Martin Dove

List of Publications by Year
in descending order

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302 papers	13,640 citations	22153 59 h-index	32842 100 g-index
307 all docs	307 docs citations	307 times ranked	10495 citing authors

#	Article	IF	Citations
1	DL_POLY_3: new dimensions in molecular dynamics simulations via massive parallelism. Journal of Materials Chemistry, 2006, 16, 1911.	6.7	1,010
2	Colossal Positive and Negative Thermal Expansion in the Framework Material Ag ₃ [Co(CN) ₆]. Science, 2008, 319, 794-797.	12.6	575
3	RMCProfile: reverse Monte Carlo for polycrystalline materials. Journal of Physics Condensed Matter, 2007, 19, 335218.	1.8	351
4	Theory of displacive phase transitions in minerals. American Mineralogist, 1997, 82, 213-244.	1.9	247
5	Structure and Properties of an Amorphous Metal-Organic Framework. Physical Review Letters, 2010, 104, 115503.	7.8	246
6	Rigid-unit phonon modes and structural phase transitions in framework silicates. American Mineralogist, 1996, 81, 1057-1079.	1.9	235
7	Origin of the negative thermal expansion in and. Journal of Physics Condensed Matter, 1996, 8, 10973-10982.	1.8	234
8	The determination of rigid-unit modes as potential soft modes for displacive phase transitions in framework crystal structures. Acta Crystallographica Section A: Foundations and Advances, 1993, 49, 697-703.	0.3	226
9	Zinc incorporation into hydroxylapatite. Biomaterials, 2009, 30, 2864-2872.	11.4	215
10	Negative thermal expansion and associated anomalous physical properties: review of the lattice dynamics theoretical foundation. Reports on Progress in Physics, 2016, 79, 066503.	20.1	211
11	Calibration of excess thermodynamic properties and elastic constant variations associated with the alpha <-->beta phase transition in quartz. American Mineralogist, 1998, 83, 2-22.	1.9	197
12	Negative Thermal Expansion inZrW2O8: Mechanisms, Rigid Unit Modes, and Neutron Total Scattering. Physical Review Letters, 2005, 95, 255501.	7.8	164
13	Nanoporous Structure and Medium-Range Order in Synthetic Amorphous Calcium Carbonate. Chemistry of Materials, 2010, 22, 3197-3205.	6.7	160
14	Adsorption and migration of alkali metals (Li, Na, and K) on pristine and defective graphene surfaces. Nanoscale, 2019, 11, 5274-5284.	5.6	149
15	Rigid unit modes in framework silicates. Mineralogical Magazine, 1995, 59, 629-639.	1.4	147
16	A detailed structural characterization of quartz on heating through the Î±â€“Î² phase transition. Mineralogical Magazine, 2001, 65, 489-507.	1.4	132
17	Geometrical Origin and Theory of Negative Thermal Expansion in Framework Structures. Journal of the American Ceramic Society, 1999, 82, 1793-1802.	3.8	130
18	Role of Disorder in the Thermodynamics and Atomic Dynamics of Glasses. Physical Review Letters, 2014, 112, 025502.	7.8	125

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19	Floppy Modes in Crystalline and Amorphous Silicates. Physical Review Letters, 1997, 78, 1070-1073.	7.8	123
20	Low-frequency floppy modes in Î²-cristobalite. Physical Review Letters, 1993, 71, 193-196.	7.8	122
21	Trapping of oxygen vacancies on twin walls of CaTiO3: a computer simulation study. Journal of Physics Condensed Matter, 2003, 15, 2301-2307.	1.8	118
22	Structural behavior, crystal chemistry, and phase transitions in substituted leucite; high-resolution neutron powder diffraction studies. American Mineralogist, 1997, 82, 16-29.	1.9	117
23	Rigid-Unit Modes and the Quantitative Determination of the Flexibility Possessed by Zeolite Frameworks. Journal of Physical Chemistry B, 1998, 102, 1759-1767.	2.6	117
