Finite strain isotherm and velocities for singleâ€crystal pressures and 300Â°K

Journal of Geophysical Research

83, 1257-1268

DOI: 10.1029/jb083ib03p01257

Citation Report

#	Article	IF	Citations
1	The elastic moduli and their pressure derivatives for tungsten carbide with different amounts of cobalt binder. Journal of Applied Physics, 1979, 50, 3331-3333.	1.1	13
2	Shock compression of solids. Physics Reports, 1979, 55, 255-379.	10.3	404
3	Physical properties of minerals and melts. Reviews of Geophysics, 1979, 17, 792-802.	9.0	52
4	Thermal expansion of LiF at high pressures. Journal of Physics and Chemistry of Solids, 1980, 41, 1019-1022.	1.9	84
5	Equation of state of sodium chloride up to 32 kbar and 500Â°Câ€. Journal of Physics and Chemistry of Solids, 1980, 41, 517-523.	1.9	181
6	Finiteâ€strain equation of state for highâ€pressure phases. Geophysical Research Letters, 1981, 8, 1219-1222.	1.5	133
7	Majorite: Vibrational and compressional properties of a highâ€pressure phase. Journal of Geophysical Research, 1981, 86, 6171-6179.	3.3	112
8	Phase transition in SrO. Journal of Geophysical Research, 1981, 86, 11773-11778.	3.3	135
9	Elastic properties of solids under pressures to 100 kbar: Experimental methods and results. Advances in Space Research, 1981, 1, 147-158.	1.2	5
10	First-principles calculation of the insulator-to-metal transition pressure in CsI. Solid State Communications, 1983, 47, 855-857.	0.9	21
11	Structural properties of III-V zinc-blende semiconductors under pressure. Physical Review B, 1983, 28, 3258-3265.	1.1	241
12	Phase transitions and mantle discontinuities. Reviews of Geophysics, 1983, 21, 51-74.	9.0	404
13	Phase transitions and equations of state for the sodium halides: NaF NaCl, NaBr, and NaI. Journal of Geophysical Research, 1983, 88, 3543-3548.	3.3	176
14	Thermal conductivity of minerals at high pressure: The effect of phase transitions. Journal of Geophysical Research, 1983, 88, 7399-7409.	3.3	48
15	Structural properties of NaCl. Physical Review B, 1984, 29, 3770-3772.	1.1	99
16	Compression of theB2high-pressure phase of NaCl. Physical Review B, 1984, 30, 6045-6050.	1.1	129
17	Structural and Bonding Changes in Cesium Iodide at High Pressures. Science, 1984, 223, 53-56.	6.0	116
18	Analysis of the Equation of State for LiF Crystal. Physica Status Solidi (B): Basic Research, 1984, 125, K21.	0.7	2

#	Article	IF	Citations
19	Lindemann Melting Law: Anharmonic correction and test of its validity for minerals. Journal of Geophysical Research, 1984, 89, 7821-7835.	3.3	80
20	The equation of state of the gold calibration standard. Journal of Applied Physics, 1984, 55, 885-893.	1.1	420
21	Equation of state and metallization of CsI. Physical Review B, 1984, 29, 2611-2621.	1.1	132
22	Pressure-Induced Structural Transition in SrS. Physica Status Solidi A, 1985, 91, 11-15.	1.7	84
23	High-pressure X-Ray diffraction and optical absorption studies of CsI. Journal of Physics and Chemistry of Solids, 1985, 46, 1179-1184.	1.9	79
24	Optical response of YbS and YbO at high pressures and the pressure-volume relation of YbS. Physical Review B, 1985, 32, 8246-8252.	1.1	49
25	High-pressure phase transition in CsBr. Physical Review B, 1985, 31, 588-590.	1.1	76
26	High-pressure phase transitions and equation of state of the III-V compound InAs up to 27 GPa. Physical Review B, 1985, 31, 7344-7348.	1.1	89
27	High-pressure phase transitions in CaTe and SrTe. Physical Review B, 1985, 32, 4066-4070.	1.1	140
28	First principles versus spherical ion models of the B1 and B2 phases of NaCl. Journal of Geophysical Research, 1985, 90, 1794-1800.	3.3	30
29	Theoretical study of solid NaF and NaCl at high pressures and temperatures. Journal of Geophysical Research, 1985, 90, 7803-7813.	3.3	90
30	Ab initio structural and thermoelastic properties of orthorhombic MgSiO₃ perovskite. Geophysical Research Letters, 1985, 12, 809-812.	1.5	86
31	Pressure-volume relations and polymorphism of europium and ytterbium to 30 GPa. Journal of Physics F: Metal Physics, 1985, 15, 543-559.	1.6	57
32	Equation of state and thermodynamic parameters of NaCl to 300 kbar in the highâ€temperature domain. Journal of Geophysical Research, 1986, 91, 4949-4954.	3.3	485
33	Hydrostatic compression of Fe_{1â€x}O WÃ¼stite. Journal of Geophysical Research, 1986, 91, 4665-4672.	3.3	82
34	Static compression of iron to 78 GPa with rare gas solids as pressureâ€transmitting media. Journal of Geophysical Research, 1986, 91, 4677-4684.	3.3	259
35	Infrared vibrational spectra of Beta-Phase Mg2SiO4 and Co2SiO4 to Pressures of 27 GPa. Physics and Chemistry of Minerals, 1986, 13, 141-145.	0.3	30
36	Effect of pressure on the valence states of Yb and Tm in Yb1-xTmxSe. Journal of Physics C: Solid State Physics, 1986, 19, 3753-3763.	1.5	6

