Neil Allan

List of Publications by Year
in descending order

161 papers	5,556 citations	109321 35 h-index	91884 69 g-index
164 all docs	164 docs citations	164 times ranked	6069 citing authors

#	Article	IF	Citations
1	Graphitic Nanofilms as Precursors to Wurtzite Films: Theory. Physical Review Letters, 2006, 96, 066102.	7.8	514
2	Ab initiostudy of MnO and NiO. Physical Review B, 1994, 50, 5041-5054.	3.2	441
3	Negative thermal expansion. Journal of Physics Condensed Matter, 2005, 17, R217-R252.	1.8	437
4	Growth of ZnO thin filmsâ€"experiment and theory. Journal of Materials Chemistry, 2005, 15, 139-148.	6.7	364
5	Strikingly Long CÂ·Â·Â·C Distances in 1,2-Disubstitutedortho-Carboranes and Their Dianions. Journal of the American Chemical Society, 2005, 127, 13538-13547.	13.7	178
6	Wetting of Water and Water/Ethanol Droplets on a Non-Polar Surface:Â A Molecular Dynamics Study. Langmuir, 2002, 18, 10462-10466.	3.5	111
7	Modeling of Wetting:Â A Study of Nanowetting at Rough and Heterogeneous Surfaces. Langmuir, 2007, 23, 1187-1194.	3.5	110
8	The â€˜zero chargeâ€™ partitioning behaviour of noble gases during mantle melting. Nature, 2003, 423, 738-741.	27.8	107
9	The embedded many-body expansion for energetics of molecular crystals. Journal of Chemical Physics, 2012, 137, 164102.	3.0	102
10	Raman spectroscopy of nanocrystalline diamond: Anab initioapproach. Physical Review B, 2006, 74, .	3.2	93
11	Thermodynamics and mechanism of theB1-B2phase transition in group-I halides and group-II oxides. Physical Review B, 1998, 57, 11164-11172.	3.2	87
12	Computer simulation of water molecules at kaolinite and silica surfaces. Physical Chemistry Chemical Physics, 2000, 2, 3663-3668.	2.8	87
13	Molecular Dynamics Study of Wetting of a Pillar Surface. Langmuir, 2003, 19, 7127-7129.	3.5	87
14	Free-energy derivatives and structure optimization within quasiharmonic lattice dynamics. Physical Review B, 1997, 56, 14380-14390.	3.2	83
15	Phosphorus carbides: theory and experiment. Dalton Transactions, 2004, , 3085.	3.3	75
16	Sputtering of grains in C-type shocks. Monthly Notices of the Royal Astronomical Society, 2000, 318, 809-816.	4.4	66
17	Calculation of properties of crystalline lithium hydride using correlated wave function theory. Physical Review B, 2009, 80, .	3.2	66
18	Displacement cascades in Gd2Ti2O7 and Gd2Zr2O7: a molecular dynamics study. Journal of Materials Chemistry, 2002, 12, 2923-2926.	6.7	65

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19	MgO addimer diffusion on MgO(100): A comparison ofab initioand empirical models. Physical Review B, 2005, 72, .	3.2	64
20	Raman spectroscopy of diamondoids. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2006, 64, 681-692.	3.9	64
21	The zero static internal stress approximation in lattice dynamics, and the calculation of isotope effects on molar volumes. Journal of Chemical Physics, 1996, 105, 8300-8303.	3.0	62
22	Towards new binary compounds: Synthesis of amorphous phosphorus carbide by pulsed laser deposition. Journal of Solid State Chemistry, 2013, 198, 466-474.	2.9	53
23	Monte Carlo and Hybrid Monte Carlo/Molecular Dynamics Approaches to Orderâ"Disorder in Alloys, Oxides, and Silicates. Journal of Physical Chemistry B, 1998, 102, 5202-5207.	2.6	51
24	Ab initio calculation of phase diagrams of ceramics and minerals. Journal of Materials Chemistry, 2001, 11, 63-68.	6.7	48
25	Carbon nitride:Ab initioinvestigation of carbon-rich phases. Physical Review B, 2009, 80, .	3.2	48
26	Thermal expansion of polymers: Mechanisms in orthorhombic polyethylene. Physical Review B, 1998, 58, 8416-8427.	3.2	44
27	Order in the disordered state: local structural entities in the fast ion conductor Ba2In2O5. Journal of Solid State Chemistry, 2005, 178, 346-355.	2.9	42
28	Ionic solids at elevated temperatures and high pressures: MgF2. Journal of Chemical Physics, 1997, 107, 4337-4344.	3.0	41
29	Simulation of mineral solid solutions at zero and high pressure using lattice statics, lattice dynamics and Monte Carlo methods. Journal of Physics Condensed Matter, 2004, 16, S2751-S2770.	1.8	41
30	Ab Initio Calculation of Phase Diagrams of Oxides. Journal of Physical Chemistry B, 2001, 105, 3594-3599.	2.6	39
31	Free energy of solid solutions and phase diagrams via quasiharmonic lattice dynamics. Physical Review B, 2001, 63, .	3.2	39
32	Free energy of formation of defects in polar solids. Faraday Discussions, 1997, 106, 377-387.	3.2	38
33	Solid phases of phosphorus carbide: Anab initiostudy. Physical Review B, 2009, 79, .	3.2	37
34	Molecular similarity of anti-HIV phospholipids. Journal of the American Chemical Society, 1993, 115, 12615-12616.	13.7	36
35	Novel potentials for modelling defect formation and oxygen vacancy migration in Gd2Ti2O7 and Gd2Zr2O7 pyrochlores. Journal of Materials Chemistry, 2012, 22, 4675.	6.7	36
36	Quasiharmonic free energy and derivatives for slabs:â€ƒOxide surfaces at elevated temperatures. Physical Review B, 1999, 59, 6742-6751.	3.2	35