24	Landau free energy and order parameter behaviour of theÎ±/Î²phase transition in cristobalite. Zeitschrift FÃ¼r Kristallographie, 1992, 201, 125-145.	1.1	116
25	Neutron total scattering method: simultaneous determination of long-range and short-range order in disordered materials. European Journal of Mineralogy, 2002, 14, 331-348.	1.3	109
26	Negative thermal expansion in beta-quartz. Physics and Chemistry of Minerals, 1998, 26, 63-77.	0.8	107
27	How the nature of the chemical bond governs resistance to amorphization by radiation damage. Physical Review B, 2005, 71, .	3.2	104
28	Crystal structure and paramagnetic behaviour of. Journal of Physics Condensed Matter, 1997, 9, 6563-6577.	1.8	100
29	Neutron powder diffraction study of the ï¿½kermanite-gehlenite solid solution series. Physics and Chemistry of Minerals, 1992, 19, 185.	0.8	99
30	Direct measurement of the Si-O bond length and orientational disorder in the high-temperature phase of cristobalite. Physics and Chemistry of Minerals, 1997, 24, 311-317.	0.8	99
31	Structure Determination of Disordered Materials from Diffraction Data. Physical Review Letters, 2010, 104, 125501.	7.8	97
32	How Floppy Modes Give Rise to Adsorption Sites in Zeolites. Physical Review Letters, 1997, 78, 3701-3704.	7.8	96
33	Application of the reverse Monte Carlo method to crystalline materials. Journal of Applied Crystallography, 2001, 34, 630-638.	4.5	94
34	Emergence and Evolution of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>k</mml:mi></mml:math> Gap in Spectra of Liquid and Supercritical States. Physical Review Letters, 2017, 118, 215502.	7.8	85
35	Computational methods for the study of energies of cation distributions: applications to cation-ordering phase transitions and solid solutions. Mineralogical Magazine, 2001, 65, 193-219.	1.4	84
36	Network Rigidity and Properties ofSiO2andGeO2Glasses under Pressure. Physical Review Letters, 2004, 93, 135502.	7.8	82

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37	Argentophilicity-Dependent Colossal Thermal Expansion in Extended Prussian Blue Analogues. Journal of the American Chemical Society, 2008, 130, 9660-9661.	13.7	82
38	Thermally-induced reversible structural isomerization in colloidal semiconductor CdS magic-size clusters. Nature Communications, 2018, 9, 2499.	12.8	79
39	Local structures of amorphous and crystalline phases of silica, SiO2, by neutron total scattering. Journal of Physics Condensed Matter, 1999, 11, 9263-9273.	1.8	78
40	Modeling of dioctahedral 2:1 phyllosilicates by means of transferable empirical potentials. Physics and Chemistry of Minerals, 2001, 28, 130-141.	0.8	78
41	Rigid unit modes and the negative thermal expansion in ZrW₂O₈. Phase Transitions, 1997, 61, 141-153.	1.3	75
42	Structural changes in zircon under Î±-decay irradiation. Physical Review B, 2002, 65, .	3.2	75
43	Simulation studies on the pyrope-grossular garnet solid solution. Physics and Chemistry of Minerals, 2000, 27, 398-418.	0.8	74
44	Magnetic Structure of MnO at 10ÂK from Total Neutron Scattering Data. Physical Review Letters, 2006, 96, 047209.	7.8	74
45	The nature of high-energy radiation damage in iron. Journal of Physics Condensed Matter, 2013, 25, 125402.	1.8	74
46	Thermodynamics of Al/Al avoidance in the ordering of Al/Si tetrahedral framework structures. Physics and Chemistry of Minerals, 1998, 25, 457-464.	0.8	72
47	Compressibility, kinetics, and phase transition in pressurized amorphous silica. Physical Review B, 2003, 67, .	3.2	72
48	Dynamic structural disorder in cristobalite: neutron total scattering measurement and reverse Monte Carlo modelling. Journal of Physics Condensed Matter, 2001, 13, 403-423.	1.8	71
