

# Potential-induced breathing model for the elastic modulus of the cubic alkaline-earth oxides

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Lattice dynamics of the potential-induced breathing model: Phonon dispersion in the alkaline-earth oxides. <i>Physical Review B</i> , 1987, 35, 5749-5760.	3.2	116
2	Lattice Dynamics and Ionicity in the High-Temperature Superconductors. <i>Materials Research Society Symposia Proceedings</i> , 1987, 99, 825.	0.1	2
3	Calculation of elasticity and high pressure instabilities in corundum and stishovite with the Potential Induced Breathing Model. <i>Geophysical Research Letters</i> , 1987, 14, 37-40.	4.0	120
4	Elasticity and equation of state of $\text{MgSiO}_3$ perovskite. <i>Geophysical Research Letters</i> , 1987, 14, 1053-1056.	4.0	115
5	Mineral and melt physics. <i>Reviews of Geophysics</i> , 1987, 25, 1265-1276.	23.0	45
6	Simple model for structural properties and crystal stability of sp <sup>3</sup> -bonded solids. <i>Physical Review B</i> , 1987, 35, 9666-9682.	3.2	162
7	Theoretical studies of charge relaxation effects on the statics and dynamics of oxides. <i>Physics and Chemistry of Minerals</i> , 1987, 14, 294-302.	0.8	71
8	X-ray diffraction of ruby ( $\text{Al}_2\text{O}_3:\text{Cr}^{3+}$ ) to 175 GPa. <i>Physica B: Physics of Condensed Matter &amp; C: Atomic, Molecular and Plasma Physics, Optics</i> , 1988, 150, 115-121.	0.9	75
9	Analysis of electronic structure and charge density of the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$ . <i>Journal of Superconductivity and Novel Magnetism</i> , 1988, 1, 111-141.	0.5	220
10	The effect of many-body forces on the elastic properties of simple oxides and olivine. <i>Physics and Chemistry of Minerals</i> , 1988, 16, 42.	0.8	11
11	Variational stabilization of the ionic charge densities in the electron-gas theory of crystals: Applications to MgO and CaO. <i>Physics and Chemistry of Minerals</i> , 1988, 15, 209-220.	0.8	71
12	First principles calculations of lattice dynamics and ionicity in $\text{La}_2\text{CuO}_4$ and $\text{YBa}_2\text{Cu}_3\text{O}_7$ . <i>Physica C: Superconductivity and Its Applications</i> , 1988, 153-155, 202-203.	1.2	4
13	Phase transitions and elasticity in zirconia. <i>Physica B: Physics of Condensed Matter &amp; C: Atomic, Molecular and Plasma Physics, Optics</i> , 1988, 150, 1-9.	0.9	50
14	Applications of ionic models to the high-temperature superconductor $\text{La}_2\text{CuO}_4$ . <i>Physica B: Physics of Condensed Matter &amp; C: Atomic, Molecular and Plasma Physics, Optics</i> , 1988, 150, 61-73.	0.9	33
15	Elastic Properties and Equations of State. , 1988, , .		8
16	Thermal expansion of periclase and olivine and their anharmonic properties. , 1988, , 361-375.		1
17	High pressure shear modulus—A many body model for oxides. <i>Geophysical Research Letters</i> , 1988, 15, 209-212.	4.0	10
18	Hugoniot equation of state of twelve rocks. , 1988, , 199-236.		0

#	ARTICLE	IF	CITATIONS
19	Raman spectroscopy and theoretical modeling of BeO at high pressure. Physical Review B, 1988, 37, 4727-4734.	3.2	72
20	Linearized augmented plane wave electronic structure calculations for MgO and CaO. Journal of Geophysical Research, 1988, 93, 8009-8022.	3.3	156
21	Static compression and equation of state of CaO to 1.35 Mbar. Journal of Geophysical Research, 1988, 93, 15279-15288.	3.3	128
22	Ionic contributions to lattice instabilities and phonon dispersion in La <sub>2</sub> CuO <sub>4</sub> . Physical Review Letters, 1988, 60, 817-820.	7.8	99
