.8	108
60	17O and29Si NMR Parameters of MgSiO3Phases from High-Resolution Solid-State NMR Spectroscopy and First-Principles Calculations. Journal of the American Chemical Society, 2007, 129, 13213-13224.	6.6	104
61	First-Principles Calculation of the17O NMR Parameters in Ca Oxide and Ca Aluminosilicates:Â the Partially Covalent Nature of the Caâ^'O Bond, a Challenge for Density Functional Theory. Journal of the American Chemical Society, 2004, 126, 12628-12635.	6.6	103
62	Dense Low-Coordination Phases of Lithium. Physical Review Letters, 2009, 102, 146401.	2.9	103
63	NMRcrystallography of oxybuprocaine hydrochloride, Modification IIÂ°. Physical Chemistry Chemical Physics, 2007, 9, 360-368.	1.3	102
64	Theory of core-hole effects in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi>s</mml:mi></mml:mrow></mml:math>core-level spectroscopy of the first-row elements. Physical Review B, 2008, 77, .	1.1	102
65	Thermodynamically Stable Phases of Carbon at Multiterapascal Pressures. Physical Review Letters, 2012, 108, 045704.	2.9	102
66	Structure and NMR assignment in calcined and as-synthesized forms of AlPO-14: a combined study by first-principles calculations and high-resolution 27Alâ€“31P MAS NMR correlation. Physical Chemistry Chemical Physics, 2008, 10, 5754.	1.3	95
67	Complex Low Energy Tetrahedral Polymorphs of Group IV Elements from First Principles. Physical Review Letters, 2018, 121, 175701.	2.9	95
68	Stone-Wales graphene: A two-dimensional carbon semimetal with magic stability. Physical Review B, 2019, 99, .	1.1	95
69	Calculation of NMR chemical shifts in organic solids: Accounting for motional effects. Journal of Chemical Physics, 2009, 130, 104701.	1.2	93
70	Structural Properties of Lanthanide and Actinide Compounds within the Plane Wave Pseudopotential Approach. Physical Review Letters, 2000, 85, 5122-5125.	2.9	92
71	Relativistic nuclear magnetic resonance chemical shifts of heavy nuclei with pseudopotentials and the zeroth-order regular approximation. Journal of Chemical Physics, 2003, 118, 5746-5753.	1.2	91
72	Superconducting graphene sheets in CaC6 enabled by phonon-mediated interband interactions. Nature Communications, 2014, 5, 3493.	5.8	91

#	Article	IF	Citations
73	Design Principles for High-Temperature Superconductors with a Hydrogen-Based Alloy Backbone at Moderate Pressure. Physical Review Letters, 2022, 128, 047001.	2.9	91
74	Low-energy tetrahedral polymorphs of carbon, silicon, and germanium. Physical Review B, 2015, 91, .	1.1	90
75	First-Principles Calculation of the 17O NMR Parameters of a Calcium Aluminosilicate Glass. Journal of Physical Chemistry B, 2005, 109, 6052-6060.	1.2	89
76	Synthesis and stability of xenon oxides Xe2O5 and Xe3O2 under pressure. Nature Chemistry, 2016, 8, 784-790.	6.6	89
77	Combinedab initio computational and experimental multinuclear solid-state magnetic resonance study of phenylphosphonic acid. Magnetic Resonance in Chemistry, 2004, 42, 445-452.	1.1	88
78	First-principles calculation of spectral features, chemical shift and absolute threshold of ELNES and XANES using a plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104204.	0.7	88
79	Garnets: Structure, compressibility, dynamics, and disorder. Jom, 2000, 52, 22-25.	0.9	87
80	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. Physical Review Letters, 2020, 125, 217001.	2.9	87
81	Electronic energy minimisation with ultrasoft pseudopotentials. Computer Physics Communications, 2006, 174, 24-29.	3.0	86
82	23Na multiple-quantum MAS NMR of the perovskites NaNbO3and NaTaO3. Physical Chemistry Chemical Physics, 2006, 8, 3423-3431.	1.3	86
83	Elucidation of the Local and Long-Range Structural Changes that Occur in Germanium Anodes in Lithium-Ion Batteries. Chemistry of Materials, 2015, 27, 1031-1041.	3.2	86
84	Hypothetical low-energy chiral framework structure of group 14 elements. Physical Review B, 2010, 81, .	1.1	84
85	Quantum Monte Carlo study of the phase diagram of solid molecular hydrogen at extreme pressures. Nature Communications, 2015, 6, 7794.	5.8	84
86	Theoretical Investigation of Oxygen-17 NMR Shielding and Electric Field Gradients in Glutamic Acid Polymorphs. Journal of Physical Chemistry A, 2004, 108, 6032-6037.	1.1	83
87	Complete 1H resonance assignment of Î²-maltose from 1Hâ€“1H DQ-SQ CRAMPS and 1H (DQ-DUMBO)â€“13C SQ refocused INEPT 2D solid-state NMR spectra and first principles GIPAW calculations. Physical Chemistry Chemical Physics, 2010, 12, 6970.	1.3	83