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37	Oxygen ion migration in La₂CuO₄. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 1991, 64, 1129-1132.	0.6	34
38	Simulations of chemical vapor deposition diamond film growth using a kinetic Monte Carlo model. Journal of Applied Physics, 2010, 108, .	2.5	33
39	Improving density functional theory for crystal polymorph energetics. Physical Chemistry Chemical Physics, 2012, 14, 7739.	2.8	32
40	Trace element incorporation into pyrope-grossular solid solutions: an atomistic simulation study. Physics and Chemistry of Minerals, 2003, 30, 217-229.	0.8	31
41	Momentum space properties and local density approximations in small molecules: A critical appraisal. Journal of Chemical Physics, 1986, 84, 5594-5605.	3.0	30
42	Local cation environments in the pyropeâ€“grossularMg3Al2Si3O12â€“Ca3Al2Si3O12garnet solid solution. Physical Review B, 2006, 74, .	3.2	30
43	Computer simulation of high-temperature, forsterite-melt partitioning. American Mineralogist, 2000, 85, 1087-1091.	1.9	29
44	Orderâ€“disorder in grossly non-stoichiometric SrFeO2.50â€” a simulation study. Physical Chemistry Chemical Physics, 2003, 5, 2237-2243.	2.8	29
45	Simple refinements of Brillouin zone integration. Journal of Physics Condensed Matter, 2000, 12, 549-558.	1.8	28
46	Collective ionic motion in oxide fast-ion-conductors. Physical Chemistry Chemical Physics, 2004, 6, 3052-3055.	2.8	28
47	Activityâ€“composition relations in the system CaCO3â€“MgCO3 predicted from static structure energy calculations and Monte Carlo simulations. Geochimica Et Cosmochimica Acta, 2007, 71, 974-983.	3.9	28
48	Bulk and surface energetics of crystalline lithium hydride: Benchmarks from quantum Monte Carlo and quantum chemistry. Physical Review B, 2010, 82, .	3.2	27
49	Ionic solids at high pressures and elevated temperatures: MgO (periclase). Journal of Chemical Physics, 1991, 95, 6792-6799.	3.0	26
50	Ionic solids at elevated temperatures and/or high pressures: lattice dynamics, molecular dynamics, Monte Carlo and ab initio studies. Physical Chemistry Chemical Physics, 2000, 2, 1099-1111.	2.8	26
51	Light Metals on Oxygen-Terminated Diamond (100): Structure and Electronic Properties. Chemistry of Materials, 2015, 27, 1306-1315.	6.7	26
52	Three-dimensional kinetic Monte Carlo simulations of diamond chemical vapor deposition. Journal of Chemical Physics, 2015, 142, 214707.	3.0	26
53	Momentum-space electron densities and quantum molecular similarity. Topics in Current Chemistry, 1995, , 85-111.	4.0	25
54	Atomistic simulations of trace element incorporation into the large site of MgSiO3 and CaSiO3 perovskites. Physics of the Earth and Planetary Interiors, 2003, 139, 113-127.	1.9	24