49	Atomistic simulations of resistance to amorphization by radiation damage. Physical Review B, 2006, 73, .	3.2	68
50	Molecular dynamics simulation of alpha - and beta -cristobalite. Journal of Physics Condensed Matter, 1995, 7, 1771-1788.	1.8	67
51	Rigid unit modes in crystal structures with octahedrally coordinated atoms. American Mineralogist, 1998, 83, 476-479.	1.9	67
52	Monte Carlo methods for the study of cation ordering in minerals. Mineralogical Magazine, 2001, 65, 221-248.	1.4	67
53	The phenomenon of low Al-Si ordering temperatures in aluminosilicate framework structures. American Mineralogist, 1996, 81, 349-362.	1.9	66
54	Structural Description of Pressure-Induced Amorphization inZrW2O8. Physical Review Letters, 2007, 98, 225501.	7.8	65

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55	Impact of self-irradiation damage on the aqueous durability of zircon (ZrSiO4): implications for its suitability as a nuclear waste form. Journal of Physics Condensed Matter, 2003, 15, L597-L605.	1.8	64
56	On the displacive character of the phase transition in quartz: a hard-mode spectroscopy study. Journal of Physics Condensed Matter, 1992, 4, 571-577.	1.8	62
57	On the thermal expansion of ?-cristobalite. Physics and Chemistry of Minerals, 1995, 22, 61.	0.8	62
58	Acoustic phonons and negative thermal expansion in MOF-5. Physical Chemistry Chemical Physics, 2014, 16, 21144-21152.	2.8	61
59	A molecular dynamics simulation study of the plastic crystalline phase of sulphur hexafluoride. Journal of Physics C: Solid State Physics, 1983, 16, 5969-5983.	1.5	60
60	Neutron diffraction at simultaneous high temperatures and pressures, with measurement of temperature by neutron radiography. Mineralogical Magazine, 2001, 65, 737-748.	1.4	60
61	An interatomic potential model for carbonates allowing for polarization effects. Physics and Chemistry of Minerals, 2003, 30, 416-424.	0.8	58
62	Study of cation order-disorder in MgAl₂O₄spinel by in situ neutron diffraction up to 1600 K and 3.2 GPa. American Mineralogist, 2004, 89, 981-986.	1.9	56
63	Refinement of the Siâ€“Oâ€“Si bond angle distribution in vitreous silica. Journal of Physics Condensed Matter, 2005, 17, S67-S75.	1.8	56
64	Computational study of tetrahedral Al-Si ordering in muscovite. Physics and Chemistry of Minerals, 2001, 28, 534-544.	0.8	55
65	On the application of mean-field and landau theory to displacive phase transitions. Ferroelectrics, 1992, 136, 33-49.	0.6	54
66	Low Energy Dynamics and Tunneling States in Silica Glass. Physical Review Letters, 1998, 81, 3431-3434.	7.8	54
67	Atomistic modelling of radiation damage in zircon. Journal of Physics Condensed Matter, 2001, 13, 1947-1959.	1.8	54
68	Structural disorder and loss of piezoelectric properties in Î±-quartz at high temperature. Applied Physics Letters, 2002, 81, 2968-2970.	3.3	54
69	Infrared and Raman spectroscopy studies of the ??? phase transition in cristobalite. Physics and Chemistry of Minerals, 2003, 30, 353-365.	0.8	54
70	The heat capacity of matter beyond the Dulongâ€“Petit value. Journal of Physics Condensed Matter, 2013, 25, 235401.	1.8	54
71	On the Sequence of Phase Transitions in Tridymite. Physics and Chemistry of Minerals, 1998, 26, 171-179.	0.8	52
72	Reverse Monte Carlo modelling of crystalline disorder. Journal of Physics Condensed Matter, 2005, 17, S15-S22.	1.8	52

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73	Frenkel line and solubility maximum in supercritical fluids. Physical Review E, 2015, 91, 012112.	2.1	52
74	Simultaneous analysis of changes in long-range and short-range structural order at the displacive phase transition in quartz. Journal of Physics Condensed Matter, 2000, 12, L723-L730.	1.8	51
