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	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
2	The ferroelastic phase transition in hydrogen cyanide studied by density functional theory. Journal of Physics Condensed Matter, 2021, , .	0.7	1
3	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> <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, .	2.9	23
4	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
5	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
6	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 Î± and Î´ phases. Journal of Physics Condensed Matter, 2019, 31, 255401.	0.7	0
7	Diffusion mechanism in the sodium-ion battery material sodium cobaltate. Scientific Reports, 2018, 8, 3210.	1.6	31
8	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
9	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
10	Nanoscale momentum-resolved vibrational spectroscopy. Science Advances, 2018, 4, eaar7495.	4.7	111
11	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:mrow><mml:mn	2.9	48
12	Topological triplon modes and bound states in a Shastryâ€“Sutherland magnet. Nature Physics, 2017, 13, 736-741.	6.5	70
13	Molecular (and Lattice) Dynamics to Analyse Neutron Scattering Experiments 2016â€”MDANSE2016. Neutron News, 2017, 28, 17-18.	0.1	0
14	Lattice dynamics and Mg/Ti order in orthorhombic pseudobrookite-type MgTi2 O5. Journal of Alloys and Compounds, 2017, 699, 16-24.	2.8	12
15	A local Fock-exchange potential in Kohnâ€“Sham equations. Journal of Physics Condensed Matter, 2017, 29, 04LT01.	0.7	12
16	High pressure elasticity of FeCO 3 -MgCO 3 carbonates. Physics of the Earth and Planetary Interiors, 2017, 271, 57-63.	0.7	22
17	Hopping Time Scales and the Phonon-Liquid Electron-Crystal Picture in Thermoelectric Copper Selenide. Physical Review Letters, 2017, 118, 145901.	2.9	77
18	Self-interaction free local exchange potentials applied to metallic systems. Journal of Physics Condensed Matter, 2017, 29, 374002.	0.7	4

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19	Mechanism of enhancement of ferroelectricity of croconic acid with temperature. Physical Chemistry Chemical Physics, 2017, 19, 32216-32225.	1.3	7
20	Lattice dynamics and elasticity of SrCO₃. Journal of Applied Crystallography, 2016, 49, 1982-1990.	1.9	21
21	Visualization and processing of computed solid-state NMR parameters: MagresView and MagresPython. Solid State Nuclear Magnetic Resonance, 2016, 78, 64-70.	1.5	57
22	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
23	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
24	Dimer-mediated cation diffusion in the stoichiometric ionic conductor Li₃N. Physical Chemistry Chemical Physics, 2016, 18, 5605-5613.	1.3	6
25	Assignment of the Internal Vibrational Modes of C₇₀ by Inelastic Neutron Scattering Spectroscopy and Periodicâ€DFT. ChemistryOpen, 2015, 4, 620-625.	0.9	10
26	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:mi>x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mi>Fe</mml:mi><mml:mn>0.8</m Physical Review B, 2015, 91, .	1.1	10
27	Ferroelectric soft mode of polarZnTiO3investigated by Raman spectroscopy at high pressure. Physical Review B, 2015, 91, .	1.1	15
28	Structure and spectroscopy of CuH preparedviaborohydride reduction. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2015, 71, 608-612.	0.5	11
29	How the Surface Structure Determines the Properties of CuH. Inorganic Chemistry, 2015, 54, 2213-2220.	1.9	27
30	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
31	Transition metal incorporation into mackinawite (tetragonal FeS). American Mineralogist, 2015, 100, 1509-1517.	0.9	26
32	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
33	Lattice dynamics ofÎ±-cristobalite and the Boson peak in silica glass. Journal of Physics Condensed Matter, 2015, 27, 305401.	0.7	18
34	A first-principles study of the vibrational properties of crystalline tetracene under pressure. Journal of Physics Condensed Matter, 2015, 27, 375402.	0.7	13
35	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
36	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

