Keith Refson

List of Publications by Year
in descending order

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133 papers	16,728 citations	70961 41 h-index	14156 128 g-index
137 all docs	137 docs citations	137 times ranked	18055 citing authors

#	Article	IF	Citations
1	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
3	Variational density-functional perturbation theory for dielectrics and lattice dynamics. Physical Review B, 2006, 73, .	1.1	735
4	Moldy: a portable molecular dynamics simulation program for serial and parallel computers. Computer Physics Communications, 2000, 126, 310-329.	3.0	328
5	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
6	Water chemisorption and reconstruction of the MgO surface. Physical Review B, 1995, 52, 10823-10826.	1.1	232
7	Computer simulation of interlayer water in 2:1 clays. Journal of Chemical Physics, 1991, 94, 7434-7445.	1.2	211
8	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
9	Spin Singlet Formation inMgTi2O4: Evidence of a Helical Dimerization Pattern. Physical Review Letters, 2004, 92, 056402.	2.9	178
10	Suppression of thermal conductivity by rattling modes in thermoelectric sodium cobaltate. Nature Materials, 2013, 12, 1028-1032.	13.3	163
11	Novel Rhenium Nitrides. Physical Review Letters, 2010, 105, 085504.	2.9	148
12	Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses. Physical Review Letters, 2014, 112, 025502.	2.9	125
13	Mechanisms of nickel sorption by a bacteriogenic birnessite. Geochimica Et Cosmochimica Acta, 2010, 74, 3076-3089.	1.6	117
14	Nanoscale momentum-resolved vibrational spectroscopy. Science Advances, 2018, 4, eaar7495.	4.7	111
15	The kinetics and mechanism of MgO dissolution. Chemical Physics Letters, 1999, 314, 558-563.	1.2	110
16	Molecular Dynamics Simulation of Water Mobility in Magnesium-Smectite Hydrates. Journal of the American Chemical Society, 2000, 122, 11459-11464.	6.6	100
17	Defect-Induced Photoconductivity in Layered Manganese Oxides: A Density Functional Theory Study. Physical Review Letters, 2008, 100, 146601.	2.9	98
18	Structural, electronic and vibrational properties of tetragonal zirconia under pressure: a density functional theory study. Journal of Physics Condensed Matter, 2009, 21, 485404.	0.7	97

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19	Understanding the trends in transition metal sorption by vacancy sites in birnessite. Geochimica Et Cosmochimica Acta, 2013, 101, 222-232.	1.6	90
20	An ab initio study of hydrogen in forsterite and a possible mechanism for hydrolytic weakening. Journal of Geophysical Research, 2000, 105, 18977-18982.	3.3	87
21	On the role of Mn(IV) vacancies in the photoreductive dissolution of hexagonal birnessite. Geochimica Et Cosmochimica Acta, 2009, 73, 4142-4150.	1.6	87
22	Hopping Time Scales and the Phonon-Liquid Electron-Crystal Picture in Thermoelectric Copper Selenide. Physical Review Letters, 2017, 118, 145901.	2.9	77
23	Local Atomic Order and Infrared Spectra of Biogenic Calcite. Angewandte Chemie - International Edition, 2007, 46, 291-294.	7.2	76
24	Probing the sorption reactivity of the edge surfaces in birnessite nanoparticles using nickel(II). Geochimica Et Cosmochimica Acta, 2015, 164, 191-204.	1.6	75
25	Surface complexation of Pb(II) by hexagonal birnessite nanoparticles. Geochimica Et Cosmochimica Acta, 2010, 74, 6731-6740.	1.6	73
26	Periclase surface hydroxylation during dissolution. Geochimica Et Cosmochimica Acta, 1995, 59, 1875-1881.	1.6	72
27	Topological triplon modes and bound states in a Shastryâ€“Sutherland magnet. Nature Physics, 2017, 13, 736-741.	6.5	70
28	Zinc surface complexes on birnessite: A density functional theory study. Geochimica Et Cosmochimica Acta, 2009, 73, 1273-1284.	1.6	63
29	Anharmonicity of inner-OH stretching modes in hydrous phyllosilicates: assessment from first-principles frozen-phonon calculations. Physics and Chemistry of Minerals, 2007, 34, 621-625.	0.3	62
30	Molecular dynamics simulation of dilute aqueous DMSO solutions. A temperature-dependence study of the hydrophobic and hydrophilic behaviour around DMSO. Physical Chemistry Chemical Physics, 2004, 6, 94.	1.3	60
31	Lifetimes of cagelike water clusters immersed in bulk liquid water: A molecular dynamics study on gas hydrate nucleation mechanisms. Journal of Chemical Physics, 2004, 121, 1542-1547.	1.2	60
32	Ab Initio Computational Crystallography of 2:1 Clay Minerals:Â 1. Pyrophyllite-1Tc. Journal of Physical Chemistry B, 2003, 107, 13376-13383.	1.2	58
33	Magnetic ordering in tetragonal FeS: Evidence for strong itinerant spin fluctuations. Physical Review B, 2011, 83, .	1.1	57
34	Visualization and processing of computed solid-state NMR parameters: MagresView and MagresPython. Solid State Nuclear Magnetic Resonance, 2016, 78, 64-70.	1.5	57
35	Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953.	0.9	54
36	Modeling steps and kinks on the surface of calcite. Journal of Chemical Physics, 2004, 121, 8511.	1.2	52