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55	Simplified Monte Carlo simulations of chemical vapour deposition diamond growth. Journal of Physics Condensed Matter, 2009, 21, 364203.	1.8	24
56	Atomistic lattice simulations of the ternary fluorides AMF3(A = Li, Na, K, Rb, Cs; M = Mg, Ca, Sr, Ba). Journal of Materials Chemistry, 1991, 1, 1035.	6.7	23
57	Topography of the Potential Energy Hypersurface and Criteria for Fast-Ion Conduction in Perovskite-Related A2B2O5 Oxides. Journal of Physical Chemistry B, 2005, 109, 12362-12365.	2.6	22
58	GaPâ€ZnS Solid Solutions: Semiconductors for Efficient Visible Light Absorption and Emission. Advanced Materials, 2013, 25, 2989-2993.	21.0	22
59	Semigrand-canonical ensemble simulations of the phase diagrams of alloys. Modelling and Simulation in Materials Science and Engineering, 2003, 11, 115-126.	2.0	21
60	Interfacial storage of noble gases and other trace elements in magmatic systems. Earth and Planetary Science Letters, 2012, 319-320, 287-294.	4.4	21
61	Growth of nano-domains in Gdâ€“CeO₂ mixtures: hybrid Monte Carlo simulations. Journal of Materials Chemistry A, 2016, 4, 4592-4602.	10.3	21
62	Atomistic Simulation of High-Tc Oxides. Journal of the American Ceramic Society, 1990, 73, 3175-3184.	3.8	20
63	Applications of momentum-space similarity. Journal of Computer-Aided Molecular Design, 1995, 9, 331-340.	2.9	20
64	Structureâ€”property relationships and momentum space quantities: Hammett Ïƒâ€”constants. Molecular Physics, 2003, 101, 3159-3162.	1.7	20
65	Ba2In2O4(OH)2: Proton sites, disorder and vibrational properties. Journal of Solid State Chemistry, 2007, 180, 3388-3392.	2.9	20
66	Simulations of chemical vapor deposition diamond film growth using a kinetic Monte Carlo model and two-dimensional models of microwave plasma and hot filament chemical vapor deposition reactors. Journal of Applied Physics, 2010, 108, .	2.5	20
67	Titanium in subduction zone fluids: First insights from ab initio molecular metadynamics simulations. Geochimica Et Cosmochimica Acta, 2010, 74, 2797-2810.	3.9	20
68	Impurity cations in the bulk and the {001} surface of muscovite: an atomistic simulation study. Journal of Materials Chemistry, 1997, 7, 1947-1951.	6.7	19
69	Simulation of radiation damage in gadolinium pyrochlores. Journal of Physics Condensed Matter, 2006, 18, 2217-2234.	1.8	19
70	Super stretchable hexagonal boron nitride Kirigami. Thin Solid Films, 2017, 632, 35-43.	1.8	19
71	Simulations of doped CeO2 at finite dopant concentrations. Solid State Ionics, 2017, 299, 32-37.	2.7	19
72	Ionic halides and oxides at high pressure: calculated Hugoniots, isotherms and thermal pressures. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 4369.	1.7	18