23	Ab initio calculations of static lattice properties for NaCl and a test of the Decker equation of state. Physical Review B, 1988, 37, 4784-4787.	3.2	8
24	The bulk modulus-volume relationship for oxide compounds and related geophysical problems. , 1988, , 153-165.		1
25	Effects of temperature and pressure on interatomic distances in oxygen-based minerals. , 1988, , 407-413.		35
26	Derivation of Wachtman's equation for the temperature dependence of the elastic moduli of oxide compounds. , 1988, , 166-170.		1
27	The bulk modulus-volume relationship for oxides. , 1988, , 283-289.		32
28	The single-crystal elastic moduli of stishovite. , 1988, , 459-465.		0
29	Some elastic constant data on minerals relevant to geophysics. , 1988, , 237-270.		2
30	Composition of the upper mantle: Geophysical tests of two petrological models. , 1988, , 513-516.		1
31	Homogeneity and constitution of the Earth's lower mantle and outer core. , 1988, , 341-348.		0
32	Elasticity and constitution of the Earth's interior. , 1988, , 31-90.		3
33	Theory of binding of ionic crystals: Application to alkali-halide and alkaline-Earth-dihalide crystals. , 1988, , 314-320.		1
34	The determination of the elastic constants of natural almandine-pyrope garnet by rectangular parallelepiped resonance method. , 1988, , 376-383.		8
35	The velocity of compressional waves in rocks to 10 kilobars, part 2. , 1988, , 91-116.		8
36	The elastic properties of composite materials. , 1988, , 384-406.		1

#	ARTICLE	IF	CITATIONS
37	The effect of pressure upon the elastic parameters of isotropic solids, according to Murnaghan's theory of finite strain. , 1988, , 21-30.		0
38	Temperature coefficients of elastic constants of single crystal MgO between 80 And 1,300 K. , 1988, , 503-512.		0
39	Density distribution in the Earth. , 1988, , 1-20.		6
40	X-ray diffraction and optical observations on crystalline solids up to 300 kbar. , 1988, , 193-198.		0
41	Thermal expansion of silicate perovskite and atratification of the Earth's mantle. , 1988, , 521-523.		0
42	Reflection properties of phase transition and compositional change models of the 670-km Discontinuity. , 1988, , 488-502.		0
43	Ab initio structural and thermoelastic properties of orthorhombic MgSiO <sub>3</sub> perovskite. , 1988, , 517-520.		0
44	Static compression of iron T78 GPa with rare gas solids as pressure-transmitting media. , 1988, , 524-531.		0
45	Equations of state of iron sulfide and constraints on the sulfur content of the Earth. , 1988, , 427-440.		0
46	Post-oxide phases of forsterite and enstatite. , 1988, , 358-360.		0
47	Velocity-density systematics and its implications for the iron content of the mantle. , 1988, , 335-340.		0
48	Composition of the Earth's mantle. , 1988, , 117-133.		0
49	Hydrostatic compression of perovskite-type MgSiO <sub>3</sub> . , 1988, , 466-474.		0
50	Some geophysical constraints on the chemical composition of the Earth's lower mantle. , 1988, , 475-487.		0
51	Pressure dependence of the thermal Gr <sup>1/4</sup> neisen parameter, with application to the Earth's lower mantle and outer core. , 1988, , 349-357.		0
52	Elasticity of coesite. , 1988, , 414-426.		0
53	Velocity-density systematics: Derivation from Debye theory and the effect of ionic size. , 1988, , 305-313.		0
54	Elasticity of pyroxene-garnet and pyroxene-ilmenite phase transformations in germanates. , 1988, , 321-334.		64

#	ARTICLE	IF	CITATIONS
55	A seismic equation of state. , 1988, , 171-192.		0
56	Elastic constants of single-crystal forsterite as a function of temperature and pressure. , 1988, , 271-282.		1