#	Article	IF	Citations
37	7. The Multianvil Press. Methods in Experimental Physics, 1987, , 237-270.	0.1	0
38	Synthesis and Equation of State of (Mg,Fe) SiO3 Perovskite to Over 100 Gigapascals. Science, 1987, 235, 668-670.	6.0	401
39	High-pressure studies of NaH to 54 GPa. Physical Review B, 1987, 36, 7664-7667.	1.1	80
40	Phase transitions in GaSb to 110 GPa (1.1 Mbar). Physical Review B, 1987, 36, 4543-4546.	1.1	53
41	Sodium chloride structural properties: Linearized augmented-plane-wave calculations and pressure calibration. Physical Review B, 1987, 35, 6395-6398.	1.1	19
42	High-pressure phases of III-V zinc-blende semiconductors. Physical Review B, 1987, 35, 7604-7610.	1.1	220
43	High precision optical strain measurements at high pressures. Geophysical Monograph Series, 1987, , 41-51.	0.1	5
44	Thermodynamics for (Mg, Fe)2SiO4 from the Hugoniot. Geophysical Monograph Series, 1987, , 373-384.	0.1	20
45	Theoretical study of the structural properties and equations of state of MgSiO3 and CaSiO3 perovskites: Implications for lower mantle composition. Geophysical Monograph Series, 1987, , 313-331.	0.1	42
46	Elasticity and equation of state of MgSiO₃ perovskite. Geophysical Research Letters, 1987, 14, 1053-1056.	1.5	115
47	Vibrational spectrum of MgSiO₃ perovskite: Zeroâ€pressure Raman and midâ€infrared spectra to 27 GPa. Journal of Geophysical Research, 1987, 92, 8116-8128.	3.3	94
48	Pyrite: Shock compression, isentropic release, and composition of the Earth's core. Journal of Geophysical Research, 1987, 92, 10363-10375.	3.3	115
49	Static compression of MnO manganosite to 60 GPa. Journal of Geophysical Research, 1987, 92, 11433-11436.	3.3	83
50	Frequency-dependent equation of state of fused silica to 10 GPa. Physical Review B, 1987, 35, 236-244.	1.1	116
51	Theoretical study of the structure, lattice dynamics, and equations of state of perovskite-type MgSiO3 and CaSiO3. Physics and Chemistry of Minerals, 1987, 14, 2-12.	0.3	148
52	Lindemann law revisited. Il Nuovo Cimento Della SocietÃ Italiana Di Fisica C, 1987, 10, 479-494.	0.2	5
53	Is the inner core of the Earth pure iron?. Nature, 1987, 325, 332-335.	13.7	196
54	Simple covalent potential models of tetrahedral SiO2: Applications to ?-quartz and coesite at pressure. Physics and Chemistry of Minerals, 1988, 16, 199.	0.3	50

#	Article	IF	Citations
55	Quasi-hydrostatic compression of ruby to 500 Kbar. Physics and Chemistry of Minerals, 1988, 16, 207.	0.3	96
56	Variational stabilization of the ionic charge densities in the electron-gas theory of crystals: Applications to MgO and CaO. Physics and Chemistry of Minerals, 1988, 15, 209-220.	0.3	71
57	A MEG study of the olivine and spinel forms of Mg2SiO4. Physics and Chemistry of Minerals, 1988, 15, 514-520.	0.3	7
58	Validity of the Sutherland-Lindemann law and melting temperatures in the Earth's interior. Geophysical Journal International, 1988, 92, 269-282.	1.0	11
59	The validity of the common approximate expressions for the Gruneisen parameter. Geophysical Journal International, 1988, 93, 505-519.	1.0	16
60	Phase transitions and elasticity in zirconia. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1988, 150, 1-9.	0.9	50
61	Elastic Properties and Equations of State. , 1988, , .		8
62	Thermal expansion of periclase and olivine and their anharmonic properties. , 1988, , 361-375.		1
63	Ultrasonic investigation of melts in the system Na2Oî—¸Al2O3î—¸SiO2. Geochimica Et Cosmochimica Acta, 1988, 52, 283-293.	1.6	93
64	Hugoniot equation of state of twelve rocks. , 1988, , 199-236.		0
65	The equation of state of molybdenum at 1400â€‰Â°C. Journal of Applied Physics, 1988, 63, 4469-4475.	1.1	39
66	Yield strength of the B1 and B2 phases of NaCl. Journal of Geophysical Research, 1988, 93, 3270-3274.	3.3	51
67	Temperature and pressure derivatives of elastic constants with application to the mantle. Journal of Geophysical Research, 1988, 93, 4688-4700.	3.3	106
68	Linearized augmented plane wave electronic structure calculations for MgO and CaO. Journal of Geophysical Research, 1988, 93, 8009-8022.	3.3	156
69	Static compression and equation of state of CaO to 1.35 Mbar. Journal of Geophysical Research, 1988, 93, 15279-15288.	3.3	128
70	High-pressure x-ray diffraction study ofCeO2to 70 GPa and pressure-induced phase transformation from the fluorite structure. Physical Review B, 1988, 38, 7755-7758.	1.1	177
71	Pressure profiles at multimegabar pressures in a diamond anvil cell using xâ€ray diffraction. Review of Scientific Instruments, 1988, 59, 318-321.	0.6	18
72	Universality relationships in condensed matter: Bulk modulus and sound velocity. Physical Review B, 1988, 37, 4351-4357.	1.1	36