88	Evidence for supercritical behaviour of high-pressure liquid hydrogen. Nature, 2020, 585, 217-220.	13.7	83
89	Polyhydride CeH9 with an atomic-like hydrogen clathrate structure. Nature Communications, 2019, 10, 3461.	5.8	81
90	Assigning powders to crystal structures by high-resolution1Hâ€“1H double quantum and1Hâ€“13C J-INEPT solid-state NMR spectroscopy and first principles computation. A case study of penicillin G. Physical Chemistry Chemical Physics, 2006, 8, 3418-3422.	1.3	79

#	Article	IF	Citations
91	Synthesis of sodium polyhydrides at high pressures. Nature Communications, 2016, 7, 12267.	5.8	79
92	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
93	Core-level spectroscopy calculation and the plane wave pseudopotential method. Journal of Physics Condensed Matter, 2009, 21, 104203.	0.7	78
94	A first principles theory of nuclear magnetic resonance J-coupling in solid-state systems. Journal of Chemical Physics, 2007, 127, 204107.	1.2	76
95	Probing Heteronuclear ¹⁵Nâ^'¹⁷O and ¹³Câ^'¹⁷O Connectivities and Proximities by Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2009, 131, 1820-1834.	6.6	76
96	Quantum simulation of low-temperature metallic liquid hydrogen. Nature Communications, 2013, 4, 2064.	5.8	75
97	Metallic Icosahedron Phase of Sodium at Terapascal Pressures. Physical Review Letters, 2015, 114, 125501.	2.9	75
98	Predicted Formation of Superconducting Platinum-Hydride Crystals under Pressure in the Presence of Molecular Hydrogen. Physical Review Letters, 2011, 107, 117002.	2.9	74
99	Applicability of a quantum mechanical `virtual crystal approximation' to study Al/Si-disorder. Chemical Physics Letters, 2002, 362, 266-270.	1.2	72
100	Electron energy-loss spectroscopy of electron states in isolated carbon nanostructures. Physical Review B, 2001, 63, .	1.1	71
101	Structures at high pressure from random searching. Physica Status Solidi (B): Basic Research, 2009, 246, 536-540.	0.7	71
102	Thermodynamically stable lithium silicides and germanides from density functional theory calculations. Physical Review B, 2014, 90, .	1.1	71
103	Systematic prediction of crystal structures: An application tosp3-hybridized carbon polymorphs. Physical Review B, 2004, 70, .	1.1	70
104	Decomposition and Terapascal Phases of Water Ice. Physical Review Letters, 2013, 110, 245701.	2.9	70
105	Structures and stability of calcium and magnesium carbonates at mantle pressures. Physical Review B, 2015, 91, .	1.1	70
106	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2017, 56, 8144-8148.	7.2	70
107	Multiple superionic states in heliumâ€“water compounds. Nature Physics, 2019, 15, 1065-1070.	6.5	69
108	Calculation of near edge structure. Ultramicroscopy, 1999, 78, 175-183.	0.8	68

#	Article	IF	Citations
109	Quantum MonteÂCarlo Study of a Positron in an Electron Gas. Physical Review Letters, 2011, 107, 207402.	2.9	68
110	High-Pressure Phase Stability and Superconductivity of Pnictogen Hydrides and Chemical Trends for Compressed Hydrides. Chemistry of Materials, 2016, 28, 1746-1755.	3.2	68
111	Crystal Structure of the ZrO Phase at Zirconium/Zirconium Oxide Interfaces. Advanced Engineering Materials, 2015, 17, 211-215.	1.6	66
112	Data-driven learning and prediction of inorganic crystal structures. Faraday Discussions, 2018, 211, 45-59.	1.6	66
113	First-principles calculations of solid-state17O and29Si NMR spectra of Mg2SiO4polymorphs. Physical Chemistry Chemical Physics, 2007, 9, 1587-1598.	1.3	65
114	Time Averaging of NMR Chemical Shifts in the MLF Peptide in the Solid State. Journal of the American Chemical Society, 2010, 132, 5993-6000.	6.6	65
115	Electron-Phonon Coupling and the Metallization of Solid Helium at Terapascal Pressures. Physical Review Letters, 2014, 112, 055504.	2.9	64
116	Density Functional Theory Calculations of Hydrogen-Bond-Mediated NMR J Coupling in the Solid State. Journal of the American Chemical Society, 2008, 130, 12663-12670.	6.6	63
117	First-Principles Calculation of17O and25Mg NMR Shieldings in MgO at Finite Temperature: Rovibrational Effect in Solids. Journal of Physical Chemistry B, 2005, 109, 7245-7250.	1.2	62
118	Density Functional Study of the 13C NMR Chemical Shifts in Small-to-Medium-Diameter Infinite Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2006, 110, 11995-12004.	1.1	62
119	Cation Disorder in Pyrochlore Ceramics: ⁸⁹Y MAS NMR and First-Principles Calculations. Journal of Physical Chemistry C, 2009, 113, 18874-18883.	1.5	62