57	Equation of state of polycrystalline and single-crystal MgO to 8 kilobars and 800Å°K. , 1988, , 290-304.		0
58	The use of ultrasonic measurements under modest compression to estimate compression at high pressure. , 1988, , 134-152.		0
59	The temperature of shock compressed iron. , 1988, , 532-541.		0
60	The equation of state for iron and the Earth's core. , 1988, , 446-458.		5
61	GrÅ¼neisen parameter of quartz, quartzite, and fluorite at high pressure. , 1988, , 441-445.		0
62	High-density structures and phase transition in an ionic model ofH2O ice. Physical Review B, 1989, 40, 2716-2718.	3.2	13
63	The properties and behaviour of mantle minerals: a computer-simulation approach. Philosophical Transactions of the Royal Society A, 1989, 328, 391-407.	1.1	29
64	Electronic structure of the high-temperature oxide superconductors. Reviews of Modern Physics, 1989, 61, 433-512.	45.6	1,309
65	A study of thermal and elastic properties of ionic crystals within the framework of compressible ion theory. Journal of Physics and Chemistry of Solids, 1990, 51, 141-145.	4.0	5
66	Structural phase diagram of BaBiO3 in the potential induced breathing model. Solid State Communications, 1990, 76, 1267-1272.	1.9	10
67	Thermodynamic and elastic properties of a many-body model for simple oxides. Physical Review B, 1990, 41, 7755-7766.	3.2	41
68	Simulation of ionic crystals: Theab initio perturbed-ion method and application to alkali hydrides and halides. Physical Review B, 1990, 41, 3800-3814.	3.2	124
69	Structural and elastic properties of sodium halides at high pressure. Physical Review B, 1990, 42, 1810-1816.	3.2	30
70	Quantum-mechanical description of ions in crystals: Electronic structure of magnesium oxide. Physical Review B, 1990, 42, 1791-1801.	3.2	44
71	Theoretical study of the elastic and thermodynamic properties of sodium chloride under pressure. Physical Review B, 1990, 41, 2150-2157.	3.2	21
72	Local Density Functional Theories of Ionic and Molecular Solids. Advances in Quantum Chemistry, 1990, , 341-363.	0.8	18

#	ARTICLE	IF	CITATIONS
73	Monte carlo calculations of the equation of state of alkaline earth oxides. <i>Ferroelectrics</i> , 1990, 111, 33-41.	0.6	1
74	Elastic constants and electronic structure of fluorite (CaF <sub>2</sub> ): an ab initio Hartree-Fock study. <i>Journal of Physics Condensed Matter</i> , 1991, 3, 4151-4164.	1.8	100
75	Quantum-mechanical Hartree-Fock self-consistent-field study of the elastic constants and chemical bonding of MgF <sub>2</sub> (sellaite). <i>Physical Review B</i> , 1991, 44, 3509-3517.	3.2	70
76	Interionic Potentials: A Users Guide. , 1991, , 159-182.		4
77	Calculation of the equation of state and elastic moduli of MgO using molecular orbital theory. <i>Physics and Chemistry of Minerals</i> , 1991, 17, 622.	0.8	2
78	Comment on "Thermodynamic and elastic properties of a many-body model for simple oxides". <i>Physical Review B</i> , 1991, 44, 7106-7107.	3.2	3
79	Modified potential-induced-breathing model of potentials between close-shell ions. <i>Physical Review B</i> , 1991, 44, 2495-2503.	3.2	92
80	Reply to "Comment on "Thermodynamic and elastic properties of a many-body model for simple oxides". <i>Physical Review B</i> , 1991, 44, 7108-7110.	3.2	0
81	Hellmann potential extended to next-nearest neighbors for alkali halide crystals. <i>Physical Review B</i> , 1991, 43, 9924-9930.	3.2	1
82	Molecular Dynamics and Diffusion in Silicate Melts. , 1991, , 1-50.		8
83	Periodic Hartree-Fock study of B1 → B2 reactions: phase transition in CaO. <i>Physics of the Earth and Planetary Interiors</i> , 1992, 72, 286-298.	1.9	9