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37	Solidâ€“aqueous equilibrium in the BaSO4â€“RaSO4â€“H2O system: First-principles calculations and a thermodynamic assessment. Geochimica Et Cosmochimica Acta, 2013, 122, 398-417.	1.6	48
38	Multiband One-Dimensional Electronic Structure and Spectroscopic Signature of Tomonaga-Luttinger Liquid Behavior in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">K</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow><mml:m Physical Review Letters, 2017, 118, 097002.	2.9	48
39	Emergence of Crystal-like Atomic Dynamics in Glasses at the Nanometer Scale. Physical Review Letters, 2013, 110, 185503.	2.9	47
40	High-pressure properties of diaspore, AlO(OH). Physics and Chemistry of Minerals, 2007, 34, 145-157.	0.3	45
41	Soft modes in strained and unstrained rutileTiO2. Physical Review B, 2010, 81, .	1.1	44
42	On optical phonons and elasticity in the hcp transition metals Fe, Ru and Re at high pressure. Europhysics Letters, 2001, 53, 504-510.	0.7	42
43	Dynamics of a Highly Charged Ion in Aqueous Solutions:Â MD Simulations of Dilute CrCl3Aqueous Solutions Using Interaction Potentials Based on the Hydrated Ion Concept. Journal of Physical Chemistry B, 1998, 102, 3272-3282.	1.2	41
44	Molecular dynamics studies of the condensed phases of n-butane and their transitions. Molecular Physics, 1987, 61, 669-692.	0.8	40
45	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:ma low-temperature Raman-scattering measurements and first-principles calculations. Physical Review B, 2009, 80, .	1.1	37
46	Density functional theory study of the relative stability of the iron disulfide polymorphs pyrite and marcasite. Physical Review B, 2010, 81, .	1.1	35
47	Molecular dynamics simulation of solid n-butane. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1985, 131, 256-266.	0.9	34
48	Viscosity and stress autocorrelation function in supercooled water: a molecular dynamics study. Molecular Physics, 2002, 100, 2617-2627.	0.8	34
49	Characterization of Hydrous Palladium Oxide: Implications for Low-Temperature Carbon Monoxide Oxidation. Journal of Physical Chemistry C, 2010, 114, 14164-14172.	1.5	34
50	Framework flexibility and the negative thermal expansion mechanism of copper(I) oxide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Cu</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m mathvariant="normal">O</mml:mi></mml:math>. Physical Review B, 2014, 89, .	1.1	34
51	Molecular-dynamics simulation of liquid water with anab initioflexible water-water interaction potential. II. The effect of internal vibrations on the time correlation functions. Physical Review A, 1987, 36, 3935-3942.	1.0	33
52	Structural compression and vibrational properties of Bi₁₂SiO₂₀sillenite from experiment and theory. Journal of Physics Condensed Matter, 2010, 22, 505401.	0.7	33
53	Quantum Delocalization of Molecular Hydrogen in Alkali-Graphite Intercalates. Physical Review Letters, 2008, 101, 126101.	2.9	32
54	Complete assignment of the vibrational modes of C60 by inelastic neutron scattering spectroscopy and periodic-DFT. Physical Chemistry Chemical Physics, 2011, 13, 7789.	1.3	32