#	Article	IF	Citations
73	Ab initiocalculations of static lattice properties for NaCl and a test of the Decker equation of state. Physical Review B, 1988, 37, 4784-4787.	1.1	8
74	Universal equation of state. Physical Review B, 1988, 38, 805-807.	1.1	90
75	X-ray diffraction using synchrotron radiation at CHESS in the multimegabar regime. High Pressure Research, 1988, 1, 3-21.	0.4	14
76	The bulk modulus-volume relationship for oxide compounds and related geophysical problems. , 1988, , 153-165.		1
77	Effects of temperature and pressure on interatomic distances in oxygen-based minerals. , 1988, , 407-413.		35
78	Derivation of Wachtman's equation for the temperature dependence of the elastic moduli of oxide compounds. , 1988, , 166-170.		1
79	The bulk modulus-volume relationship for oxides. , 1988, , 283-289.		32
80	The single-crystal elastic moduli of stishovite. , 1988, , 459-465.		0
81	Some elastic constant data on minerals relevant to geophysics. , 1988, , 237-270.		2
82	Composition of the upper mantle: Geophysical tests of two petrological models. , 1988, , 513-516.		1
83	Homogeneity and constitution of the Earth's lower mantle and outer core. , 1988, , 341-348.		0
84	Elasticity and constitution of the Earth's interior. , 1988, , 31-90.		3
85	Theory of binding of ionic crystals: Application to alkali-halide and alkaline-Earth-dihalide crystals. , 1988, , 314-320.		1
86	The determination of the elastic constants of natural almandine-pyrope garnet by rectangular parallelepiped resonance method. , 1988, , 376-383.		8
87	The velocity of compressional waves in rocks to 10 kilobars, part 2. , 1988, , 91-116.		8
88	The elastic properties of composite materials. , 1988, , 384-406.		1
89	The effect of pressure upon the elastic parameters of isotropic solids, according to Murnaghan's theory of finite strain. , 1988, , 21-30.		0
90	Temperature coefficients of elastic constants of single crystal MgO between 80 And 1,300 K. , 1988, , 503-512.		0

#	Article	IF	Citations
91	Density distribution in the Earth. , 1988, , 1-20.		6
92	X-ray diffraction and optical observations on crystalline solids up to 300 kbar. , 1988, , 193-198.		0
93	Thermal expansion of silicate perovskite and atratification of the Earth's mantle. , 1988, , 521-523.		0
94	Reflection properties of phase transition and compositional change models of the 670-km Discontinuity. , 1988, , 488-502.		0
95	Ab initio structural and thermoelastic properties of orthorhombic MgSiO3 perovskite. , 1988, , 517-520.		0
96	Static compression of iron T78 GPa with rare gas solids as pressure-transmitting media. , 1988, , 524-531.		0
97	Equations of state of iron sulfide and constraints on the sulfur content of the Earth. , 1988, , 427-440.		0
98	Post-oxide phases of forsterite and enstatite. , 1988, , 358-360.		0
99	Velocity-density systematics and its implications for the iron content of the mantle. , 1988, , 335-340.		0
100	Composition of the Earth's mantle. , 1988, , 117-133.		0
101	Hydrostatic compression of perovskite-type MgSiO3. , 1988, , 466-474.		0
102	Some geophysical constraints on the chemical composition of the Earth's lower mantle. , 1988, , 475-487.		0
103	Pressure dependence of the thermal GrÃ¼neisen parameter, with application to the Earth's lower mantle and outer core. , 1988, , 349-357.		0
104	Elasticity of coesite. , 1988, , 414-426.		0
105	Velocity-density systematics: Derivation from Debye theory and the effect of ionic size. , 1988, , 305-313.		0
106	Elasticity of pyroxene-garnet and pyroxene-ilmenite phase transformations in germanates. , 1988, , 321-334.		64
107	A seismic equation of state. , 1988, , 171-192.		0
108	Elastic constants of single-crystal forsterite as a function of temperature and pressure. , 1988, , 271-282.		1