84	Properties of ordered intermetallic alloys: first-principles and approximate methods. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 1993, 170, 49-57.	5.6	27
85	A self consistent atomic deformation model for total energy calculations: Application to ferroelectrics. <i>Ferroelectrics</i> , 1993, 150, 13-24.	0.6	27
86	Ionic halides and oxides at high pressure: calculated Hugoniot, isotherms and thermal pressures. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1993, 89, 4369.	1.7	18
87	Crystal-structure calculations with distorted ions. <i>Physical Review B</i> , 1993, 48, 2889-2908.	3.2	55
88	Phase stability of wurtzite at high pressure from first-principles linearized augmented plane-wave calculations. <i>Physical Review B</i> , 1993, 47, 7720-7731.	3.2	56
89	Variational charge relaxation in ionic crystals: An efficient treatment of statics and dynamics. <i>Physical Review B</i> , 1994, 50, 15559-15574.	3.2	27
90	Calculated phonon dispersion of infinite-layer compounds and the effects of charge fluctuations. <i>European Physical Journal B</i> , 1994, 95, 417-425.	1.5	1

#	ARTICLE	IF	CITATIONS
91	Derivation and application of ab initio Nb <sup>5+</sup> -O <sup>2-</sup> short-range effective pair potentials in shell-model simulations of KNbO <sub>3</sub> and KTaO <sub>3</sub> . Physical Review B, 1994, 49, 3746-3754.	3.2	28
92	Theoretical study of cation ordering in the system Pb(Sc <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> . Ferroelectrics, 1994, 151, 331-336.	0.6	20
93	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
94	Nonempirical calculation of the Pb(Sc <sub>0.5</sub> Ta <sub>0.5</sub> )O <sub>3</sub> -PbTiO <sub>3</sub> quasibinary phase diagram. Physical Review B, 1995, 52, 792-797.	3.2	22
95	Modeling the O <sup>2-</sup> -O <sup>2-</sup> interaction for atomistic simulations. Physical Review B, 1995, 51, 11289-11295.	3.2	7
96	First principles study of cation ordering in the system Pb(Sc <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> and (1 - X) Pb(Sc <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> - X PbTiO <sub>3</sub> . Ferroelectrics, 1995, 164, 201-212.	0.6	2
97	Breathing instability and disproportionation of Bi <sup>4+</sup> ions in BaBiO <sub>3</sub> . Ferroelectrics, 1995, 164, 169-175.	0.6	8
98	Self-Consistent potential induced breathing model calculations for longitudinal modes in MgO. Ferroelectrics, 1995, 164, 177-181.	0.6	6
99	Electronic and structural properties of alkaline-earth oxides under high pressure. Physical Review B, 1995, 52, 4-7.	3.2	81
100	Molecular dynamics simulations of compressible ions. Journal of Chemical Physics, 1996, 104, 8068-8081.	3.0	94
101	Structure and bonding in the deep mantle and core. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 1996, 354, 1461-1479.	3.4	12
102	Spherical self-consistent atomic deformation model for first-principles energy calculations in ionic crystalline solids. Physical Review B, 1996, 54, 7729-7736.	3.2	19
103	Theoretical and experimental investigation of the equations of state and phase stabilities of MgS and CaS. Journal of Physics Condensed Matter, 1996, 8, 8251-8265.	1.8	33
104	Long-range order effects in Pb(Zr <sub>1/2</sub> Ti <sub>1/2</sub> )O <sub>3</sub> . Ferroelectrics, 1997, 194, 287-298.	0.6	20
105	Cation ordering in some ABO <sub>3</sub> perovskites. Ferroelectrics, 1997, 194, 187-206.	0.6	9
106	Pressure induced structural phase transition in MgS and CaS. Journal of Physics and Chemistry of Solids, 1998, 59, 599-603.	4.0	16