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55	Diffusion mechanism in the sodium-ion battery material sodium cobaltate. Scientific Reports, 2018, 8, 3210.	1.6	31
56	AbÂinitioNonequilibrium Molecular Dynamics in the Solid Superionic Conductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LiBH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 095901.	2.9	30
57	The structure and orientational disorder in solid n-butane by neutron powder diffraction. Acta Crystallographica Section B: Structural Science, 1986, 42, 402-410.	1.8	27
58	How the Surface Structure Determines the Properties of CuH. Inorganic Chemistry, 2015, 54, 2213-2220.	1.9	27
59	An ab initio study of the compressional behavior of forsterite. American Mineralogist, 1996, 81, 257-260.	0.9	26
60	Agâ€“Ag dispersive interaction and physical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">Ag</mml:mi></mml:mrow><mml:mn>3</mml:mn></mml:msub><mml:mi>Co</mml:mi><mml:mo>(</mml:mo><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	26
61	Transition metal incorporation into mackinawite (tetragonal FeS). American Mineralogist, 2015, 100, 1509-1517.	0.9	26
62	The effect of molecular vibrations on calculated second virial coefficients. Journal of Chemical Physics, 1987, 87, 3634-3638.	1.2	25
63	The structure of interlayer water in a hydrated 2:1 clay. Chemical Physics Letters, 1990, 166, 141-145.	1.2	25
64	Finite-size effect at both high and low temperatures in molecular dynamics calculations of the self-diffusion coefficient and viscosity of liquid silica. Journal of Physics Condensed Matter, 2004, 16, 9127-9135.	0.7	25
65	Spectroscopic and Ab Initio Characterization of the [ReH9]2-Ion. Inorganic Chemistry, 2006, 45, 10951-10957.	1.9	25
66	Vibrational properties ofRe3Nfrom experiment and theory. Physical Review B, 2010, 82, .	1.1	24
67	Experimental evidence of librational vibrations determining the stability of calcium borohydride. Physical Review B, 2011, 83, .	1.1	24
68	Assignment of the vibrational spectra of lithium hydroxide monohydrate, LiOHÂ·H2O. Journal of Chemical Physics, 2011, 134, 084503.	1.2	24
69	Strong physisorption site for H2 in K- and Li-doped porous carbons. Journal of Chemical Physics, 2008, 129, 224701.	1.2	23
70	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
71	Structure determination of adsorbed hydrogen on a real catalyst. Chemical Communications, 2010, 46, 2959.	2.2	22
72	High pressure elasticity of FeCO 3 -MgCO 3 carbonates. Physics of the Earth and Planetary Interiors, 2017, 271, 57-63.	0.7	22

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73	Diffusion in Li₂O studied by non-equilibrium molecular dynamics for 873 < T/K < 1603. Physical Chemistry Chemical Physics, 2015, 17, 21470-21475.	1.3	21
74	Lattice dynamics and elasticity of SrCO₃. Journal of Applied Crystallography, 2016, 49, 1982-1990.	1.9	21
75	High-pressure crystal structure prediction of calcium borohydride using density functional theory. Physical Review B, 2011, 83, .	1.1	20
76	New insights into the lattice dynamics ofÎ±-quartz. Zeitschrift FÃ¼r Kristallographie, 2012, 227, 84-91.	1.1	20
77	Many-body renormalization of forces in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> -electron materials. Physical Review B, 2018, 98, .	1.1	20
78	Dispersion Relation of an OH-Stretching Vibration from Inelastic X-Ray Scattering. Physical Review Letters, 2008, 101, 065501.	2.9	19
79	Optimized effective potential using the Hylleraas variational method. Physical Review B, 2012, 85, .	1.1	19
80	Lattice dynamics of stishovite from powder inelastic Xâ€ray scattering. Geophysical Research Letters, 2009, 36, .	1.5	18
81	Molecular dynamics investigation of the disordered crystal structure of hexagonal LiBH4. Physical Chemistry Chemical Physics, 2013, 15, 8081.	1.3	18
82	Ferroelectric behaviour in solid croconic acid using neutron scattering and first-principles density functional theory. Chemical Physics, 2013, 427, 95-100.	0.9	18
83	Lattice dynamics ofÎ±-cristobalite and the Boson peak in silica glass. Journal of Physics Condensed Matter, 2015, 27, 305401.	0.7	18
84	Chemical Descriptors of Yttria-Stabilized Zirconia at Low Defect Concentration: An ab Initio Study. Journal of Physical Chemistry A, 2015, 119, 6412-6420.	1.1	16
85	The influence of pressure on the structure and dynamics of hydrogen bonds in zoisite and clinozoisite. Physics and Chemistry of Minerals, 2008, 35, 25-35.	0.3	15
86	Pressure dependence of the lattice dynamics of diaspore, Î±-AlO(OH), from Raman spectroscopy and density functional perturbation theory. Physics and Chemistry of Minerals, 2011, 38, 693-700.	0.3	15
87	Inelastic incoherent neutron scattering study of the molecular properties of pure hydrogen peroxide and its water mixtures of different concentration. Journal of Chemical Physics, 2014, 140, 164504.	1.2	15
88	Ferroelectric soft mode of polarZnTiO3investigated by Raman spectroscopy at high pressure. Physical Review B, 2015, 91, .	1.1	15
89	3DÂImaging of the Fermi Surface by Thermal Diffuse Scattering. Physical Review Letters, 2009, 103, 076403.	2.9	14
90	Molecular dynamics studies of the condensed phases of n-butane and their transitions. Molecular Physics, 1987, 61, 693-709.	0.8	13

