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	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
2	Design Principles for High-Temperature Superconductors with a Hydrogen-Based Alloy Backbone at Moderate Pressure. Physical Review Letters, 2022, 128, 047001.	2.9	91
3	High-pressure phase behaviors of titanium dioxide revealed by a Î”-learning potential. Journal of Chemical Physics, 2022, 156, 074106.	1.2	2
4	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
5	Suppression of the superconducting phase in new structures of elemental sulfur at terapascal pressures. Physical Review B, 2022, 105, .	1.1	2
6	Structural diversity and hydrogen storage properties in the system Kâ€“Siâ€“H. Physical Chemistry Chemical Physics, 2022, 24, 13033-13039.	1.3	3
7	Ephemeral data derived potentials for random structure search. Physical Review B, 2022, 106, .	1.1	15
8	Revisiting metal fluorides as lithium-ion battery cathodes. Nature Materials, 2021, 20, 841-850.	13.3	109
9	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
10	Random Structure Searching with Orbital-Free Density Functional Theory. Journal of Physical Chemistry A, 2021, 125, 1650-1660.	1.1	8
11	Superionic iron oxideâ€“hydroxide in Earthâ€™s deep mantle. Nature Geoscience, 2021, 14, 174-178.	5.4	36
12	Anataselike Grain Boundary Structure in Rutile Titanium Dioxide. Nano Letters, 2021, 21, 2745-2751.	4.5	9
13	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
14	High-temperature phase transitions in dense germanium. Journal of Chemical Physics, 2021, 154, 174702.	1.2	6
15	Synthesis of Weaireâ€“Phelan Barium Polyhydride. Journal of Physical Chemistry Letters, 2021, 12, 4910-4916.	2.1	13
16	Ab initio random structure searching for battery cathode materials. Journal of Chemical Physics, 2021, 154, 174111.	1.2	19
17	From Slater to Mott physics by epitaxially engineering electronic correlations in oxide interfaces. Npj Computational Materials, 2021, 7, .	3.5	1
18	Multistep Dissociation of Fluorine Molecules under Extreme Compression. Physical Review Letters, 2021, 126, 225704.	2.9	10

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19	Study of disorder in pulsed laser deposited double perovskite oxides by first-principle structure prediction. Npj Computational Materials, 2021, 7, .	3.5	4
20	Pressure-Induced Superionicity of H^{â€“} in Hypervalent Sodium Silicon Hydrides. Journal of Physical Chemistry Letters, 2021, 12, 7166-7172.	2.1	2
21	High-throughput discovery of high-temperature conventional superconductors. Physical Review B, 2021, 104, .	1.1	45
22	Phase behaviours of superionic water at planetary conditions. Nature Physics, 2021, 17, 1228-1232.	6.5	26
23	Diaphite-structured nanodiamonds with six- and twelve-fold symmetries. Diamond and Related Materials, 2021, 119, 108573.	1.8	16
24	Computationally Directed Discovery of MoBi₂. Journal of the American Chemical Society, 2021, 143, 214-222.	6.6	17
25	High T _c Superconductivity in Heavy Rare Earth Hydrides. Chinese Physics Letters, 2021, 38, 107401.	1.3	40
26	Perspectives for next generation lithium-ion battery cathode materials. APL Materials, 2021, 9, .	2.2	44
27	Visualizing Energy Landscapes through Manifold Learning. Physical Review X, 2021, 11, .	2.8	10
28	Structural and vibrational properties of methane up to 71 GPa. Physical Review B, 2021, 104, .	1.1	2
29	Accelerating cathode material discovery through ab initio random structure searching. APL Materials, 2021, 9, 121111.	2.2	13
30	Reply to: On the liquidâ€“liquid phase transition of dense hydrogen. Nature, 2021, 600, E15-E16.	13.7	2
31	Navigating the Ti-C-O and Al-C-O ternary systems through theory-driven discovery. Physical Review Materials, 2021, 5, .	0.9	2
32	Superconducting Hydrides Under Pressure. Annual Review of Condensed Matter Physics, 2020, 11, 57-76.	5.2	149
33	Chemical and structural stability of superconducting In5Bi3 driven by spinâ€“orbit coupling. JPhys Materials, 2020, 3, 015007.	1.8	1
34	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
35	Superconducting Zirconium Polyhydrides at Moderate Pressures. Journal of Physical Chemistry Letters, 2020, 11, 646-651.	2.1	26
36	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