120	Stable All-Nitrogen Metallic Salt at Terapascal Pressures. Physical Review Letters, 2013, 111, 175502.	2.9	62
121	High Energy Density Mixed Polymeric Phase from Carbon Monoxide and Nitrogen. Physical Review Letters, 2013, 111, 235501.	2.9	62
122	The effect of radiation damage on local structure in the crystalline fraction of ZrSiO₄: Investigating the²⁹Si NMR response to pressure in zircon and reidite. American Mineralogist, 2003, 88, 1663-1667.	0.9	61
123	Solid-State 17O NMR Spectroscopy of Hydrous Magnesium Silicates: Evidence for Proton Dynamics. Journal of Physical Chemistry C, 2009, 113, 465-471.	1.5	61
124	Controlling the Bonding and Band Gaps of Solid Carbon Monoxide with Pressure. Physical Review Letters, 2011, 106, 145502.	2.9	60
125	Inorganic Doubleâ€Helix Structures of Unusually Simple Lithiumâ€“Phosphorus Species. Angewandte Chemie - International Edition, 2012, 51, 8330-8333.	7.2	60
126	Crystal Structure of Ammonia Monohydrate Phase II. Journal of the American Chemical Society, 2009, 131, 13508-13515.	6.6	59

#	Article	IF	Citations
127	Predicted Pressure-Induced<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>s</mml:mi></mml:math>-Band Ferromagnetism in Alkali Metals. Physical Review Letters, 2011, 107, 087201.	2.9	59
128	Ab Initio Calculations of NMR Parameters of Highly Coordinated Oxygen Sites in Aluminosilicates. Journal of Physical Chemistry B, 2004, 108, 13249-13253.	1.2	57
129	Mapping uncharted territory in iceÂfrom zeolite networks to ice structures. Nature Communications, 2018, 9, 2173.	5.8	57
130	Density Functional Study of the ¹³C NMR Chemical Shifts in Single-Walled Carbon Nanotubes with Stoneâ^'Wales Defects. Journal of Physical Chemistry C, 2008, 112, 11744-11750.	1.5	56
131	Persistence and Eventual Demise of Oxygen Molecules at Terapascal Pressures. Physical Review Letters, 2012, 108, 045503.	2.9	55
132	Extrapolative approaches to Brillouin-zone integration. Physical Review B, 1999, 59, 4685-4693.	1.1	54
133	Cubic boron nitride: Experimental and theoretical energy-loss near-edge structure. Physical Review B, 2001, 64, .	1.1	54
134	Prediction of 10-fold coordinated TiO ₂ and SiO ₂ structures at multimegabar pressures. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6898-6901.	3.3	54
135	Structure and Metallicity of Phase V of Hydrogen. Physical Review Letters, 2018, 120, 255701.	2.9	54
136	Nonlocal Pseudopotentials and Magnetic Fields. Physical Review Letters, 2003, 91, 196401.	2.9	53
137	Systematic prediction of crystal structures. Chemical Physics Letters, 2001, 337, 36-42.	1.2	52
138	DFT calculations of quadrupolar solidâ€state NMR properties: Some examples in solidâ€state inorganic chemistry. Journal of Computational Chemistry, 2008, 29, 2279-2287.	1.5	52
139	Predicting interface structures: From<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>to graphene. Physical Review B, 2014, 90, .	1.1	52
140	Experimental and theoretical evidence for an ionic crystal of ammonia at high pressure. Physical Review B, 2014, 89, .	1.1	52
141	Carbon nitride frameworks and dense crystalline polymorphs. Physical Review B, 2016, 94, .	1.1	51
142	Ab Initio Quality NMR Parameters in Solid-State Materials Using a High-Dimensional Neural-Network Representation. Journal of Chemical Theory and Computation, 2016, 12, 765-773.	2.3	51
143	¹¹⁹Sn MAS NMR and first-principles calculations for the investigation of disorder in stannate pyrochlores. Physical Chemistry Chemical Physics, 2011, 13, 488-497.	1.3	49
144	Theoretical and experimental insights into applicability of solid-state 93Nb NMR in catalysis. Physical Chemistry Chemical Physics, 2013, 15, 5115.	1.3	48

#	Article	IF	Citations
145	A Density Functional Study of the13C NMR Chemical Shifts in Functionalized Single-Walled Carbon Nanotubes. Journal of the American Chemical Society, 2007, 129, 4430-4439.	6.6	47
146	Characterizing Slight Structural Disorder in Solids by Combined Solid-State NMR and First Principles Calculations. Journal of Physical Chemistry A, 2009, 113, 902-911.	1.1	47
147	Hydrogen/silicon complexes in silicon from computational searches. Physical Review B, 2008, 78, .	1.1	46
148	What are the possible structures for CNx compounds? The example of C3N. Chemical Physics Letters, 2000, 325, 53-60.	1.2	45
149	Theoretical investigation of bonding in diaspore. European Journal of Mineralogy, 2001, 13, 343-349.	0.4	45