#	Article	IF	Citations
109	Equation of state of polycrystalline and single-crystal MgO to 8 kilobars and 800Â°K. , 1988, , 290-304.		0
110	The use of ultrasonic measurements under modest compression to estimate compression at high pressure. , 1988, , 134-152.		0
111	The temperature of shock compressed iron. , 1988, , 532-541.		0
112	The equation of state for iron and the Earth's core. , 1988, , 446-458.		5
113	GrÃ¼neisen parameter of quartz, quartzite, and fluorite at high pressure. , 1988, , 441-445.		0
114	Compressibility and stability of icosahedral Al-Mn up to 28 GPa. Physical Review B, 1989, 39, 2654-2660.	1.1	27
115	Structural phase transitions in InSb to 66 GPa. Physical Review B, 1989, 40, 12450-12456.	1.1	31
116	Highâ€pressure equations of state of krypton and xenon by a statistical mechanical theory. Journal of Chemical Physics, 1989, 91, 3133-3147.	1.2	29
117	Evidence for the Insulator-Metal Transition in Xenon from Optical, X-Ray, and Band-Structure Studies to 170 GPa. Physical Review Letters, 1989, 62, 669-672.	2.9	131
118	Structural phase transitions in GaAs to 108 GPa. Physical Review B, 1989, 39, 1280-1285.	1.1	119
119	First-principles equation of state of gold. Physical Review B, 1989, 40, 7501-7507.	1.1	45
120	Density and composition of the lower mantle. Philosophical Transactions of the Royal Society A, 1989, 328, 377-389.	1.3	120
121	Equation of state of solid ammonia (NH3) to 56 GPa. Journal of Physics and Chemistry of Solids, 1989, 50, 171-175.	1.9	18
122	Inverted isothermal equations of state and determination of B0, B'0 and B0. Journal of Physics and Chemistry of Solids, 1989, 50, 263-268.	1.9	68
123	Pressure dependent properties of cubic boron nitride. Solid State Communications, 1989, 71, 1055-1058.	0.9	27
124	Experimental and theoretical equation of state of cubic boron nitride. Nature, 1989, 337, 349-352.	13.7	307
125	Seismic velocities in mantle minerals and the mineralogy of the upper mantle. Journal of Geophysical Research, 1989, 94, 1895-1912.	3.3	558
126	Bulk moduli of magnesiowÃ¼stites from static compression measurements. Journal of Geophysical Research, 1989, 94, 3037-3045.	3.3	53

#	Article	IF	Citations
127	Shock wave equation of state and finite strain theory. Journal of Geophysical Research, 1989, 94, 5873-5886.	3.3	140
128	Theoretical Study of a new Transition Sequence in III-V Compounds: High-Pressure Phases of InSb. Materials Research Society Symposia Proceedings, 1990, 193, 89.	0.1	0
129	First Principles Calculations of the Equilibrium Mechanical Properties of Simple Metals and Ordered Intermetallic Alloys. Materials Research Society Symposia Proceedings, 1990, 186, 277.	0.1	12
130	Thermal expansion, heat capacity, and entropy of MgO at mantle pressures. Physics and Chemistry of Minerals, 1990, 17, 142.	0.3	81
131	Thermal properties of forsterite at mantle pressures derived from vibrational spectroscopy. Physics and Chemistry of Minerals, 1990, 17, 149.	0.3	126
132	High precision powder xâ€ray diffraction measurements at high pressures. Review of Scientific Instruments, 1990, 61, 2571-2580.	0.6	36
133	Miniaturization techniques for obtaining static pressures comparable to the pressure at the center of the earth: Xâ€ray diffraction at 416 GPa. Review of Scientific Instruments, 1990, 61, 3830-3833.	0.6	142
134	Total-energy calculations of solid H, Li, Na, K, Rb, and Cs. Physical Review B, 1990, 42, 11637-11643.	1.1	56
135	New high-pressure phase transition in zirconium metal. Physical Review Letters, 1990, 64, 204-207.	2.9	211
136	Static compression of metals Mo, Pb, and Pt to 272 GPa: Comparison with shock data. Physical Review B, 1990, 42, 8651-8654.	1.1	98
137	Equations of state of alkali hydrides at high pressures. Physical Review B, 1990, 41, 7883-7886.	1.1	45
138	Pressure dependence of the4T2and4T1absorption bands of ruby to 35 GPa. Physical Review B, 1990, 41, 5372-5381.	1.1	114
139	Yield strength ofAl2O3at high pressures. Physical Review B, 1990, 42, 2532-2535.	1.1	40
140	Pressure-inducedsâ†'dtransfer and the equation of state of molybdenum. Physical Review B, 1990, 41, 7440-7445.	1.1	30
141	Metallization pressure for NaCl in theB2 structure. Physical Review B, 1990, 42, 2752-2760.	1.1	12
142	Optical properties of diamond at pressures of the center of Earth. Applied Physics Letters, 1990, 57, 1007-1009.	1.5	22
143	Static compression of Ca(OH)₂ at room temperature: Observations of amorphization and equation of state measurements to 10.7 GPa. Geophysical Research Letters, 1990, 17, 1157-1160.	1.5	157
144	Thermodynamically consistent decompression: Implications for lower mantle composition. Journal of Geophysical Research, 1990, 95, 12583-12593.	3.3	43