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37	Speed of sound from fundamental physical constants. Science Advances, 2020, 6, .	4.7	27
38	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
39	Hydrogen Pentagraphenelike Structure Stabilized by Hafnium: A High-Temperature Conventional Superconductor. Physical Review Letters, 2020, 125, 217001.	2.9	87
40	Evidence for supercritical behaviour of high-pressure liquid hydrogen. Nature, 2020, 585, 217-220.	13.7	83
41	Predicting the phase diagram of titanium dioxide with random search and pattern recognition. Physical Chemistry Chemical Physics, 2020, 22, 12697-12705.	1.3	22
42	Efficient prediction of nucleus independent chemical shifts for polycyclic aromatic hydrocarbons. Physical Chemistry Chemical Physics, 2020, 22, 13746-13755.	1.3	10
43	Hierarchically Structured Allotropes of Phosphorus from Dataâ€Driven Exploration. Angewandte Chemie - International Edition, 2020, 59, 15880-15885.	7.2	26
44	Coexistence of plastic and partially diffusive phases in a helium-methane compound. National Science Review, 2020, 7, 1540-1547.	4.6	33
45	Hierarchically Structured Allotropes of Phosphorus from Dataâ€Driven Exploration. Angewandte Chemie, 2020, 132, 16014-16019.	1.6	1
46	Prediction of quasi-one-dimensional superconductivity in metastable two-dimensional boron. Physical Review B, 2020, 101, .	1.1	12
47	The discontinuous effect of pressure on twin boundary strength in MgO. Physics and Chemistry of Minerals, 2020, 47, 1.	0.3	1
48	Stability and superconductivity of lanthanum and yttrium decahydrides. Physical Review B, 2020, 101, .	1.1	19
49	Plastic and Superionic Helium Ammonia Compounds under High Pressure and High Temperature. Physical Review X, 2020, 10, .	2.8	28
50	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></mml:math> studied by Raman spectroscopy, x-ray diffraction, and density functional theory calculations. Physical Review Materials, 2020, 4, .	0.9	23
51	Exotic silicon phases synthesized through ultrashort laser-induced microexplosion: Characterization with Raman microspectroscopy. Physical Review Materials, 2020, 4, .	0.9	9
52	Ternary hypervalent silicon hydrides via lithium at high pressure. Physical Review Materials, 2020, 4, .	0.9	4
53	Polyhydride CeH9 with an atomic-like hydrogen clathrate structure. Nature Communications, 2019, 10, 3461.	5.8	81
54	Multiple superionic states in heliumâ€“water compounds. Nature Physics, 2019, 15, 1065-1070.	6.5	69