107	Structure and elasticity of CaO at high pressure. Journal of Geophysical Research, 1998, 103, 12405-12411.	3.3	46
108	The phase transition in alkaline-earth oxides: a comparison of ab initio Hartree-Fock and density functional calculations. Journal of Physics Condensed Matter, 1998, 10, 6897-6909.	1.8	91

#	ARTICLE	IF	CITATIONS
109	The melting curve and premelting of MgO. Geophysical Monograph Series, 1998, , 185-196.	0.1	12
110	Employment of curvilinear coordinates in ab initio calculations of insulators using pseudopotentials. Physics of the Solid State, 1999, 41, 213-218.	0.6	0
111	Calcium oxide (CaO) crystal structure, lattice parameters, thermal expansion. , 0, , 1-3.		0
112	Magnesium oxide (MgO) crystal structure, lattice parameters, thermal expansion. , 0, , 1-6.		5
113	Strontium oxide (SrO) crystal structure, lattice parameters, thermal expansion. , 0, , 1-3.		0
114	Barium oxide (BaO) crystal structure, lattice parameters, thermal expansion. , 0, , 1-3.		0
115	Structures, compressibilities and relative stabilities of the $\hat{A}$ , $\hat{A}$ and $\hat{A}$ phases of Mg <sub>2</sub> SiO <sub>4</sub> deduced from an electron-gas ionic Hamiltonian. Geophysical Journal International, 2000, 143, 295-301.	2.4	3
116	Elasticity of MgO and a primary pressure scale to 55 GPa. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 13494-13499.	7.1	410
117	High-pressure elastic properties of major materials of Earth's mantle from first principles. Reviews of Geophysics, 2001, 39, 507-534.	23.0	240
118	Systematics of elasticity: Ab initio study in B1-type alkaline earth oxides. Journal of Chemical Physics, 2001, 114, 10086-10093.	3.0	125
119	Ab-initio studies of pressure induced phase transitions in BaO. Journal of Computer-Aided Materials Design, 2001, 8, 193-202.	0.7	19
120	Deformation of polycrystalline MgO at pressures of the lower mantle. Journal of Geophysical Research, 2002, 107, ECV 3-1-ECV 3-17.	3.3	207
121	Multipoles and interaction potentials in ionic materials from planewave-DFT calculations. Faraday Discussions, 2003, 124, 171.	3.2	85
122	Interionic potentials from ab initio molecular dynamics: The alkaline earth oxides CaO, SrO, and BaO. Journal of Chemical Physics, 2003, 118, 5704-5717.	3.0	65
123	Ab initio calculations of the physical properties of ionic crystals. Physics-Uspokhi, 2004, 47, 1075-1099.	2.2	28
124	Thermodynamics of Oxides with Substitutional Disorder: A Microscopic Model and Evaluation of Important Energy Contributions. Journal of the American Ceramic Society, 1998, 81, 517-525.	3.8	32
125	Generalized Guinan-Steinberg formula for the shear modulus at all pressures. Physical Review B, 2005, 71, .	3.2	14
126	Structural and magnetic phase transitions in simple oxides using hybrid functionals. Molecular Simulation, 2005, 31, 367-377.	2.0	28



#	ARTICLE	IF	CITATIONS
127	Ab initio interionic potentials for CaO by multiple lattice inversion. Journal of Alloys and Compounds, 2005, 388, 195-207.	5.5	15
128	Stability of alkali-metal oxides as a function of pressure: Theoretical calculations. Physical Review B, 2006, 73, .	3.2	47
129	First-principles study of the elastic and thermodynamic properties of CaSiO <sub>3</sub> perovskite. Journal of Physics Condensed Matter, 2007, 19, 246103.	1.8	7
130	Thermoelasticity of MgO at High Pressures. Chinese Journal of Chemical Physics, 2007, 20, 65-70.	1.3	8
131	Thermoelasticity of CaO from first principles. Chinese Physics B, 2007, 16, 499-505.	1.3	14