150	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	6.6	45
151	High-throughput discovery of high-temperature conventional superconductors. Physical Review B, 2021, 104, .	1.1	45
152	Solid-state NMR calculations for metal oxides and gallates: Shielding and quadrupolar parameters for perovskites and related phases. Journal of Magnetic Resonance, 2010, 204, 1-10.	1.2	44
153	OptaDOS - a new tool for EELS calculations. Journal of Physics: Conference Series, 2012, 371, 012062.	0.3	44
154	Computational searches for iron oxides at high pressures. Journal of Physics Condensed Matter, 2015, 27, 455501.	0.7	44
155	Hexagonal structure of phase III of solid hydrogen. Physical Review B, 2016, 94, .	1.1	44
156	Perspectives for next generation lithium-ion battery cathode materials. APL Materials, 2021, 9, .	2.2	44
157	Solid-state NMR and computational studies of 4-methyl-2-nitroacetanilide. Magnetic Resonance in Chemistry, 2006, 44, 325-333.	1.1	43
158	New perspectives in the PAW/GIPAW approach: JP-O-Si coupling constants, antisymmetric parts of shift tensors and NQR predictions. Magnetic Resonance in Chemistry, 2010, 48, S86-S102.	1.1	42
159	Accurate kinetic energy evaluation in electronic structure calculations with localized functions on real space grids. Computer Physics Communications, 2001, 140, 315-322.	3.0	41
160	High T _c Superconductivity in Heavy Rare Earth Hydrides. Chinese Physics Letters, 2021, 38, 107401.	1.3	40
161	Second-orderkâ‹…pperturbation theory with Vanderbilt pseudopotentials and plane waves. Physical Review B, 2000, 62, 4383-4388.	1.1	39
162	Probing the surface structure of hydroxyapatite using NMR spectroscopy and first principles calculations. Physical Chemistry Chemical Physics, 2008, 10, 600-606.	1.3	39

#	Article	IF	Citations
163	New insights into the structure and chemistry of Titanâ€™s tholins via 13C and 15N solid state nuclear magnetic resonance spectroscopy. Icarus, 2012, 221, 844-853.	1.1	39
164	Stable phases of iron at terapascal pressures. Journal of Physics Condensed Matter, 2009, 21, 452205.	0.7	38
165	Backbone NxH compounds at high pressures. Journal of Chemical Physics, 2015, 142, 214308.	1.2	38
166	Structure and properties of aluminosilicate garnets and katoite: an ab initio study. Computational Materials Science, 2000, 17, 141-145.	1.4	37
167	Crystal structures of curium compounds: an ab initio study. Journal of Nuclear Materials, 2003, 322, 165-179.	1.3	37
168	Pressure-Stabilized Cubic Perovskite Oxyhydride BaScO₂H. Inorganic Chemistry, 2017, 56, 4840-4845.	1.9	36
169	Superionic iron oxideâ€“hydroxide in Earthâ€™s deep mantle. Nature Geoscience, 2021, 14, 174-178.	5.4	36
170	Graphite intercalation compounds under pressure: A first-principles density functional theory study. Physical Review B, 2007, 75, .	1.1	35
171	Computational searches for iron carbide in the Earth's inner core. Physical Review B, 2011, 84, .	1.1	35
172	EPRg-tensor of paramagnetic centers in yttria-stabilized zirconia from first-principles calculations. Physical Review B, 2006, 73, .	1.1	34
173	Systematic ab initio study of the compressibility of silicate garnets. Acta Crystallographica Section B: Structural Science, 2001, 57, 163-177.	1.8	33
174	Coexistence of plastic and partially diffusive phases in a helium-methane compound. National Science Review, 2020, 7, 1540-1547.	4.6	33
175	Calculating NMR parameters in aluminophosphates: evaluation of dispersion correction schemes. Physical Chemistry Chemical Physics, 2014, 16, 2660.	1.3	32
176	Density-functional study of charge disordering inCs2Au(I)Au(III)Cl6under pressure. Physical Review B, 2001, 63, .	1.1	31
177	Postaragonite phases of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaCO</mml:mi><mml:mn>3</mml:mn></mml:msub><m at lower mantle pressures. Physical Review Materials, 2018, 2, .	1.0	31
178	Gauge invariance of the spin-other-orbit contribution to the g-tensors of electron paramagnetic resonance. Journal of Chemical Physics, 2005, 122, 214101.	1.2	30
179	Determining the Diameter of Functionalized Single-Walled Carbon Nanotubes with 13C NMR: A Theoretical Study. Journal of Physical Chemistry C, 2008, 112, 9267-9271.	1.5	30
180	Dense close-packed phase of tin above 157 GPa observed experimentally via angle-dispersive x-ray diffraction. Physical Review B, 2011, 84, .	1.1	30

#	Article	IF	Citations
181	Generalized convex hull construction for materials discovery. Physical Review Materials, 2018, 2, .	0.9	30