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91	Effect of H-bond topology on the lifetimes of cagelike water clusters immersed in liquid water and the probability distribution of these lifetimes: Implications for hydrate nucleation mechanisms. Chemical Physics Letters, 2005, 413, 415-419.	1.2	13
92	A first-principles study of the vibrational properties of crystalline tetracene under pressure. Journal of Physics Condensed Matter, 2015, 27, 375402.	0.7	13
93	Hydrogen Bonding in the Organic Ferroelectric Croconic Acid: Insights from Experiment and First-Principles Modelling. Journal of the Physical Society of Japan, 2013, 82, SA001.	0.7	12
94	Lattice dynamics and Mg/Ti order in orthorhombic pseudobrookite-type MgTi2 O5. Journal of Alloys and Compounds, 2017, 699, 16-24.	2.8	12
95	A local Fock-exchange potential in Kohnâ€“Sham equations. Journal of Physics Condensed Matter, 2017, 29, 04LT01.	0.7	12
96	Effect of Basicity on the Hydrolysis of the Bi(III) Aqua Ion in Solution: An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry A, 2018, 122, 1905-1915.	1.1	12
97	A combined experimental inelastic neutron scattering, Raman and ab initio lattice dynamics study of Î±-lithium amidoborane. Physical Chemistry Chemical Physics, 2011, 13, 12249.	1.3	11
98	Structure and spectroscopy of CuH preparedviaborohydride reduction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 608-612.	0.5	11
99	Experimental evidence for the structural models of Re<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>N and Re<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>C from micro-Raman spectroscopy. Physical Review B, 2012, 86, .	1.1	10
100	Assignment of Metalâ€“Ligand Modes in Pt(II) Diimine Complexes Relevant to Solar Energy Conversion. Inorganic Chemistry, 2012, 51, 9748-9756.	1.9	10
101	Diffuse scattering in metallic tin polymorphs. Journal of Physics Condensed Matter, 2014, 26, 115401.	0.7	10
102	Assignment of the Internal Vibrational Modes of C₇₀ by Inelastic Neutron Scattering Spectroscopy and Periodicâ€ĐFT. ChemistryOpen, 2015, 4, 620-625.	0.9	10
103	Two-dimensional Cs-vacancy superstructure in iron-based superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Cs</mml:mi><mml:mrow /></mml:msub><mml:mn>0.8</mml:mn></mml:mrow></mml:math>Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Se<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2015, 91, .	1.1	10
104	Comment on â€œFirst-principles study of the influence of (110)-oriented strain on the ferroelectric properties of rutile TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>â€• Physical Review B, 2013, 88, .	1.1	9
105	Room temperature single-crystal diffuse scattering andab initiolattice dynamics in CaTiSiO5. Journal of Physics Condensed Matter, 2013, 25, 315402.	0.7	8
106	Pressure-induced Pbâ€“Pb bonding and phase transition in Pb₂SnO₄. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2020, 76, 979-991.	0.5	8
107	A molecular dynamics study on Rh3+ hydration: development and application of a first principles hydrated ionâ€“water interaction potential. Theoretical Chemistry Accounts, 2004, 111, 101-109.	0.5	7
108	Mechanism of enhancement of ferroelectricity of croconic acid with temperature. Physical Chemistry Chemical Physics, 2017, 19, 32216-32225.	1.3	7