#	Article	IF	Citations
145	Fundamental thermodynamic relations and silicate melting with implications for the constitution of Dâ€³. Journal of Geophysical Research, 1990, 95, 19311-19325.	3.3	123
146	Structural and electronic properties of Fe₂SiO₄â€fayalite at ultrahigh pressures: Amorphization and gap closure. Journal of Geophysical Research, 1990, 95, 21549-21563.	3.3	107
147	Static compression of iron to 300 GPa and Fe_{0.8}Ni_{0.2} alloy to 260 GPa: Implications for composition of the core. Journal of Geophysical Research, 1990, 95, 21737-21742.	3.3	475
148	Structural properties of ordered high-melting-temperature intermetallic alloys from first-principles total-energy calculations. Physical Review B, 1990, 41, 10311-10323.	1.1	386
149	High-pressure properties of wurtzite- and rocksalt-type aluminum nitride. Physical Review B, 1991, 44, 9056-9059.	1.1	167
150	Calculated elastic constants and structural properties of Mo andMoSi2. Physical Review B, 1991, 43, 6500-6509.	1.1	162
151	The effect of nonhydrostaticity on measuring the pressure in metals by energy dispersive X-ray diffraction in the diamond anvil cell. High Pressure Research, 1991, 6, 183-186.	0.4	13
152	High-Pressure X-Ray Diffraction Study on Electronics-dTransition in Zirconium. Journal of the Physical Society of Japan, 1991, 60, 3211-3214.	0.7	89
153	Equations of state for strong compression. High Pressure Research, 1991, 7, 290-292.	0.4	16
154	The highâ€pressure phase diagram of Fe_{0.94}O: A possible constituent of the Earth's core. Journal of Geophysical Research, 1991, 96, 16169-16180.	3.3	89
155	Thermal properties of Î²â€Mg₂SiO₄ at mantle pressures derived from vibrational spectroscopy: Implications for the mantle at 400 km depth. Journal of Geophysical Research, 1991, 96, 11817-11829.	3.3	68
156	The shock wave equation of state of brucite Mg(OH)₂. Journal of Geophysical Research, 1991, 96, 14319-14330.	3.3	52
157	Compressional study of katoite [Ca₃Al₂(O₄H₄)₃] and grossular garnet. Journal of Geophysical Research, 1991, 96, 14313-14318.	3.3	55
158	Carbonate stability in the Earth's mantle: A vibrational spectroscopic study of aragonite and dolomite at high pressures and temperatures. Journal of Geophysical Research, 1991, 96, 17997-18009.	3.3	94
159	Calculations of the total energy, electron-phonon interaction and Stoner parameter in the 5d transition metal hydrides. Journal of the Less Common Metals, 1991, 172-174, 401-410.	0.9	4
160	The closing diamond anvil optical window in multimegabar research. Journal of Applied Physics, 1991, 69, 6413-6416.	1.1	56
161	Earth's Core-Mantle Boundary: Results of Experiments at High Pressures and Temperatures. Science, 1991, 251, 1438-1443.	6.0	359
162	Static strength and equation of state of rhenium at ultra-high pressures. Nature, 1991, 349, 687-689.	13.7	76