182	Double-layer ice from first principles. Physical Review B, 2017, 95, .	1.1	29
183	The aperiodic states of zircon: an ab initio molecular dynamics study. American Mineralogist, 2003, 88, 1769-1777.	0.9	28
184	When is H2O not water?. Journal of Chemical Physics, 2007, 127, 244503.	1.2	28
185	A Density Functional Study of the 13C NMR Chemical Shifts in Fluorinated Single-Walled Carbon Nanotubes. Journal of Physical Chemistry A, 2009, 113, 4117-4124.	1.1	28
186	Temperature effects in first-principles solid state calculations of the chemical shielding tensor made simple. Journal of Chemical Physics, 2014, 141, 134113.	1.2	28
187	Calcium peroxide from ambient to high pressures. Physical Chemistry Chemical Physics, 2015, 17, 6889-6895.	1.3	28
188	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. Physical Review X, 2020, 10, .	2.8	28
189	Speed of sound from fundamental physical constants. Science Advances, 2020, 6, .	4.7	27
190	Resolving the Different Silicon Clusters in Li₁₂Si₇ by ²⁹Si and ^{6,7}Li Solidâ€State NMR Spectroscopy. Angewandte Chemie - International Edition, 2011, 50, 12591-12594.	7.2	26
191	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie, 2017, 129, 8256-8260.	1.6	26
192	Superconducting Zirconium Polyhydrides at Moderate Pressures. Journal of Physical Chemistry Letters, 2020, 11, 646-651.	2.1	26
193	Hierarchically Structured Allotropes of Phosphorus from Dataâ€Driven Exploration. Angewandte Chemie - International Edition, 2020, 59, 15880-15885.	7.2	26
194	Phase behaviours of superionic water at planetary conditions. Nature Physics, 2021, 17, 1228-1232.	6.5	26
195	Prediction of a nanoporous sp2-carbon framework structure by combining graph theory with quantum mechanics. Chemical Physics Letters, 1999, 312, 536-541.	1.2	25
196	Hydrogen/nitrogen/oxygen defect complexes in silicon from computational searches. Physical Review B, 2009, 80, .	1.1	25
197	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. Journal of Physics Condensed Matter, 2013, 25, 085402.	0.7	25
198	High-pressure phases of group-II difluorides: Polymorphism and superionicity. Physical Review B, 2017, 95, .	1.1	25

#	Article	IF	Citations
199	Is there theoretical evidence for a metallic carbon polymorph with space group symmetry at ambient conditions?. Diamond and Related Materials, 2001, 10, 2225-2227.	1.8	24
200	Strong coupling superconductivity in a quasiperiodic host-guest structure. Science Advances, 2018, 4, eaao4793.	4.7	24
201	Helium-Iron Compounds at Terapascal Pressures. Physical Review Letters, 2018, 121, 015301.	2.9	24
202	High-pressure ionic and molecular phases of ammonia within density functional theory. Physical Review B, 2012, 86, .	1.1	23
203	Ab initio random structure searching of organic molecular solids: assessment and validation against experimental data. Physical Chemistry Chemical Physics, 2017, 19, 25949-25960.	1.3	23
204	Phase stabilities of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgCO</mml:mi><mml:mn>3</mml:mn></mml:msub></m xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MgCO</mml:mi><mml:mn>3</mml:mn></mml:msub></m studied by Raman spectroscopy, x-ray diffraction, and density functional theory calculations. Physical Review Materials, 2020, 4, .	0.9	23
205	An ab initio study of hydrogarnets. American Mineralogist, 2000, 85, 1706-1715.	0.9	22
206	Lithiation of silicon via lithium Zintl-defect complexes from first principles. Physical Review B, 2013, 87, .	1.1	22
207	Ground state structure of high-energy-density polymeric carbon monoxide. Physical Review B, 2017, 95, .	1.1	22
208	Pressureâ€Tuneable Visibleâ€Range Band Gap in the Ionic Spinel Tin Nitride. Angewandte Chemie - International Edition, 2018, 57, 11623-11628.	7.2	22
209	Structures of CdSe and CdS Nanoclusters from Ab Initio Random Structure Searching. Journal of Physical Chemistry C, 2019, 123, 29370-29378.	1.5	22
210	Weak Intermolecular CHÂ·Â·Â·N Hydrogen Bonding: Determination of ¹³CHâ€“¹⁵N Hydrogen-Bond Mediated J Couplings by Solid-State NMR Spectroscopy and First-Principles Calculations. Journal of Physical Chemistry A, 2020, 124, 560-572.	1.1	22
211	Predicting the phase diagram of titanium dioxide with random search and pattern recognition. Physical Chemistry Chemical Physics, 2020, 22, 12697-12705.	1.3	22
212	Density Functional Theory Calculations of ⁹⁵Mo NMR Parameters in Solidâ€State Compounds. ChemPhysChem, 2009, 10, 3320-3329.	1.0	21