75	Direct measurement of the thermal expansion of the Si-O bond by neutron total scattering. Journal of Physics Condensed Matter, 2000, 12, L425-L430.	1.8	51
76	Dynamics of silica glass: two-level tunnelling states and low-energy floppy modes. Journal of Physics Condensed Matter, 2000, 12, 8041-8064.	1.8	51
77	Pressure-induced softening as a common feature of framework structures with negative thermal expansion. Physical Review B, 2013, 87, .	3.2	49
78	Densification of silica glass under pressure. Journal of Physics Condensed Matter, 2002, 14, 7449-7459.	1.8	48
79	A molecular dynamics simulation study of the orientationally disordered phase of sulphur hexafluoride. Journal of Physics C: Solid State Physics, 1984, 17, 6581-6599.	1.5	47
80	Crystal structure of the high-pressure monoclinic phase-II of cristobalite, SiO2. Mineralogical Magazine, 2000, 64, 569-576.	1.4	47
81	Origin of Ferroelectricity in Two Prototypical Hybrid Organicâ€“Inorganic Perovskites. Journal of the American Chemical Society, 2022, 144, 816-823.	13.7	47
82	Monte Carlo simulations of ordering of Al, Fe, and Mg cations in the octahedral sheet of smectites and illites. American Mineralogist, 2003, 88, 1033-1045.	1.9	46
83	Simulation study of pressure and temperature dependence of the negative thermal expansion in Zn(CN)<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>. Physical Review B, 2013, 88, .	3.2	46
84	Finding best-fit polyhedral rotations with geometric algebra. Journal of Physics Condensed Matter, 2002, 14, 4567-4584.	1.8	45
85	Large swelling and percolation in irradiated zircon. Journal of Physics Condensed Matter, 2003, 15, L1-L7.	1.8	45
86	DFT study of the cation arrangements in the octahedral and tetrahedral sheets of dioctahedral 2:1 phyllosilicates. Physics and Chemistry of Minerals, 2006, 33, 655-666.	0.8	45
87	Neutron powder diffraction study of the ferroelastic phase transition and lattice melting in sodium carbonate, Na2CO3. Journal of Physics Condensed Matter, 1995, 7, 4395-4417.	1.8	44
88	Disordering of MgAl2O4 spinel from first principles. Mineralogical Magazine, 2000, 64, 311-317.	1.4	44
89	Ferroelectric nanoscale domains and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>905</mml:mn><mml:mspace width="0.3em" /><mml:mi mathvariant="normal">K</mml:mi></mml:mrow></mml:math>phase transition in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sr</mml:mi><mml:mi mathvariant="normal">Sn</mml:mi><mml:msub><mml:mi	3.2	44
90	Electronic effects in high-energy radiation damage in iron. Journal of Physics Condensed Matter, 2014, 26, 085401.	1.8	44

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91	Local structure of the metalâ€“organic perovskite dimethylammonium manganese(<scp>ii</scp>) formate. Dalton Transactions, 2016, 45, 4380-4391.	3.3	44
92	Real-space rigid-unit-mode analysis of dynamic disorder in quartz, cristobalite and amorphous silica. Journal of Physics Condensed Matter, 2002, 14, 4645-4657.	1.8	43
93	Discreteâ€“element modelling: methods and applications in the environmental sciences. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2004, 362, 1797-1816.	3.4	42
94	Common origin of negative thermal expansion and other exotic properties in ceramic and hybrid materials. Physical Review B, 2014, 89, .	3.2	42
95	Orientational ordering and the low temperature structure of SF6. Molecular Physics, 1987, 62, 1127-1141.	1.7	41
96	Surface relaxations in hydroxyapatite. Journal of Physics Condensed Matter, 2000, 12, 9829-9841.	1.8	41
97	Scaling of thermodynamic mixing properties in garnet solid solutions. Physics and Chemistry of Minerals, 2001, 28, 177-187.	0.8	41