#	Article	IF	Citations
163	Molecular dynamics simulations of pressure and temperature effects on MgSiO3 and Mg2SiO4 melts and glasses. Physics and Chemistry of Minerals, 1991, 17, 661.	0.3	96
164	Static compression of ?-MnS at 298 K to 21 GPa. Physics and Chemistry of Minerals, 1991, 17, 636.	0.3	22
165	Theory of high-pressure phases of Pb. Physical Review B, 1991, 43, 1795-1798.	1.1	37
166	First-principles calculation of the elastic moduli ofNi3Al. Physical Review B, 1991, 43, 1805-1807.	1.1	31
167	Pressure strengthening: A possible route to obtaining 9 Mbar and metallic diamonds. Journal of Applied Physics, 1991, 70, 2066-2070.	1.1	46
168	Structural properties of a three-dimensional all-sp2phase of carbon. Physical Review B, 1991, 43, 6742-6745.	1.1	86
169	Theoretical study of high-pressure phases of tin. Physical Review B, 1991, 43, 9251-9254.	1.1	34
170	Molecular Dynamics and Diffusion in Silicate Melts. , 1991, , 1-50.		8
171	The effect of a tapered aperture on xâ€•ray diffraction from a sample with a pressure gradient: Studies on three samples with a maximum pressure of 560 GPa. Review of Scientific Instruments, 1992, 63, 4342-4348.	0.6	104
172	Pressure-induced phase transformations in alkali-metal hydrides calculated using an improved linear-muffin-tin-orbitalâ€“atomic-sphere-approximation energy scheme. Physical Review B, 1992, 45, 90-96.	1.1	22
173	Total energy and band structure of the 3d, 4d, and 5dmetals. Physical Review B, 1992, 45, 5777-5783.	1.1	115
174	Comparison of carbon and boron nitride in a hypothetical all-sp2-bonded tetragonal phase. Physical Review B, 1992, 45, 12746-12751.	1.1	16
175	Effect of Pressure on Order and Stability in Alloys: The Case of Al-Ge. Materials Research Society Symposia Proceedings, 1992, 291, 153.	0.1	0
176	Theoretical study of a hypothetical metallic phase of carbon. Physical Review B, 1992, 45, 4579-4581.	1.1	64
177	General-potential study of the electronic and magnetic structure of FeCo. Physical Review B, 1992, 46, 11145-11148.	1.1	36
178	A High-Pressure Test of Birch's Law. Science, 1992, 257, 66-68.	6.0	32
179	Zinc-blendeâ€“wurtzite polytypism in semiconductors. Physical Review B, 1992, 46, 10086-10097.	1.1	977
180	Synchrotron X-ray diffraction studies on the transition metal alloy Moî—¸Re under high pressures. Scripta Metallurgica Et Materialia, 1992, 26, 1395-1398.	1.0	3

#	Article	IF	Citations
181	Alexandrite as a highâ€temperature pressure calibrant, and implications for the rubyâ€fluorescence scale. Journal of Applied Physics, 1992, 71, 1579-1582.	1.1	41
182	Superconductivity in simple cubic phase of arsenic. Phase Transitions, 1992, 38, 61-68.	0.6	2
183	Comment [on â€œPressure derivative of the bulk modulusâ€•by A. M. Hofmeister]. Journal of Geophysical Research, 1992, 97, 15273-15273.	3.3	2
184	Reply [to â€œComment on â€˜Pressure derivative of the bulk modulusâ€™ by A. M. Hofmeisterâ€]. Journal of Geophysical Research, 1992, 97, 15275-15275.	3.3	0
185	Calculation of Elastic Properties from Thermodynamic Equation of State Principles. Annual Review of Earth and Planetary Sciences, 1992, 20, 527-552.	4.6	78
186	Shock-induced transformations in the system NaAlSiO4?SiO2: a new interpretation. Physics and Chemistry of Minerals, 1992, 18, 359.	0.3	16
187	P-V-T equation of state of magnesiowï¿½stite (Mg0.6Fe0.4)O. Physics and Chemistry of Minerals, 1992, 18, 416.	0.3	111
188	Mï¿½ssbauer studies of iron silicate spinel at high pressure. Physics and Chemistry of Minerals, 1992, 19, 236.	0.3	17
189	Theoretical study of diamond under strong anisotropic stresses. Solid State Communications, 1992, 84, 731-733.	0.9	17
190	X-ray and optical study of AgReO4 under pressure. Journal of Physics and Chemistry of Solids, 1992, 53, 631-638.	1.9	10
191	Sound velocities at high pressure and temperature and their geophysical implications. Journal of Geophysical Research, 1992, 97, 4503-4520.	3.3	85
192	Polynomial approximations to a universal equation of state. Journal of Physics and Chemistry of Solids, 1992, 53, 485-492.	1.9	4
193	The dependence of the Anderson-GrÃ¼neisen parameter ÎT upon compression at extreme conditions. Journal of Physics and Chemistry of Solids, 1993, 54, 221-227.	1.9	97
194	Properties of ordered intermetallic alloys: first-principles and approximate methods. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1993, 170, 49-57.	2.6	27
195	Systematics and anomalies in the equations of states for the lanthanide and actinide elements. Physica B: Condensed Matter, 1993, 190, 21-30.	1.3	14
196	Compression of ?-MnS (alabandite) and a new high-pressure phase. Physics and Chemistry of Minerals, 1993, 20, 63.	0.3	23
197	Accuracy in measurements and the temperature and volume dependence of thermoelastic parameters. Pure and Applied Geophysics, 1993, 141, 327-339.	0.8	4
198	High-pressure structure of gallium nitride: Wurtzite-to-rocksalt phase transition. Physical Review B, 1993, 47, 12925-12928.	1.1	167