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37	Discussion: Nuclear Quantum Dynamics - Protons and Beyond. Journal of Physics: Conference Series, 2014, 571, 012004.	0.3	3
38	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:mo></mml:mo><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	26
39	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
40	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:mi mathvariant="normal">O</mml:mi></mml:math>. Physical Review B, 2014, 89, .	1.1	34
41	Diffuse scattering in metallic tin polymorphs. Journal of Physics Condensed Matter, 2014, 26, 115401.	0.7	10
42	Density functional theory in the solid state. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130270.	1.6	242
43	Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses. Physical Review Letters, 2014, 112, 025502.	2.9	125
44	Suppression of thermal conductivity by rattling modes in thermoelectric sodium cobaltate. Nature Materials, 2013, 12, 1028-1032.	13.3	163
45	Molecular dynamics investigation of the disordered crystal structure of hexagonal LiBH4. Physical Chemistry Chemical Physics, 2013, 15, 8081.	1.3	18
46	Determining Surface Chemistry and Vibrational Properties of SOFC Anode Materials Through Ab Initio Calculations. ECS Transactions, 2013, 57, 2419-2427.	0.3	2
47	Ferroelectric behaviour in solid croconic acid using neutron scattering and first-principles density functional theory. Chemical Physics, 2013, 427, 95-100.	0.9	18
48	Origin of the large anharmonicity in the phonon modes of LiBH4. Chemical Physics, 2013, 427, 22-29.	0.9	6
49	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
50	Emergence of Crystal-like Atomic Dynamics in Glasses at the Nanometer Scale. Physical Review Letters, 2013, 110, 185503.	2.9	47
51	Understanding the trends in transition metal sorption by vacancy sites in birnessite. Geochimica Et Cosmochimica Acta, 2013, 101, 222-232.	1.6	90
52	Room temperature single-crystal diffuse scattering andab initiolattice dynamics in CaTiSiO5. Journal of Physics Condensed Matter, 2013, 25, 315402.	0.7	8
53	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
54	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

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55	Optimized effective potential using the Hylleraas variational method. Physical Review B, 2012, 85, .	1.1	19
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	Phonon dispersion and elastic moduli 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
58	Assignment of Metalâ€“Ligand Modes in Pt(II) Diimine Complexes Relevant to Solar Energy Conversion. Inorganic Chemistry, 2012, 51, 9748-9756.	1.9	10
59	New insights into the lattice dynamics ofÎ±-quartz. Zeitschrift FÃ¼r Kristallographie, 2012, 227, 84-91.	1.1	20
60	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
61	Magnetic ordering in tetragonal FeS: Evidence for strong itinerant spin fluctuations. Physical Review B, 2011, 83, .	1.1	57
62	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
63	High-pressure crystal structure prediction of calcium borohydride using density functional theory. Physical Review B, 2011, 83, .	1.1	20
64	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
65	Experimental evidence of librational vibrations determining the stability of calcium borohydride. Physical Review B, 2011, 83, .	1.1	24
66	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
67	Assignment of the vibrational spectra of lithium hydroxide monohydrate, LiOHÂ·H2O. Journal of Chemical Physics, 2011, 134, 084503.	1.2	24
68	Ab initiolattice dynamics and thermal diffuse scattering in CaTiSiO5. Acta Crystallographica Section A: Foundations and Advances, 2011, 67, C417-C418.	0.3	0
69	Electron and vibrational spectroscopies using DFT, plane waves and pseudopotentials: CASTEP implementation. Computational and Theoretical Chemistry, 2010, 954, 22-35.	1.5	205
70	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
71	Vibrational properties ofRe3Nfrom experiment and theory. Physical Review B, 2010, 82, .	1.1	24
72	Density functional theory study of the relative stability of the iron disulfide polymorphs pyrite and marcasite. Physical Review B, 2010, 81, .	1.1	35

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73	Structure determination of adsorbed hydrogen on a real catalyst. Chemical Communications, 2010, 46, 2959.	2.2	22
74	Structural compression and vibrational properties of Bi₁₂SiO₂₀sillenite from experiment and theory. Journal of Physics Condensed Matter, 2010, 22, 505401.	0.7	33
75	Characterization of Hydrous Palladium Oxide: Implications for Low-Temperature Carbon Monoxide Oxidation. Journal of Physical Chemistry C, 2010, 114, 14164-14172.	1.5	34
76	Mechanisms of nickel sorption by a bacteriogenic birnessite. Geochimica Et Cosmochimica Acta, 2010, 74, 3076-3089.	1.6	117
77	Surface complexation of Pb(II) by hexagonal birnessite nanoparticles. Geochimica Et Cosmochimica Acta, 2010, 74, 6731-6740.	1.6	73
78	Novel Rhenium Nitrides. Physical Review Letters, 2010, 105, 085504.	2.9	148
79	Soft modes in strained and unstrained rutileTiO2. Physical Review B, 2010, 81, .	1.1	44
80	Evidence for hydrogen transport in deuterated<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LiBH</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>low-temperature Raman-scattering measurements and first-principles calculations. Physical Review B, 2009, 80, .	1.1	37
81	Time and Frequency Resolved Hydrogen Dynamics in deuterated LiBH₄. Materials Research Society Symposia Proceedings, 2009, 1216, 1.	0.1	0
82	Vibrational spectroscopy of a compound with a CS₇ ring. Journal of Raman Spectroscopy, 2009, 40, 703-708.	1.2	3
83	3DÂImaging of the Fermi Surface by Thermal Diffuse Scattering. Physical Review Letters, 2009, 103, 076403.	2.9	14
84	Zinc surface complexes on birnessite: A density functional theory study. Geochimica Et Cosmochimica Acta, 2009, 73, 1273-1284.	1.6	63
85	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
86	Lattice dynamics of stishovite from powder inelastic Xâ€ray scattering. Geophysical Research Letters, 2009, 36, .	1.5	18
87	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
88	Theoretical infrared absorption coefficient of OH groups in minerals. American Mineralogist, 2008, 93, 950-953.	0.9	54
89	Strong physisorption site for H2 in K- and Li-doped porous carbons. Journal of Chemical Physics, 2008, 129, 224701.	1.2	23
90	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