98	Thermodynamic properties of MgSiO3 perovskite derived from large scale molecular dynamics simulations. Physics and Chemistry of Minerals, 1992, 18, 407.	0.8	40
99	Rigid unit modes in the high-temperature phase of SiO2 tridymite: calculations and electron diffraction. Physics and Chemistry of Minerals, 1996, 23, 56.	0.8	40
100	Ab initiosimulations of cation ordering in oxides: application to spinel. Journal of Physics Condensed Matter, 2000, 12, L43-L48.	1.8	40
101	Reverse Monte Carlo with geometric analysis â€“ RMC+GA. Journal of Applied Crystallography, 2004, 37, 536-544.	4.5	40
102	What do Landau free energies really look like for structural phase transitions?. Journal of Physics Condensed Matter, 1989, 1, 8327-8335.	1.8	39
103	Theoretical modelling of cis â€Š-vacant and trans â€Š-vacant configurations in the octahedral sheet of illites and smectites. Physics and Chemistry of Minerals, 2001, 28, 322-331.	0.8	39
104	Radiation damage effects and percolation theory. Journal of Physics Condensed Matter, 2004, 16, S2623-S2627.	1.8	39
105	Anatomy of a structural phase transition: theoretical analysis of the displacive phase transition in quartz and other silicates. Physics and Chemistry of Minerals, 1999, 26, 344-353.	0.8	38
106	Rigid Unit Modes in Framework Structures: Theory, Experiment and Applications. Reviews in Mineralogy and Geochemistry, 2000, 39, 1-33.	4.8	38
107	Total scattering and reverse Monte Carlo study of the 105 K displacive phase transition in strontium titanate. Journal of Physics Condensed Matter, 2005, 17, S111-S124.	1.8	38
108	Distortions of framework structures. Phase Transitions, 1996, 58, 121-143.	1.3	37

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109	Intermediate state in pressurized silica glass: Reversibility window analogue. Physical Review B, 2003, 67, .	3.2	37
110	A computational study of Al/Si ordering in cordierite. Physics and Chemistry of Minerals, 1996, 23, 127.	0.8	35
111	Radiation damage effects in the perovskiteCaTiO3and resistance of materials to amorphization. Physical Review B, 2004, 70, .	3.2	35
112	Anomalous inelastic neutron scattering from calcite. Journal of Physics Condensed Matter, 1992, 4, 2761-2774.	1.8	34
113	A computer simulation study of Al/Si ordering in gehlenite and the paradox of the low transition temperature. Physics and Chemistry of Minerals, 1994, 21, 110.	0.8	34
114	Phase transitions in tridymite studied using â€˜Rigid Unit Modeâ€™ theory, Reverse Monte Carlo methods and molecular dynamics simulations. Mineralogical Magazine, 2000, 64, 267-283.	1.4	34
115	Local structure in Ag₃[Co(CN)₆]: colossal thermal expansion, rigid unit modes and argentophilic interactions. Journal of Physics Condensed Matter, 2008, 20, 255225.	1.8	34
116	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:mathvariant="normal">O</mml:mi></mml:math>. Physical Review B, 2014, 89, .	3.2	34
117	Octahedral cation ordering of illite and smectite. Theoretical exchange potential determination and Monte Carlo simulations. Physics and Chemistry of Minerals, 2003, 30, 382-392.	0.8	33
118	Rigid unit modes and dynamic disorder: SiO 2 cristobalite and quartz. Physics and Chemistry of Minerals, 1999, 26, 484-495.	0.8	32
119	Anisotropic ionic transport in quartz: the effect of twin boundaries. Journal of Physics Condensed Matter, 2001, 13, 9445-9454.	1.8	32
120	An introduction to the use of neutron scattering methods in mineral sciences. European Journal of Mineralogy, 2002, 14, 203-224.	1.3	32
121	Model-independent extraction of dynamical information from powder diffraction data. Physical Review B, 2005, 72, .	3.2	32