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73	Density functional theory and interionic potentials. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 69, 871-878.	0.6	18
74	Adaptive kinetic Monte Carlo simulation of solid oxide fuel cell components. Journal of Materials Chemistry A, 2014, 2, 13407-13414.	10.3	18
75	Quantum molecular similarity via momentumâ€space indices. Journal of Mathematical Chemistry, 1998, 23, 51-60.	1.5	17
76	Simulation of thermodynamic mixing properties of garnet solid solutions at high temperatures and pressures. Chemical Geology, 2006, 225, 336-346.	3.3	17
77	The Practical Calculation of Interionic Potentials in Solids using Electron Gas Theory. Molecular Simulation, 1990, 4, 269-283.	2.0	16
78	Solid phosphorus carbide?. Chemical Communications, 2002, , 2494-2495.	4.1	16
79	Binary phosphorus-carbon compounds: The series P4C3+8n. International Journal of Quantum Chemistry, 2003, 95, 546-553.	2.0	16
80	Sr and Ga substituted Ba2In2O5: Linking ionic conductivity and the potential energy surface. Solid State Ionics, 2006, 177, 223-228.	2.7	16
81	Molecular modelling of rare earth element complexation in subduction zone fluids. Geochimica Et Cosmochimica Acta, 2009, 73, 3934-3947.	3.9	16
82	Hybrid Monte Carlo and lattice dynamics simulations: the enthalpy of mixing of binary oxides. Chemical Communications, 1998, , 627-628.	4.1	15
83	A study of the electronic, magnetic, structural and dynamic properties of low-dimensional NiO on MgO(100) surfaces. Faraday Discussions, 1999, 114, 105-127.	3.2	15
84	Novel exchange mechanisms in the surface diffusion of oxides. Journal of Physics Condensed Matter, 2004, 16, L187-L192.	1.8	15
85	Size mismatch effects in oxide solid solutions using Monte Carlo and configurational averaging. Physical Chemistry Chemical Physics, 2005, 7, 1127-1135.	2.8	15
86	Investigating the utility of momentum-space descriptors for predicting bloodâ€“brain barrier penetration. Journal of Molecular Graphics and Modelling, 2007, 26, 607-612.	2.4	15
87	Use of massively parallel molecular dynamics simulations for radiation damage in pyrochlores. Journal of Materials Science, 2007, 42, 1920-1930.	3.7	15
88	Band Gap Modification of ZnO and ZnS through Solid Solution Formation for Applications in Photocatalysis. Energy Procedia, 2014, 60, 32-36.	1.8	15
89	Negative electron affinity from aluminium on the diamond (1â€‰0â€‰0) surface: a theoretical study. Journal of Physics Condensed Matter, 2018, 30, 235002.	1.8	15
90	Atomistic simulation of mineralâ€“melt trace-element partitioning. Physics of the Earth and Planetary Interiors, 2003, 139, 93-111.	1.9	14

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91	The use of momentum-space descriptors for predicting octanolâ€“water partition coefficients. Computational and Theoretical Chemistry, 2005, 727, 57-61.	1.5	14
92	Surface diffusion and surface growth in nanofilms of mixed rocksalt oxides. Physical Chemistry Chemical Physics, 2005, 7, 1839.	2.8	14
93	Monte Carlo simulation of GaN/InN mixtures. Journal of Materials Chemistry, 2005, 15, 785.	6.7	14
94	Simulation Studies of the Phase Stability of the Ruddlesdenâ€“Popper Phases. Journal of the American Ceramic Society, 2013, 96, 2316-2321.	3.8	14
95	Dopant incorporation into garnet solid solutionsâ€”a breakdown of Goldschmidtâ€™s first ruleElectronic supplementary information (ESI) available: (1) comparison between observed and calculated structural parameters of the end-members pyrope and grossular. (2) GULP input file for configuration 1. See http://www.rsc.org/suppdata/cc/b2/b211249c/. Chemical Communications, 2003, , 786-787.	4.1	13
96	Design of three-dimensional solid-state boron oxide networks:Ab initiocalculations using density functional theory. Physical Review B, 2010, 82, .	3.2	13
97	Piezoelectric effects in boron nitride nanotubes predicted by the atomistic finite element method and molecular mechanics. Nanotechnology, 2017, 28, 355705.	2.6	13
98	Theoretical studies of fluorocarbons. Part I. Small perfluoroalkane molecules. Journal of Fluorine Chemistry, 1990, 46, 317-337.	1.7	12
99	Quasiharmonic free energy and derivatives for three-body interactions. Physical Review B, 1999, 59, 353-363.	3.2	12
100	Classification of reaction pathways via momentumâ€“space and quantum molecular similarity measures. Chemical Physics Letters, 2003, 367, 207-213.	2.6	12
101	Beyond the point defect limit: solid solutions, phase diagrams and trace-element partitioning. Physical Chemistry Chemical Physics, 2003, 5, 2190-2196.	2.8	12
102	Structural forms of fluorides in bone tissue of animals under chronic fluoride intoxication. Journal of Structural Chemistry, 2006, 47, 258-266.	1.0	12
103	Predicting crystal structures ab initio: group 14 nitrides and phosphides. Physical Chemistry Chemical Physics, 2010, 12, 8620.	2.8	12
104	Evaluation of Thermodynamic Properties of Solids by Quasiharmonic Lattice Dynamics. International Journal of Thermophysics, 2001, 22, 535-546.	2.1	11
105	Ternary silicon germanium nitrides: A class of tunable band gap materials. Physical Review B, 2011, 84, .	3.2	11
106	Polar Solids at High Pressure: NaF. Molecular Simulation, 1992, 9, 161-169.	2.0	10
107	Potentials for B-metal compounds: The stannates ASnO₃ (A = Ca, Sr or Ba) and SnO₂. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1996, 73, 33-39.	0.6	10
108	Monte Carlo simulation of segregation in ceramic thin films. Physical Chemistry Chemical Physics, 2005, 7, 3601.	2.8	10