132	Theory and Practice “ Lattice Vibrations and Spectroscopy of Mantle Phases. , 2007, , 153-196.		2
133	Elastic properties of alkaline earth oxides under high pressure. Physica B: Condensed Matter, 2007, 391, 307-311.	2.7	16
134	Phase transition and elastic constants of CaO from first-principle calculations. Physica B: Condensed Matter, 2007, 392, 229-232.	2.7	41
135	Mercury Species and SO <sub>2</sub> Adsorption on CaO(100). Journal of Physical Chemistry C, 2008, 112, 16484-16490.	3.1	73
136	Self-consistent atomic deformation method for application of density functional theory. Physical Review B, 2008, 78, .	3.2	8
137	Free enthalpy landscape of SrO. Journal of Chemical Physics, 2008, 128, 194712.	3.0	23
138	High sensitivity of O17 NMR to p-d hybridization in transition metal perovskites: First principles calculations of large anisotropic chemical shielding. Journal of Chemical Physics, 2009, 131, 184511.	3.0	4
139	Simulating solid state phase transitions with the roots of transformation matrices. Journal of Physics Condensed Matter, 2009, 21, 245404.	1.8	1
140	Elasticity of the B2 phase and the effect of the B1“B2 phase transition on the elasticity of MgO. Phase Transitions, 2009, 82, 87-97.	1.3	6
141	Phonon and elastic instabilities in rocksalt calcium oxide under pressure: a first-principles study. Journal of Physics Condensed Matter, 2009, 21, 015402.	1.8	13
142	Role of temperature in the numerical analysis of CaO under high pressure. Open Chemistry, 2010, 8, 126-133.	1.9	8
143	First-principles calculations of structural, elastic, electronic and optical properties of XO (X=Ca, Sr) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 92-101.	4.0	27
144	Universal Phase Transitions of <i>B</i>-1-Structured Stoichiometric Transition Metal Carbides. Inorganic Chemistry, 2011, 50, 9266-9272.	4.0	11

#	ARTICLE	IF	CITATIONS
145	The first principles study on the TmSb compound. Solid State Sciences, 2011, 13, 1291-1298.	3.2	5
146	Lattice energy and phase transition of alkaline earth chalcogenide. Phase Transitions, 2011, 84, 624-638.	1.3	1
147	High pressure phase transitions in Mg <sub>1-x</sub> Ca <sub>x</sub> O: Theory. Physica Status Solidi (B): Basic Research, 2011, 248, 1901-1907.	1.5	11
148	High pressure lattice dynamics and thermodynamics in BaO. Physica Status Solidi (B): Basic Research, 2011, 248, 1405-1411.	1.5	10
149	Effects of pressure and temperature on the isothermal bulk modulus of CaO. Physica B: Condensed Matter, 2011, 406, 293-296.	2.7	10
150	High pressure lattice dynamics, dielectric and thermodynamic properties of SrO. Physica B: Condensed Matter, 2011, 406, 3410-3416.	2.7	12
151	Electron momentum density and phase transition in SrO. Phase Transitions, 2012, 85, 1098-1108.	1.3	9
152	Ab initio lattice dynamics and thermodynamic properties of SrO under pressure. Journal of Physics and Chemistry of Solids, 2012, 73, 129-135.	4.0	25
153	A first-principle study of the structural, elastic, lattice dynamical and thermodynamic properties of PrX (X=P, As). Physica B: Condensed Matter, 2012, 407, 316-323.	2.7	8
154	Raman spectroscopy and lattice dynamics of MgSiO <sub>3</sub> -perovskite at high pressure. Geophysical Monograph Series, 0, , 35-44.	0.1	26
155	Electronic Structure and Total Energy Calculations for Oxide Perovskites and Superconductors. Geophysical Monograph Series, 0, , 55-66.	0.1	11
156	Development of semi-ab initio interionic potential for CaO and MgO. Molecular Simulation, 2013, 39, 956-967.	2.0	1
157	Theoretical investigation of high-pressure phase transitions in Mg <sub>1-x</sub> Sr <sub>x</sub> O. Phase Transitions, 2014, 87, 126-135.	1.3	2