122	Modelling the percolation-type transition in radiation damage. Journal of Applied Physics, 2000, 87, 7702-7707.	2.5	30
123	A computational investigation of the Al/Fe/Mg order-disorder behavior in the dioctahedral sheet of phyllosilicates. American Mineralogist, 2004, 89, 164-175.	1.9	30
124	Aperiodicity, structure, and dynamics inNi(CN)2. Physical Review B, 2009, 80, .	3.2	30
125	Neutron powder diffraction study of the orientational orderâ€“disorder phase transition in calcite, CaCO3. Physics and Chemistry of Minerals, 2005, 32, 493-503.	0.8	29
126	Total scattering studies of silica polymorphs: similarities in glass and disordered crystalline local structure. Mineralogical Magazine, 2000, 64, 447-457.	1.4	28

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127	Floppy modes in silica glass under pressure. Journal of Physics Condensed Matter, 2002, 14, 1143-1152.	1.8	28
128	Phonons from Powder Diffraction: A Quantitative Model-Independent Evaluation. Physical Review Letters, 2004, 93, 075502.	7.8	28
129	Flexibility of zeolitic imidazolate framework structures studied by neutron total scattering and the reverse Monte Carlo method. Journal of Physics Condensed Matter, 2013, 25, 395403.	1.8	28
130	A simulation study of the disordered phase of CBr4. I. Single-particle properties. Journal of Physics C: Solid State Physics, 1986, 19, 3325-3341.	1.5	27
131	Effect of surface relaxations on the equilibrium growth morphology of crystals: platelet formation. Journal of Physics Condensed Matter, 1999, 11, 7385-7410.	1.8	27
132	Temperature measurement in a Paris-Edinburgh cell by neutron resonance spectroscopy. Journal of Applied Physics, 2005, 98, 064905.	2.5	27
133	Temperature-dependent pressure-induced softening in Zn(CN)<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>. Physical Review B, 2013, 88, .	3.2	27
134	High-energy radiation damage in zirconia: Modeling results. Journal of Applied Physics, 2014, 115, .	2.5	27
135	The Ginzburg interval in soft-mode phase transitions: consequences of the rigid unit mode picture. Journal of Physics Condensed Matter, 1994, 6, 3171-3196.	1.8	26
136	Local structure in ZrW₂O₈from neutron total scattering. Journal of Physics Condensed Matter, 2007, 19, 335215.	1.8	26
137	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:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	3.2	26
138	The use of Monte Carlo methods to determine the distribution of Al and Si cations in framework aluminosilicates from²⁹Si MAS NMR data. American Mineralogist, 1996, 81, 39-44.	1.9	25
139	Simulation studies of at high pressure. Journal of Physics Condensed Matter, 1998, 10, 8417-8428.	1.8	25
140	Flexibility of network materials and the Rigid Unit Mode model: a personal perspective. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2019, 377, 20180222.	3.4	25
141	Comment on â€˜â€˜First-principles studies on structural properties of Î²-cristobaliteâ€™â€™. Physical Review Letters, 1993, 71, 3610-3610.	7.8	24
142	Rigid Unit Modes in disordered nepheline: a study of a displacive incommensurate phase transition. Physics and Chemistry of Minerals, 2000, 27, 285-290.	0.8	24
143	Pair distribution functions calculated from interatomic potential models using theGeneral Utility Lattice Program. Journal of Applied Crystallography, 2007, 40, 589-594.	4.5	24
144	Direct links between dynamical, thermodynamic, and structural properties of liquids: Modeling results. Physical Review E, 2017, 95, 032116.	2.1	24

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145	Collective modes and gapped momentum states in liquid Ga: Experiment, theory, and simulation. Physical Review B, 2020, 101, .	3.2	24