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109	Molecular dynamics simulations on a parallel computer plastic crystals and related systems. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1985, 82, 249-257.	0.2	7
110	Origin of the large anharmonicity in the phonon modes of LiBH4. Chemical Physics, 2013, 427, 22-29.	0.9	6
111	Dimer-mediated cation diffusion in the stoichiometric ionic conductor Li₃N. Physical Chemistry Chemical Physics, 2016, 18, 5605-5613.	1.3	6
112	Computation of diffuse scattering arising from one-phonon excitations in a neutron time-of-flight single-crystal Laue diffraction experiment. Journal of Applied Crystallography, 2015, 48, 1122-1129.	1.9	6
113	The high resolution inelastic neutron scattering spectrum of ammonium fluoride. Physical Chemistry Chemical Physics, 2005, 7, 3685.	1.3	5
114	Negative thermal expansion of cubic silicon dicarbodiimide, Si(NCN)₂, studied by ab initio lattice dynamics. Journal of Physics Condensed Matter, 2020, 32, 465402.	0.7	5
115	The ab initio study of the stability of low temperature Al/Si ordered albite, NaAlSi₃O₈. American Mineralogist, 2000, 85, 1681-1685.	0.9	4
116	Terascale materials modelling on high performance system HPCx. Journal of Materials Chemistry, 2006, 16, 1885.	6.7	4
117	Stabilization of 3d Transition Metal Hydrido Complexes in SrH₂Mg₂[Co(I)H₅], BaH₂Mg₅[Co(â"I)H₄]₂, and RbH₂Mg₅[Co(â"I)H₄ Ni(0)H₄] via Easily Polarizable Hydride Ligands. Inorganic Chemistry, 2016, 55, 3576-3582.	1.9	4
118	Self-interaction free local exchange potentials applied to metallic systems. Journal of Physics Condensed Matter, 2017, 29, 374002.	0.7	4
119	Electronic, Structural, and Mechanical Properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Glass at High Pressure Inferred from its Refractive Index. Physical Review Letters, 2022, 128, 077403.	2.9	4
120	Refinement of the orientational distribution function in plasticn-butane guided by computer simulations. Acta Crystallographica Section A: Foundations and Advances, 1987, 43, 727-731.	0.3	3
121	Core beliefs. Nature, 2001, 413, 27-29.	13.7	3
122	Vibrational spectroscopy of a compound with a CS₇ ring. Journal of Raman Spectroscopy, 2009, 40, 703-708.	1.2	3
123	Influence of deuteration on lithium acetate dihydrate studied by inelastic X-ray scattering, density functional theory, thermal expansion, elastic and thermodynamic measurements. Dalton Transactions, 2011, 40, 1737.	1.6	3
124	Discussion: Nuclear Quantum Dynamics - Protons and Beyond. Journal of Physics: Conference Series, 2014, 571, 012004.	0.3	3
125	Determining Surface Chemistry and Vibrational Properties of SOFC Anode Materials Through Ab Initio Calculations. ECS Transactions, 2013, 57, 2419-2427.	0.3	2
126	Correlations in the plastic crystal phase of n-butane. Computer Physics Communications, 1991, 62, 279-288.	3.0	1

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127	Na3O(CN):â€ƒAb initiocalculations on a multidomain structure. Physical Review B, 2004, 70, .	1.1	1
128	The ferroelastic phase transition in hydrogen cyanide studied by density functional theory. Journal of Physics Condensed Matter, 2021, , .	0.7	1
129	Time and Frequency Resolved Hydrogen Dynamics in deuterated LiBH₄. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	0
130	Evidence for Hydrogen Transport in Deuterated LiBH₄ from Raman-Scattering Measurements and First-Principles Calculations. Advances in Science and Technology, 2010, 72, 150-157.	0.2	0
131	Molecular (and Lattice) Dynamics to Analyse Neutron Scattering Experiments 2016â€”MDANSE2016. Neutron News, 2017, 28, 17-18.	0.1	0
132	Structural phase transitions in malononitrile, CH2(CN)2: crystal structure of the Î´ phase by neutron powder diffraction, and ab initio calculations of the structures and phonons of the Îµ and Î´ phases. Journal of Physics Condensed Matter, 2019, 31, 255401.	0.7	0
133	Ab initiolattice dynamics and thermal diffuse scattering in CaTiSiO5. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C417-C418.	0.3	0