213	Energetics of hydrogen/lithium complexes in silicon analyzed using the Maxwell construction. Physical Review B, 2011, 84, .	1.1	21
214	High pressure ionic and molecular crystals of ammonia monohydrate within density functional theory. Journal of Chemical Physics, 2012, 137, 064506.	1.2	21
215	Polytypism in the ground state structure of the Lennard-Jonesium. Physical Chemistry Chemical Physics, 2017, 19, 19369-19376.	1.3	21
216	Improving sensitivity and resolution of MQMAS spectra: A 45 Sc-NMR case study of scandium sulphate pentahydrate. Journal of Magnetic Resonance, 2010, 203, 226-235.	1.2	20

#	Article	IF	Citations
217	Probing Intermolecular Hydrogen Bonding in Sibenadet Hydrochloride Polymorphs by High-Resolution 1H Double-Quantum Solid-State NMR Spectroscopy. Journal of Pharmaceutical Sciences, 2012, 101, 1821-1830.	1.6	20
218	Prediction of pressure-induced stabilization of noble-gas-atom compounds with alkali oxides and alkali sulfides. Physical Review Materials, 2019, 3, .	0.9	20
219	A combined⁷⁷Se NMR and molecular dynamics contribution to the structural understanding of the chalcogenide glasses. Physical Chemistry Chemical Physics, 2014, 16, 17975-17982.	1.3	19
220	Hunting for hydrogen: random structure searching and prediction of NMR parameters of hydrous wadsleyite. Physical Chemistry Chemical Physics, 2016, 18, 10173-10181.	1.3	19
221	Revealing and exploiting hierarchical material structure through complex atomic networks. Npj Computational Materials, 2017, 3, .	3.5	19
222	Determining interface structures in vertically aligned nanocomposite films. APL Materials, 2019, 7, .	2.2	19
223	High-Pressure Polymorphs of LaHO with Anion Coordination Reversal. Journal of the American Chemical Society, 2019, 141, 8717-8720.	6.6	19
224	Stability and superconductivity of lanthanum and yttrium decahydrides. Physical Review B, 2020, 101, .	1.1	19
225	Ab initio random structure searching for battery cathode materials. Journal of Chemical Physics, 2021, 154, 174111.	1.2	19
226	Effects of Aromatic Substitution on the Photodimerization Kinetics of Î²-trans Cinnamic Acid Derivatives Studied with ¹³C Solid-State NMR. Journal of Physical Chemistry C, 2012, 116, 12212-12218.	1.5	17
227	Crystal structure of ammonia dihydrate II. Journal of Chemical Physics, 2012, 136, 174512.	1.2	17
228	Synthesis, Crystal Structure, and Solid-State NMR Investigations of Heteronuclear Zn/Co Coordination Networks â€" A Comparative Study. Inorganic Chemistry, 2013, 52, 4431-4442.	1.9	17
229	Dirac cones in two-dimensional borane. Physical Review B, 2017, 96, .	1.1	17
230	Computationally Directed Discovery of MoBi₂. Journal of the American Chemical Society, 2021, 143, 214-222.	6.6	17
231	Diaphite-structured nanodiamonds with six- and twelve-fold symmetries. Diamond and Related Materials, 2021, 119, 108573.	1.8	16
232	ON THE STRUCTURE OF i-CARBON. Journal of Theoretical and Computational Chemistry, 2006, 05, 175-185.	1.8	15
233	First-principles method for impurities in quantum fluids: Positron in an electron gas. Physical Review B, 2010, 82, .	1.1	15
234	77Se solid-state NMR of As2Se3, As4Se4 and As4Se3 crystals: a combined experimental and computational study. Physical Chemistry Chemical Physics, 2013, 15, 6284.	1.3	15

#	Article	IF	Citations
235	Electrostatic force driven helium insertion into ammonia and water crystals under pressure. Communications Chemistry, 2019, 2, .	2.0	15
236	Hyperspatial optimization of structures. Physical Review B, 2019, 99, .	1.1	15
237	A structure determination protocol based on combined analysis of 3D-ED data, powder XRD data, solid-state NMR data and DFT-D calculations reveals the structure of a new polymorph of<scp>l</scp>-tyrosine. Chemical Science, 2022, 13, 5277-5288.	3.7	15
238	Ephemeral data derived potentials for random structure search. Physical Review B, 2022, 106, .	1.1	15
239	Theoretical investigation of xenon-hydrogen solids under pressure usingab initioDFT and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations. Physical Review B, 2011, 84, .	1.1	13
240	A Picture of Disorder in Hydrous Wadsleyiteâ€”Under the Combined Microscope of Solid-State NMR Spectroscopy and Ab Initio Random Structure Searching. Journal of the American Chemical Society, 2019, 141, 3024-3036.	6.6	13
241	Synthesis of Weaireâ€“Phelan Barium Polyhydride. Journal of Physical Chemistry Letters, 2021, 12, 4910-4916.	2.1	13