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55	Determining interface structures in vertically aligned nanocomposite films. APL Materials, 2019, 7, .	2.2	19
56	Electrostatic force driven helium insertion into ammonia and water crystals under pressure. Communications Chemistry, 2019, 2, .	2.0	15
57	Stone-Wales graphene: A two-dimensional carbon semimetal with magic stability. Physical Review B, 2019, 99, .	1.1	95
58	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
59	Computational discovery and characterization of new B₂O phases. Physical Chemistry Chemical Physics, 2019, 21, 2499-2506.	1.3	7
60	High-Pressure Polymorphs of LaHO with Anion Coordination Reversal. Journal of the American Chemical Society, 2019, 141, 8717-8720.	6.6	19
61	Managing uncertainty in data-derived densities to accelerate density functional theory. JPhys Materials, 2019, 2, 034001.	1.8	9
62	Nuclear Magnetic Resonance Spectroscopy as a Dynamical Structural Probe of Hydrogen under High Pressure. Physical Review Letters, 2019, 122, 135501.	2.9	9
63	Structure prediction drives materials discovery. Nature Reviews Materials, 2019, 4, 331-348.	23.3	402
64	Hyperspatial optimization of structures. Physical Review B, 2019, 99, .	1.1	15
65	Structures of CdSe and CdS Nanoclusters from Ab Initio Random Structure Searching. Journal of Physical Chemistry C, 2019, 123, 29370-29378.	1.5	22
66	X-rays glimpse solid hydrogenâ€™s structure. Nature, 2019, 573, 504-505.	13.7	1
67	Prediction of pressure-induced stabilization of noble-gas-atom compounds with alkali oxides and alkali sulfides. Physical Review Materials, 2019, 3, .	0.9	20
68	Data-Driven Learning of Total and Local Energies in Elemental Boron. Physical Review Letters, 2018, 120, 156001.	2.9	150
69	Data-driven learning and prediction of inorganic crystal structures. Faraday Discussions, 2018, 211, 45-59.	1.6	66
70	Strong coupling superconductivity in a quasiperiodic host-guest structure. Science Advances, 2018, 4, eaao4793.	4.7	24
71	Stochastic generation of complex crystal structures combining group and graph theory with application to carbon. Physical Review B, 2018, 97, .	1.1	114
72	Carbon network evolution from dimers to sheets in superconducting ytrrium dicarbide under pressure. Communications Chemistry, 2018, 1, .	2.0	8

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73	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
74	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</m 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
75	Complex Low Energy Tetrahedral Polymorphs of Group IV Elements from First Principles. Physical Review Letters, 2018, 121, 175701.	2.9	95
76	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
77	Helium-Iron Compounds at Terapascal Pressures. Physical Review Letters, 2018, 121, 015301.	2.9	24
78	Pressureâ€Tuneable Visibleâ€Range Band Gap in the Ionic Spinel Tin Nitride. Angewandte Chemie - International Edition, 2018, 57, 11623-11628.	7.2	22
79	Mapping uncharted territory in iceÂfrom zeolite networks to ice structures. Nature Communications, 2018, 9, 2173.	5.8	57
80	Structure and Metallicity of Phase V of Hydrogen. Physical Review Letters, 2018, 120, 255701.	2.9	54
81	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, .	0.9	31
82	Generalized convex hull construction for materials discovery. Physical Review Materials, 2018, 2, .	0.9	30
83	Pressure-Stabilized Cubic Perovskite Oxyhydride BaScO₂H. Inorganic Chemistry, 2017, 56, 4840-4845.	1.9	36
84	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
85	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie, 2017, 129, 8256-8260.	1.6	26
86	Encapsulation and Polymerization of White Phosphorus Inside Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2017, 56, 8144-8148.	7.2	70
87	Double-layer ice from first principles. Physical Review B, 2017, 95, .	1.1	29
88	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
89	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
90	Revealing and exploiting hierarchical material structure through complex atomic networks. Npj Computational Materials, 2017, 3, .	3.5	19

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91	Dirac cones in two-dimensional borane. Physical Review B, 2017, 96, .	1.1	17
92	Ground state structure of high-energy-density polymeric carbon monoxide. Physical Review B, 2017, 95, .	1.1	22
93	Polytypism in the ground state structure of the Lennard-Jonesium. Physical Chemistry Chemical Physics, 2017, 19, 19369-19376.	1.3	21
94	High-pressure phases of group-II difluorides: Polymorphism and superionicity. Physical Review B, 2017, 95, .	1.1	25
95	Multiphase modelling of Pb(Zr1-xTix)O3 structure. Ferroelectrics, 2017, 520, 1-9.	0.3	2
96	Perspective: Role of structure prediction in materials discovery and design. APL Materials, 2016, 4, 053210.	2.2	114
97	Ab Initio Study of Phosphorus Anodes for Lithium- and Sodium-Ion Batteries. Chemistry of Materials, 2016, 28, 2011-2021.	3.2	182
98	Single-Layered Hittorfâ€™s Phosphorus: A Wide-Bandgap High Mobility 2D Material. Nano Letters, 2016, 16, 2975-2980.	4.5	219
99	Hexagonal structure of phase III of solid hydrogen. Physical Review B, 2016, 94, .	1.1	44
100	Carbon nitride frameworks and dense crystalline polymorphs. Physical Review B, 2016, 94, .	1.1	51
101	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
102	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
103	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
104	Synthesis of sodium polyhydrides at high pressures. Nature Communications, 2016, 7, 12267.	5.8	79
105	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
106	Synthesis and stability of xenon oxides Xe2O5 and Xe3O2 under pressure. Nature Chemistry, 2016, 8, 784-790.	6.6	89
107	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
108	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113