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91	Dispersion Relation of an OH-Stretching Vibration from Inelastic X-Ray Scattering. Physical Review Letters, 2008, 101, 065501.	2.9	19
92	Quantum Delocalization of Molecular Hydrogen in Alkali-Graphite Intercalates. Physical Review Letters, 2008, 101, 126101.	2.9	32
93	Defect-Induced Photoconductivity in Layered Manganese Oxides: A Density Functional Theory Study. Physical Review Letters, 2008, 100, 146601.	2.9	98
94	Local Atomic Order and Infrared Spectra of Biogenic Calcite. Angewandte Chemie - International Edition, 2007, 46, 291-294.	7.2	76
95	High-pressure properties of diaspore, AlO(OH). Physics and Chemistry of Minerals, 2007, 34, 145-157.	0.3	45
96	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
97	Variational density-functional perturbation theory for dielectrics and lattice dynamics. Physical Review B, 2006, 73, .	1.1	735
98	Spectroscopic and Ab Initio Characterization of the [ReH9]2-Ion. Inorganic Chemistry, 2006, 45, 10951-10957.	1.9	25
99	Terascale materials modelling on high performance system HPCx. Journal of Materials Chemistry, 2006, 16, 1885.	6.7	4
100	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
101	The high resolution inelastic neutron scattering spectrum of ammonium fluoride. Physical Chemistry Chemical Physics, 2005, 7, 3685.	1.3	5
102	First principles methods using CASTEP. Zeitschrift Fur Kristallographie - Crystalline Materials, 2005, 220, .	0.4	9,458
103	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
104	Modeling steps and kinks on the surface of calcite. Journal of Chemical Physics, 2004, 121, 8511.	1.2	52
105	Spin Singlet Formation inMgTi2O4: Evidence of a Helical Dimerization Pattern. Physical Review Letters, 2004, 92, 056402.	2.9	178
106	Na3O(CN):â€ƒAb initiocalculations on a multidomain structure. Physical Review B, 2004, 70, .	1.1	1
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	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

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109	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
110	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
111	Viscosity and stress autocorrelation function in supercooled water: a molecular dynamics study. Molecular Physics, 2002, 100, 2617-2627.	0.8	34
112	Core beliefs. Nature, 2001, 413, 27-29.	13.7	3
113	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
114	The ab initio study of the stability of low temperature Al/Si ordered albite, NaAlSi₃O₈. American Mineralogist, 2000, 85, 1681-1685.	0.9	4
115	Moldy: a portable molecular dynamics simulation program for serial and parallel computers. Computer Physics Communications, 2000, 126, 310-329.	3.0	328
116	Molecular Dynamics Simulation of Water Mobility in Magnesium-Smectite Hydrates. Journal of the American Chemical Society, 2000, 122, 11459-11464.	6.6	100
117	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
118	The kinetics and mechanism of MgO dissolution. Chemical Physics Letters, 1999, 314, 558-563.	1.2	110
119	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
120	An ab initio study of the compressional behavior of forsterite. American Mineralogist, 1996, 81, 257-260.	0.9	26
121	Water chemisorption and reconstruction of the MgO surface. Physical Review B, 1995, 52, 10823-10826.	1.1	232
122	Periclase surface hydroxylation during dissolution. Geochimica Et Cosmochimica Acta, 1995, 59, 1875-1881.	1.6	72
123	Computer simulation of interlayer water in 2:1 clays. Journal of Chemical Physics, 1991, 94, 7434-7445.	1.2	211
124	Correlations in the plastic crystal phase of n-butane. Computer Physics Communications, 1991, 62, 279-288.	3.0	1
125	The structure of interlayer water in a hydrated 2:1 clay. Chemical Physics Letters, 1990, 166, 141-145.	1.2	25
126	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

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127	The effect of molecular vibrations on calculated second virial coefficients. Journal of Chemical Physics, 1987, 87, 3634-3638.	1.2	25
128	Molecular dynamics studies of the condensed phases of n-butane and their transitions. Molecular Physics, 1987, 61, 669-692.	0.8	40
129	Molecular dynamics studies of the condensed phases of n-butane and their transitions. Molecular Physics, 1987, 61, 693-709.	0.8	13
130	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
131	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
132	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
133	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