#	Article	IF	Citations
199	Condensed-Matter Energetics from Diatomic Molecular Spectra. Science, 1993, 260, 649-652.	6.0	17
200	Thermal expansivity, bulk modulus, and melting curve of H2Oâ€“ice VII to 20 GPa. Journal of Chemical Physics, 1993, 99, 5369-5373.	1.2	163
201	Thorium under strong compressionâ€”a test case for the evaluation of EOS data by different forms and procedures. High Pressure Research, 1993, 11, 223-237.	0.4	31
202	Î²-Po phase of sulfur at 162 GPa: X-ray diffraction study to 212 GPa. Physical Review Letters, 1993, 71, 2943-2946.	2.9	109
203	Structural, bonding, and electronic properties of IIA-IV antifluorite compounds. Physical Review B, 1993, 48, 17138-17144.	1.1	92
204	Pressure dependence of the elastic moduli in aluminum-rich Al-Li compounds. Physical Review B, 1993, 47, 2493-2500.	1.1	397
205	Deviatoric stress in a quasiâ€hydrostatic diamond anvil cell: Effect on the volumeâ€based pressure calibration. Geophysical Research Letters, 1993, 20, 1147-1150.	1.5	108
206	Refractive index determination at high pressures using the Fourier transform signal of an FT spectrometer. Measurement Science and Technology, 1993, 4, 237-239.	1.4	4
207	Analytic expressions of band structure potentials and transferability studies. Modelling and Simulation in Materials Science and Engineering, 1993, 1, 307-313.	0.8	0
208	Phase stability of wÃ¼stite at high pressure from first-principles linearized augmented plane-wave calculations. Physical Review B, 1993, 47, 7720-7731.	1.1	56
209	Weighted-density-approximation ground-state studies of solids. Physical Review B, 1993, 48, 14099-14103.	1.1	27
210	Pressureâ€induced rocksalt phase of aluminum nitride: A metastable structure at ambient condition. Journal of Applied Physics, 1993, 73, 8198-8200.	1.1	202
211	X-ray-diffraction study of sulfur to 32 GPa: Amorphization at 25 GPa. Physical Review B, 1993, 48, 569-572.	1.1	63
212	Energetics, structure, and compressibility of NaF determined by the periodic Hartreeâ€“Fock method. Journal of Chemical Physics, 1993, 99, 336-344.	1.2	10
213	Optical probing of hot expanded states produced by shock release. Physical Review E, 1993, 47, 3547-3565.	0.8	49
214	Theoretical study of high-pressure orthorhombic silicon. Physical Review B, 1993, 48, 16144-16147.	1.1	35
215	BP at megabar pressures and its equation of state to 110 GPa. Journal of Applied Physics, 1993, 74, 1660-1662.	1.1	47
216	Pressure-induced phase transition in SiC. Physical Review B, 1993, 48, 10587-10590.	1.1	205

#	Article	IF	Citations
217	Equation of State. , 1993, , 75-113.		99
218	Chapter 113 High-pressure studies â€" Structural aspects. Fundamental Theories of Physics, 1993, 17, 245-300.	0.1	28
219	X-ray measurements of the compressibility of an Al5.1Li3Cu quasi-crystal. Journal of Physics Condensed Matter, 1994, 6, 2185-2188.	0.7	1
220	Electronic structure and stability of the transition metal oxide Ni2Ti4O. Journal of Physics Condensed Matter, 1994, 6, 2861-2868.	0.7	2
221	Universal equation of state for compressed solids. Physical Review B, 1994, 49, 3049-3060.	1.1	79
222	Magnetic and electronic structure of CoH. Physical Review B, 1994, 49, 12801-12804.	1.1	6
223	Ab initiopseudopotential calculations for aluminum-rich cobalt compounds. Physical Review B, 1994, 50, 2075-2084.	1.1	17
224	Variational charge relaxation in ionic crystals: An efficient treatment of statics and dynamics. Physical Review B, 1994, 50, 15559-15574.	1.1	27
225	High pressure study of AlP: Transformation to a metallic NiAs phase. Journal of Applied Physics, 1994, 76, 7296-7299.	1.1	49
226	Ab initiocalculation of melting and thermodynamic properties of crystal and liquid aluminum. Physical Review B, 1994, 50, 5055-5061.	1.1	43
227	High-pressure structural study of barium to 90 GPa. Physical Review B, 1994, 50, 16238-16246.	1.1	45
228	Elastic properties ofB2-NiTi andB2-PdTi. Physical Review B, 1994, 50, 13113-13117.	1.1	41
229	Bonding in the molybdenum silicides. Physical Review B, 1994, 50, 10742-10760.	1.1	42
230	Electronic structure and physical properties of bcc selenium under high pressure. High Pressure Research, 1994, 12, 111-118.	0.4	0
231	Lattice instability in Î²â€SiC and simulation of brittle fracture. Journal of Applied Physics, 1994, 76, 2719-2725.	1.1	58
232	Al as a Simple Solid: High Pressure Study to 220 GPa (2.2 Mbar). Physical Review Letters, 1994, 73, 2075-2078.	2.9	133
233	Hydrostatic compression of ?-Mg2SiO4 to mantle pressures and 700 K: Thermal equation of state and related thermoelastic properties. Physics and Chemistry of Minerals, 1994, 21, 407.	0.3	81
234	Structural change of GeO2 under pressure. Physics and Chemistry of Minerals, 1994, 20, 531-535.	0.3	26