242	Accelerating cathode material discovery through ab initio random structure searching. APL Materials, 2021, 9, 121111.	2.2	13
243	Structure of Cu6PbO8. Acta Crystallographica Section B: Structural Science, 2000, 56, 22-26.	1.8	12
244	Virtual crystal approximation study of nitridosilicates and oxonitridoaluminosilicates. Journal of Physics and Chemistry of Solids, 2008, 69, 1861-1868.	1.9	12
245	95Mo nuclear magnetic resonance parameters of molybdenum hexacarbonyl from density functional theory: appraisal of computational and geometrical parameters. Physical Chemistry Chemical Physics, 2011, 13, 19471.	1.3	12
246	⁹⁵Mo Solid-State Nuclear Magnetic Resonance Spectroscopy and Quantum Simulations: Synergetic Tools for the Study of Molybdenum Cluster Materials. Inorganic Chemistry, 2013, 52, 617-627.	1.9	12
247	First-principles structure determination of interface materials: The<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>Ni</mml:mtext><mml:mi>x</mml:mi> Physical Review B, 2015, 92, .	1.1	12
248	Prediction of quasi-one-dimensional superconductivity in metastable two-dimensional boron. Physical Review B, 2020, 101, .	1.1	12
249	Pressure-Induced Enhancement of Thermoelectric Figure of Merit and Structural Phase Transition in TiNiSn. Journal of Physical Chemistry Letters, 2021, 12, 1046-1051.	2.1	12
250	Ultrasoft spin-dependent pseudopotentials. Journal of Chemical Physics, 2005, 123, 214101.	1.2	11
251	Theoretical investigation of moganite. European Journal of Mineralogy, 2005, 17, 21-30.	0.4	11
252	Equation of state and phase transition of deuterated ammonia monohydrate (ND3â‹…D2O) measured by high-resolution neutron powder diffraction up to 500 MPa. Journal of Chemical Physics, 2009, 131, 154503.	1.2	11

#	Article	IF	Citations
253	Rules of formation of Hâ€“Câ€“Nâ€“O compounds at high pressure and the fates of planetary ices. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	11
254	Post-cotunnite phase ofTeO2obtained from first-principles density-functional theory methods with random-structure searching. Physical Review B, 2009, 80, .	1.1	10
255	Oxygen K-edge electron energy loss spectra of hydrous and anhydrous compounds. Journal of Physics Condensed Matter, 2013, 25, 485401.	0.7	10
256	Impact of Te on the structure and⁷⁷Se NMR spectra of Se-rich Geâ€“Teâ€“Se glasses: a combined experimental and computational investigation. Physical Chemistry Chemical Physics, 2015, 17, 29020-29026.	1.3	10
257	Covalency is Frustrating: La₂Sn₂O₇ and the Nature of Bonding in Pyrochlores under High Pressureâ€“Temperature Conditions. Inorganic Chemistry, 2018, 57, 15051-15061.	1.9	10
258	Efficient prediction of nucleus independent chemical shifts for polycyclic aromatic hydrocarbons. Physical Chemistry Chemical Physics, 2020, 22, 13746-13755.	1.3	10
259	Multistep Dissociation of Fluorine Molecules under Extreme Compression. Physical Review Letters, 2021, 126, 225704.	2.9	10
260	Visualizing Energy Landscapes through Manifold Learning. Physical Review X, 2021, 11, .	2.8	10
261	Quantum mechanical study of Al/Si disorder in leucite and bicchulite. Mineralogical Magazine, 2004, 68, 819-824.	0.6	9
262	Modelling the structure of Zr-rich Pb(Zr_{1â^'x}Ti_x)O₃, x = 0.4 by a multiphase approach. Physical Chemistry Chemical Physics, 2016, 18, 28316-28324.	1.3	9
263	Managing uncertainty in data-derived densities to accelerate density functional theory. JPhys Materials, 2019, 2, 034001.	1.8	9
264	Nuclear Magnetic Resonance Spectroscopy as a Dynamical Structural Probe of Hydrogen under High Pressure. Physical Review Letters, 2019, 122, 135501.	2.9	9
265	Anataselike Grain Boundary Structure in Rutile Titanium Dioxide. Nano Letters, 2021, 21, 2745-2751.	4.5	9
266	Exotic silicon phases synthesized through ultrashort laser-induced microexplosion: Characterization with Raman microspectroscopy. Physical Review Materials, 2020, 4, .	0.9	9
267	Carbon network evolution from dimers to sheets in superconducting ytrrium dicarbide under pressure. Communications Chemistry, 2018, 1, .	2.0	8
268	Random Structure Searching with Orbital-Free Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 1650-1660.	1.1	8
269	Calculations of Magnetic Resonance Parameters in Solids and Liquids Using Periodic Boundary Conditions. , 2004, , 265-277.		7
270	The Structure of (SCN)_x: A Study Using Molecular and Solidâ€State Density Functional Theory Calculations. Chemistry - A European Journal, 2009, 15, 2687-2692.	1.7	7