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109	Solvation of Ti(iv) in aqueous solution under ambient and supercritical conditions. Physical Chemistry Chemical Physics, 2011, 13, 7371.	2.8	10
110	A theoretical study of substitutional boronâ€“nitrogen clusters in diamond. Journal of Physics Condensed Matter, 2018, 30, 425501.	1.8	10
111	Ab initio study of negative electron affinity from light metals on the oxygen-terminated diamond (1â€‰×â€‰1) surface. Journal of Physics Condensed Matter, 2019, 31, 295002.	1.8	10
112	Oxygen Interstitial Defects in High-Tc Oxides. Molecular Simulation, 1994, 12, 89-100.	2.0	9
113	Change in the bulk modulus at theB1â^'B2phase transition. Physical Review B, 1999, 60, 2968-2971.	3.2	9
114	Monte Carlo simulation of GaN/AlN and AlN/InN mixtures. Materials Chemistry and Physics, 2007, 105, 179-184.	4.0	9
115	Hunting the elusive shallow n-type donor â€“ An ab initio study of Li and N co-doped diamond. Carbon, 2021, 171, 857-868.	10.3	9
116	Ab initio predictions of ferroelectric ternary fluorides with the LiNbO3structure. Chemical Communications, 2003, , 2440-2441.	4.1	8
117	Similarity in silicate chemistry: trace elements in garnet solid solutions. Computational and Theoretical Chemistry, 2005, 727, 199-204.	1.5	8
118	Improving Hydride Conductivity in Layered Perovskites via Crystal Engineering. Chemistry of Materials, 2021, 33, 177-185.	6.7	8
119	Momentum space studies of large polyenes. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 1519.	1.1	7
120	Phase transitions in disordered solids via hybrid Monte Carlo: the orthorhombic to cubic phase transition in (Mg,Mn)SiO3 perovskite. Chemical Communications, 1999, , 707-708.	4.1	7
121	Think locally â€“ linking structure, thermodynamics and transport in grossly non-stoichiometric compounds and solid solutions. Journal of Materials Chemistry, 2008, 18, 4124.	6.7	7
122	Ultraâ€Flexible Boronâ€Oxygen 3D Solidâ€State Networks. Advanced Functional Materials, 2013, 23, 5887-5892.	14.9	7
123	GaPâ€“ZnS Multilayer Films: Visible-Light Photoelectrodes by Interface Engineering. Journal of Physical Chemistry C, 2019, 123, 3336-3342.	3.1	7
124	Mixing Thermodynamics and Photocatalytic Properties of GaPâ€“ZnS solid solutions. Advanced Theory and Simulations, 2019, 2, 1800146.	2.8	7
125	Interatomic forces breaking carbon-carbon bonds. Carbon, 2021, 175, 420-428.	10.3	7
126	Cooperative excitations in superionic PbF ₂. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20190455.	3.4	7