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109	Quantum hydrogen-bond symmetrization in the superconducting hydrogen sulfide system. Nature, 2016, 532, 81-84.	13.7	222
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	Two Dimensional Ice from First Principles: Structures and Phase Transitions. Physical Review Letters, 2016, 116, 025501.	2.9	167
112	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, .	3.7	12
113	Computational searches for iron oxides at high pressures. Journal of Physics Condensed Matter, 2015, 27, 455501.	0.7	44
114	Evaluation of95Mo Nuclear Shielding and Chemical Shift of [Mo6X14]2â€“Clusters in the Liquid Phase. Inorganic Chemistry, 2015, 54, 7673-7683.	1.9	6
115	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
116	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
117	Backbone NxH compounds at high pressures. Journal of Chemical Physics, 2015, 142, 214308.	1.2	38
118	Low-energy tetrahedral polymorphs of carbon, silicon, and germanium. Physical Review B, 2015, 91, .	1.1	90
119	Experimental evidence of new tetragonal polymorphs of silicon formed through ultrafast laser-induced confined microexplosion. Nature Communications, 2015, 6, 7555.	5.8	122
120	High-Pressure Hydrogen Sulfide from First Principles: A Strongly Anharmonic Phonon-Mediated Superconductor. Physical Review Letters, 2015, 114, 157004.	2.9	377
121	Calcium peroxide from ambient to high pressures. Physical Chemistry Chemical Physics, 2015, 17, 6889-6895.	1.3	28
122	Metallic Icosahedron Phase of Sodium at Terapascal Pressures. Physical Review Letters, 2015, 114, 125501.	2.9	75
123	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
124	Structures and stability of calcium and magnesium carbonates at mantle pressures. Physical Review B, 2015, 91, .	1.1	70
125	Quantum Monte Carlo study of the phase diagram of solid molecular hydrogen at extreme pressures. Nature Communications, 2015, 6, 7794.	5.8	84
126	Crystal Structure of the ZrO Phase at Zirconium/Zirconium Oxide Interfaces. Advanced Engineering Materials, 2015, 17, 211-215.	1.6	66

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127	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
128	Thermodynamically stable lithium silicides and germanides from density functional theory calculations. Physical Review B, 2014, 90, .	1.1	71
129	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
130	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
131	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
132	Electron-Phonon Coupling and the Metallization of Solid Helium at Terapascal Pressures. Physical Review Letters, 2014, 112, 055504.	2.9	64
133	Superconducting graphene sheets in CaC6 enabled by phonon-mediated interband interactions. Nature Communications, 2014, 5, 3493.	5.8	91
134	Reactions of xenon with iron and nickel are predicted in the Earth's inner core. Nature Chemistry, 2014, 6, 644-648.	6.6	369
135	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
136	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
137	Calculating NMR parameters in aluminophosphates: evaluation of dispersion correction schemes. Physical Chemistry Chemical Physics, 2014, 16, 2660.	1.3	32
138	Experimental and theoretical evidence for an ionic crystal of ammonia at high pressure. Physical Review B, 2014, 89, .	1.1	52
139	Experimental observation for new polymorphs of silicon formed through ultrafast-laser-induced microexplosion. , 2014, , .		0
140	Piling on the pressure. Nature, 2014, 511, 294-295.	13.7	6
141	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
142	Stable All-Nitrogen Metallic Salt at Terapascal Pressures. Physical Review Letters, 2013, 111, 175502.	2.9	62
143	Oxygen K-edge electron energy loss spectra of hydrous and anhydrous compounds. Journal of Physics Condensed Matter, 2013, 25, 485401.	0.7	10
144	High Energy Density Mixed Polymeric Phase from Carbon Monoxide and Nitrogen. Physical Review Letters, 2013, 111, 235501.	2.9	62