158	Pressure-induced phase transition and structural behavior of MgO at high temperatures: a model study. Phase Transitions, 2015, 88, 1-15.	1.3	5
159	Lattice Vibrations and Spectroscopy of Mantle Phases. , 2015, , 203-231.		3
160	Mechanical and electronic properties of Ca <sup>1+</sup> Mg O alloys. Materials Science in Semiconductor Processing, 2015, 40, 676-684.	4.0	18
161	Structural, electronic and mechanical properties of alkaline earth metal oxides MO (M=Be, Mg, Ca, Sr), Tj ETQq0 0 0 rgBT /Overlock 10 T	4.0	35
162	Effects of epitaxial strains on spontaneous polarizations and band gaps of alkaline-earth-metal oxides MO (M = Mg, Ca, Sr, Ba). Computational Materials Science, 2016, 121, 61-66.	3.0	12

#	ARTICLE	IF	CITATIONS
163	First-principles calculations of typical anisotropic cubic and hexagonal structures and homogenized moduli estimation based on the Y-parameter: Application to CaO, MgO, CH and Calcite CaCO <sub>3</sub> . Journal of Physics and Chemistry of Solids, 2017, 101, 74-89.	4.0	41
164	First principles study on the adsorption of Au dimer on metal-oxide surfaces: The implications for Au growing. Applied Surface Science, 2017, 426, 554-561.	6.1	13
165	Structural and elastic properties of KBr at high pressure and high temperature. Phase Transitions, 2017, 90, 955-963.	1.3	5
166	Theoretical study of CaO, CaS and CaSe via first-principles calculations. Results in Physics, 2018, 10, 934-945.	4.1	29
167	Structural phase transition and electronic properties of CaO under high pressure. Materials Research Express, 2018, 5, 125903.	1.6	10
168	First-principles calculations on physical properties of Ni <sub>3</sub> Sn binary system intermetallic compounds and Ni/Ni <sub>3</sub> Sn interfaces in Nickel-Tin TLPS bonding layer. Intermetallics, 2018, 101, 27-38.	3.9	19
169	Atomistic Simulation of Anisotropic Crystal Structures at Nanoscale. , 2019, , .		3
170	Bonding and Electronic Structure of Minerals. , 1999, , 201-264.		3
171	Quantum Theory of Structure: Tight-Binding Systems. Cohesion and Structure, 1989, 2, 287-362.	0.0	10
173	Bonding Models: Ionic. , 2001, , 767-771.		0
175	Computer-aided materials design - status and perspectives of atomistic approaches. , 1994, , 189-194.		0
176	Lattice Dynamics, Vibrational Spectra, Thermodynamic and Heat Properties of Minerals. , 1994, , 412-435.		0
177	Computer Modelling of Defects. , 1994, , 315-339.		0
178	Advances in Electron-gas Potential Models: Applications to Some Candidate Lower Mantle Minerals. Topics in Molecular Organization and Engineering, 1997, , 81-112.	0.1	1
180	Study of elastic properties of prototype solids under high pressure. Computational Condensed Matter, 2022, 30, e00626.	2.1	3
181	A simple derivation of a new equation of state (EOS) based on Eulerian finite strain and its applicability. Pramana - Journal of Physics, 2022, 96, .	1.5	3
182	Prediction of the melting curve and phase diagram for CaO using newly developed interatomic potentials. Vacuum, 2023, 209, 111717.	3.5	4
183	First-principles study of thermoelasticity and structural phase diagram of CaO. Physical Review B, 2023, 107, .	3.2	1

#	ARTICLE	IF	CITATIONS
184	Thermal properties of CaO and SrO and their B1-B2 phase boundaries: Validity of the quasi-harmonic approximation. <i>Physica B: Condensed Matter</i> , 2023, 657, 414816.	2.7	1
185	Structure, pressure-induced phase transition, electronic and thermal properties of alkaline earth oxide compounds. <i>Phase Transitions</i> , 2024, 97, 240-259.	1.3	0