146	Lattice simulation studies of the ferroelastic phase transitions in (Na,K)AlSi₃O₈and (Sr,Ca)Al₂Si₂O₈feldspar solid solutions. American Mineralogist, 1997, 82, 8-15.	1.9	24
147	Origin of the colossal positive and negative thermal expansion in Ag3[Co(CN)6]: anab initiodensity functional theory study. Journal of Physics Condensed Matter, 2008, 20, 255226.	1.8	23
148	Phonon stabilized polytypism in PbI2: in situ Raman spectroscopy and transferable core-shell model calculations. Journal of Physics Condensed Matter, 1991, 3, 539-550.	1.8	22
149	The origin of the compressibility anomaly in amorphous silica: a molecular dynamics study. Journal of Physics Condensed Matter, 2007, 19, 275210.	1.8	22
150	The compressibility and high pressure structure of diopside from first principles simulation. Physics and Chemistry of Minerals, 2008, 35, 359-366.	0.8	22
151	First-principles calculations of structural changes in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>B</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mte under pressure. Physical Review B, 2008, 78, .	3.2	22
152	Structures of CdSe and CdS Nanoclusters from Ab Initio Random Structure Searching. Journal of Physical Chemistry C, 2019, 123, 29370-29378.	3.1	22
153	Structural phase transitions in malononitrile. Faraday Discussions of the Chemical Society, 1980, 69, 98.	2.2	21
154	Insights into zeolite behaviour from the rigid unit mode model. Phase Transitions, 1997, 61, 155-172.	1.3	21
155	Amorphous silica from the Rigid Unit Mode approach. Mineralogical Magazine, 2000, 64, 377-388.	1.4	21
156	Exotic distributions of rigid unit modes in the reciprocal spaces of framework aluminosilicates. Journal of Physics Condensed Matter, 2007, 19, 275209.	1.8	21
157	Thermal Disorder and Bond Anharmonicity in Cesium Lead Iodide Studied by Neutron Total Scattering and the Reverse Monte Carlo Method. Journal of Physical Chemistry C, 2019, 123, 14934-14940.	3.1	21
158	Quantitative understanding of negative thermal expansion in scandium trifluoride from neutron total scattering measurements. Physical Review B, 2020, 102, .	3.2	20
159	MCGRtof: Monte CarloG(r) with resolution corrections for time-of-flight neutron diffractometers. Journal of Applied Crystallography, 2001, 34, 780-782.	4.5	19
160	Computational study of tetrahedral Alâ€“Si and octahedral Alâ€“Mg ordering in phengite. Physics and Chemistry of Minerals, 2003, 30, 293-304.	0.8	19
161	Simulation of radiation damage in gadolinium pyrochlores. Journal of Physics Condensed Matter, 2006, 18, 2217-2234.	1.8	19
162	Pressure-Induced Structural Transformation in Radiation-Amorphized Zircon. Physical Review Letters, 2007, 98, 135502.	7.8	19

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163	Molecular dynamics simulation study of various zeolitic imidazolate framework structures. Dalton Transactions, 2016, 45, 4289-4302.	3.3	19
164	Colossal Pressure-Induced Softening in Scandium Fluoride. Physical Review Letters, 2020, 124, 255502.	7.8	19
165	Floppy modes and the Boson peak in crystalline and amorphous silicates: an inelastic neutron scattering study. Mineralogical Magazine, 2000, 64, 435-440.	1.4	18
166	A phenomenological expression to describe the temperature dependence of pressure-induced softening in negative thermal expansion materials. Journal of Physics Condensed Matter, 2014, 26, 115402.	1.8	18
167	Orientational Disorder in Adamantane and Adamantanecarboxylic Acid. ChemPhysChem, 2017, 18, 459-464.	2.1	18
168	Yang etÂal. Reply:. Physical Review Letters, 2018, 120, 219602.	7.8	18
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