#	Article	IF	Citations
271	High-pressure <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>CaF</mml:mi></mml:mrow><mml:mn>2</mml:mn> revisited: A new high-temperature phase and the role of phonons in the search for superionic conductivity. Physical Review B, 2018, 98, .	1.1	7
272	Computational discovery and characterization of new B₂O phases. Physical Chemistry Chemical Physics, 2019, 21, 2499-2506.	1.3	7
273	Theoretical Investigations of Oxygen-17 NMR Chemical Shifts to Discriminate among Helical Forms. Journal of Physical Chemistry A, 2007, 111, 13099-13105.	1.1	6
274	Phase stability and superconductivity of strontium under pressure. Applied Physics Letters, 2012, 101, 052604.	1.5	6
275	Solid-state NMR/NQR and first-principles study of two niobium halide cluster compounds. Solid State Nuclear Magnetic Resonance, 2014, 59-60, 20-30.	1.5	6
276	Piling on the pressure. Nature, 2014, 511, 294-295.	13.7	6
277	Evaluation of95Mo Nuclear Shielding and Chemical Shift of [Mo6X14]2â€“Clusters in the Liquid Phase. Inorganic Chemistry, 2015, 54, 7673-7683.	1.9	6
278	Identifying aspirin polymorphs from combined DFTâ€based crystal structure prediction and solidâ€state NMR. Magnetic Resonance in Chemistry, 2020, 58, 1018-1025.	1.1	6
279	High-temperature phase transitions in dense germanium. Journal of Chemical Physics, 2021, 154, 174702.	1.2	6
280	Prediction of structural parameters and physical properties ofCsHSO3up to 60 GPa. Physical Review B, 1998, 57, 4321-4326.	1.1	5
281	Electronic structure of oxide fuels from experiment and first principles calculations. Journal of Physics: Conference Series, 2010, 241, 012062.	0.3	5
282	High pressure chemical reactivity and structural study of the Naâ€“P and Liâ€“P systems. Journal of Materials Chemistry A, 2020, 8, 21797-21803.	5.2	5
283	Study of disorder in pulsed laser deposited double perovskite oxides by first-principle structure prediction. Npj Computational Materials, 2021, 7, .	3.5	4
284	Ternary hypervalent silicon hydrides via lithium at high pressure. Physical Review Materials, 2020, 4, .	0.9	4
285	Structural diversity and hydrogen storage properties in the system Kâ€“Siâ€“H. Physical Chemistry Chemical Physics, 2022, 24, 13033-13039.	1.3	3
286	Partially Diffusive Helium-Silica Compound under High Pressure. Chinese Physics Letters, 0, , .	1.3	3
287	Multiphase modelling of Pb(Zr1-xTix)O3 structure. Ferroelectrics, 2017, 520, 1-9.	0.3	2
288	Reply to â€œComment on â€˜High-pressure phases of group-II difluorides: Polymorphism and superionicityâ€™ â€•. Physical Review B, 2018, 98, .	1.1	2

#	Article	IF	Citations
289	Pressure-Induced Superionicity of H^{â€“} in Hypervalent Sodium Silicon Hydrides. Journal of Physical Chemistry Letters, 2021, 12, 7166-7172.	2.1	2
290	Structural and vibrational properties of methane up to 71 GPa. Physical Review B, 2021, 104, .	1.1	2
291	High-pressure phase behaviors of titanium dioxide revealed by a Î”-learning potential. Journal of Chemical Physics, 2022, 156, 074106.	1.2	2
292	Reply to: On the liquidâ€“liquid phase transition of dense hydrogen. Nature, 2021, 600, E15-E16.	13.7	2
293	Navigating the Ti-C-O and Al-C-O ternary systems through theory-driven discovery. Physical Review Materials, 2021, 5, .	0.9	2
294	Suppression of the superconducting phase in new structures of elemental sulfur at terapascal pressures. Physical Review B, 2022, 105, .	1.1	2
295	A computer simulation study of domain walls in NH4Cl. Journal of Physics Condensed Matter, 2000, 12, 2093-2101.	0.7	1
296	X-rays glimpse solid hydrogenâ€™s structure. Nature, 2019, 573, 504-505.	13.7	1
297	Chemical and structural stability of superconducting In5Bi3 driven by spinâ€“orbit coupling. JPhys Materials, 2020, 3, 015007.	1.8	1
298	Hierarchically Structured Allotropes of Phosphorus from Dataâ€Driven Exploration. Angewandte Chemie, 2020, 132, 16014-16019.	1.6	1
299	The discontinuous effect of pressure on twin boundary strength in MgO. Physics and Chemistry of Minerals, 2020, 47, 1.	0.3	1
300	From Slater to Mott physics by epitaxially engineering electronic correlations in oxide interfaces. Npj Computational Materials, 2021, 7, .	3.5	1
301	Ab initio Calculations of NMR Parameters of Highly Coordinated Oxygen Sites in Aluminosilicates.. ChemInform, 2004, 35, no.	0.1	0
302	Experimental observation for new polymorphs of silicon formed through ultrafast-laser-induced microexplosion. , 2014, , .		0