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145	Theoretical and experimental insights into applicability of solid-state 93Nb NMR in catalysis. Physical Chemistry Chemical Physics, 2013, 15, 5115.	1.3	48
146	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
147	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
148	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
149	Decomposition and Terapascal Phases of Water Ice. Physical Review Letters, 2013, 110, 245701.	2.9	70
150	Lithiation of silicon via lithium Zintl-defect complexes from first principles. Physical Review B, 2013, 87, .	1.1	22
151	Quantum simulation of low-temperature metallic liquid hydrogen. Nature Communications, 2013, 4, 2064.	5.8	75
152	Classical and quantum ordering of protons in cold solid hydrogen under megabar pressures. Journal of Physics Condensed Matter, 2013, 25, 085402.	0.7	25
153	High pressure ionic and molecular crystals of ammonia monohydrate within density functional theory. Journal of Chemical Physics, 2012, 137, 064506.	1.2	21
154	OptaDOS - a new tool for EELS calculations. Journal of Physics: Conference Series, 2012, 371, 012062.	0.3	44
155	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
156	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
157	Cagelike Diamondoid Nitrogen at High Pressures. Physical Review Letters, 2012, 109, 175502.	2.9	176
158	High-pressure ionic and molecular phases of ammonia within density functional theory. Physical Review B, 2012, 86, .	1.1	23
159	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
160	Crystal structure of ammonia dihydrate II. Journal of Chemical Physics, 2012, 136, 174512.	1.2	17
161	Thermodynamically Stable Phases of Carbon at Multiterapascal Pressures. Physical Review Letters, 2012, 108, 045704.	2.9	102
162	Phase stability and superconductivity of strontium under pressure. Applied Physics Letters, 2012, 101, 052604.	1.5	6

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163	Persistence and Eventual Demise of Oxygen Molecules at Terapascal Pressures. Physical Review Letters, 2012, 108, 045503.	2.9	55
164	The Fuzzy Quantum Proton in the Hydrogen Chloride Hydrates. Journal of the American Chemical Society, 2012, 134, 8557-8569.	6.6	45
165	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
166	Inorganic Doubleâ€Helix Structures of Unusually Simple Lithiumâ€“Phosphorus Species. Angewandte Chemie - International Edition, 2012, 51, 8330-8333.	7.2	60
167	Density functional theory study of phase IV of solid hydrogen. Physical Review B, 2012, 85, .	1.1	134
168	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
169	Ab initiorandom structure searching. Journal of Physics Condensed Matter, 2011, 23, 053201.	0.7	832
170	Computational searches for iron carbide in the Earth's inner core. Physical Review B, 2011, 84, .	1.1	35
171	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
172	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
173	Crystal Structures of Dense Lithium: A Metal-Semiconductor-Metal Transition. Physical Review Letters, 2011, 106, 095502.	2.9	120
174	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
175	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
176	Energetics of hydrogen/lithium complexes in silicon analyzed using the Maxwell construction. Physical Review B, 2011, 84, .	1.1	21
177	Controlling the Bonding and Band Gaps of Solid Carbon Monoxide with Pressure. Physical Review Letters, 2011, 106, 145502.	2.9	60
178	Predicted Formation of Superconducting Platinum-Hydride Crystals under Pressure in the Presence of Molecular Hydrogen. Physical Review Letters, 2011, 107, 117002.	2.9	74
179	Quantum MonteÂCarlo Study of a Positron in an Electron Gas. Physical Review Letters, 2011, 107, 207402.	2.9	68
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