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127	Quasiharmonic free energy and derivatives for many-body interactions: The embedded atom method. Physical Review B, 2004, 69, .	3.2	6
128	The quantitative use of momentum-space descriptors. Chemical Physics Letters, 2005, 416, 376-380.	2.6	6
129	Thin films of wÃ¼rtzite materialsâ€"AlN vs. AlP. Journal of Crystal Growth, 2006, 294, 111-117.	1.5	6
130	Oxide and halide nanoclusters on ionic substrates: heterofilm formation and lattice mismatch. Journal of Materials Chemistry, 2010, 20, 10403.	6.7	6
131	Order parameter and connectivity topology analysis of crystalline ceramics for nuclear waste immobilization. Journal of Physics Condensed Matter, 2014, 26, 485011.	1.8	6
132	Graphene and novel graphitic ZnO and ZnS nanofilms: the energy landscape, non-stoichiometry and water dissociation. Nanoscale Advances, 2019, 1, 1924-1935.	4.6	6
133	Momentum-space similarity. Advances in Molecular Similarity, 1996, , 61-87.	0.5	6
134	Lattice dynamics and thermodynamic properties of Y3Al5O12 (YAG). Journal of Physics and Chemistry of Solids, 2021, 162, 110512.	4.0	6
135	Ab initio study of negative electron affinity on the scandium-terminated diamond (100) surface for electron emission devices. Carbon, 2022, 196, 176-185.	10.3	6
136	Differences Between High-T_cOxides Containing Six-, Five-, Four- And Two-Fold Coordinated Copper. Molecular Simulation, 1992, 9, 115-128.	2.0	5
137	Monte Carlo simulation of segregation in ceramic thin films: Comparison of the MgO/MnO {100} and {210} surfaces. Journal of Crystal Growth, 2006, 294, 130-136.	1.5	5
138	Monte Carlo simulation and free energies of mixed oxide nanoparticles. Physical Chemistry Chemical Physics, 2013, 15, 6219.	2.8	5
139	Adventures in boron chemistry â€“ the prediction of novel ultra-flexible boron oxide frameworks. Faraday Discussions, 2018, 211, 569-591.	3.2	5
140	Predicted strong spin-phonon interactions in Li-doped diamond. Physical Chemistry Chemical Physics, 2020, 22, 20612-20617.	2.8	5
141	Fast-ion conduction and local environments in BIMEVOX. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2021, 379, 20200430.	3.4	5
142	Energy landscapes of perfect and defective solids: from structure prediction to ion conduction. Theoretical Chemistry Accounts, 2021, 140, 1.	1.4	5
143	Momentum-space electron densities?localized orbitals in hydrocarbons, boranes, and transition metal complexes. International Journal of Quantum Chemistry, 1996, 60, 579-592.	2.0	4
144	Configurational lattice dynamics and hybrid Monte Carlo approaches to thermodynamic properties of solid solutions. Computational and Theoretical Chemistry, 2000, 506, 45-53.	1.5	4

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145	Simulating surface diffusion and surface growth in ceramics. Dalton Transactions, 2004, , 3071.	3.3	4
146	Ultrathin oxide films and heterojunctions: CaO layers on BaO and SrO. Physical Chemistry Chemical Physics, 2009, 11, 3217.	2.8	4
147	Multi-million atom Monte Carlo simulation of oxide materials and solid solutions. Computational Materials Science, 2015, 103, 244-249.	3.0	4
148	A first-principles Hartree-Fock description of MnO at high pressures. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 77, 1063-1075.	0.6	3
149	QSAR using momentum-space and trivial feature count descriptors â€“ An application to Tetrahymena pyriformis toxicity. Computational and Theoretical Chemistry, 2009, 901, 56-59.	1.5	3
150	Perovskite solid solutionsâ€“a Monte Carlo study of the deep earth analogue (K, Na)MgF3. Journal of Structural Chemistry, 2016, 57, 257-266.	1.0	3
151	Lithium oxide: a quantum-corrected and classical Monte Carlo study. Physical Chemistry Chemical Physics, 2019, 21, 14964-14972.	2.8	3
152	Calciteâ€“magnesite solid solutions: using genetic algorithms to understand non-ideality. Physics and Chemistry of Minerals, 2019, 46, 193-202.	0.8	3
153	Thermodynamics of solid solutions VIA lattice dynamics and hybrid monte carlo simulations. Radiation Effects and Defects in Solids, 1999, 151, 197-202.	1.2	2
154	Vibrational analysis of per-fluorinated-triamantane. Chemical Physics Letters, 2008, 460, 237-240.	2.6	2
155	Multiple cascade radiation damage simulations of pyrochlore. Molecular Simulation, 2021, 47, 273-283.	2.0	2
156	Structure of Nanoclusters on Oxide Substratesâ€”Bi₂O₃ on SrTiO₃. Nanoscience and Nanotechnology Letters, 2012, 4, 178-181.	0.4	2
157	Physisorption of molecular hydrogen in curved carbon nanomaterials: a computational study. WIT Transactions on Engineering Sciences, 2013, , .	0.0	2
158	Ultrathin oxide films: CaO layers on BaO and SrO. Materials Research Society Symposia Proceedings, 2008, 1148, 1.	0.1	1
159	Simulations of CVD Diamond Film Growth Using a Simplified Monte Carlo Model. Materials Research Society Symposia Proceedings, 2009, 1203, 1.	0.1	1
160	A Theoretical Study of Ultra-Thin Films with the Wurtzite and Zinc Blende Structures. Materials Research Society Symposia Proceedings, 2007, 1035, 1.	0.1	0
161	Ab initio study of structural, elastic and thermodynamic properties of Fe3S at high pressure: Implications for planetary cores. American Mineralogist, 2022, 107, 248-256.	1.9	0