#	Article	IF	Citations
235	Elastic properties of monoclinic and orthorhombic ZrO2. Journal of Materials Science Letters, 1994, 13, 514-515.	0.5	4
236	Birch Equation of State for Alkali Halide Crystals. Physica Status Solidi (B): Basic Research, 1994, 181, 387-395.	0.7	11
237	Structural phase transformation and ground state properties of cadmium telluride. Solid State Communications, 1994, 91, 607-610.	0.9	11
238	Prediction of an orthorhombic phase of germanium. Solid State Communications, 1994, 89, 483-486.	0.9	28
239	Approximate equations of state for solids from limited data sets. Journal of Physics and Chemistry of Solids, 1994, 55, 711-719.	1.9	18
240	Compression of MgS TO 54 GPa. Journal of Physics and Chemistry of Solids, 1994, 55, 413-419.	1.9	60
241	Correlation of frequency shifts with other properties in ice: a periodic Hartreeâ€"Fock study. Journal of Molecular Structure, 1994, 325, 77-84.	1.8	3
242	High-pressure polymorphism of the copper(I) halides: A neutron-diffraction study to âˆ¼10 GPa. Physical Review B, 1994, 50, 5868-5885.	1.1	202
243	Relativistic density functional calculation of the total energy and Fermi surface of gold. European Physical Journal B, 1994, 95, 145-150.	0.6	3
244	Static compression of chondrodite: Implications for water in the upper mantle. Geophysical Research Letters, 1994, 21, 1935-1938.	1.5	37
245	High-pressure acoustic wave velocities and equations of state of the alkali chlorides. Journal of Geophysical Research, 1994, 99, 11765-11774.	3.3	4
246	The equation of state, amorphization, and high-pressure phase diagram of muscovite. Journal of Geophysical Research, 1994, 99, 19785-19792.	3.3	59
247	Electronic structure and structural phase stability in BaS, BaSe, and BaTe. Physical Review B, 1994, 50, 12318-12325.	1.1	106
248	In Situ Determination of the NiAs Phase of FeO at High Pressure and Temperature. Science, 1994, 266, 1678-1680.	6.0	228
249	First-principles study of stability and local order in bcc-based Fe-Cr and Fe-V alloys. Physical Review B, 1994, 50, 15542-15558.	1.1	51
250	Sound velocity of Al2O3 to 616 kbar. Physics of the Earth and Planetary Interiors, 1994, 87, 77-83.	0.7	13
251	Phase transformation of AlAs to NiAs structure at high pressure. Physical Review Letters, 1994, 72, 2045-2048.	2.9	67
252	Structural phase transformations and the equations of state of calcium chalcogenides at high pressure. Physical Review B, 1994, 50, 16232-16237.	1.1	142

#	Article	IF	Citations
253	Stability of the wurtzite-type structure under high pressure: GaN and InN. Physical Review B, 1994, 49, 14-21.	1.1	620
254	High-pressure phase transformation and the equation of state of SrSe. Physical Review B, 1994, 49, 15341-15343.	1.1	59
255	Pressure Induced Metastable Amorphization of BAs: Evidence for a Kinetically Frustrated Phase Transformation. Physical Review Letters, 1994, 73, 2476-2479.	2.9	69
256	Raman Modes of6HPolytype of Silicon Carbide to Ultrahigh Pressures: A Comparison with Silicon and Diamond. Physical Review Letters, 1994, 72, 4105-4108.	2.9	125
257	Static compression and H disorder in brucite, Mg(OH)2, to 11 GPa: a powder neutron diffraction study. Physics and Chemistry of Minerals, 1995, 22, 200.	0.3	199
258	Single-crystal x-ray diffraction of brucite to 14 GPa. Physics and Chemistry of Minerals, 1995, 22, 277.	0.3	49
259	Total energy calculations in theDFT on binary compounds. International Journal of Quantum Chemistry, 1995, 55, 339-345.	1.0	24
260	MgAl2O4 spinel crystal structure. An ab initio perturbed ion study. International Journal of Quantum Chemistry, 1995, 56, 685-694.	1.0	3
261	Equations of State and Pressure Dependence of Bulk Modulus for NaCl Crystals. Physica Status Solidi (B): Basic Research, 1995, 189, 363-369.	0.7	13
262	High Pressure Properties of the Alkalineâ€Earth Sulphides. Physica Status Solidi (B): Basic Research, 1995, 190, 193-197.	0.7	25
263	High pressure structural study of AlSb to 50 GPa. Journal of Physics and Chemistry of Solids, 1995, 56, 517-520.	1.9	20
264	High pressure X-ray and Raman study of ZnSe. Journal of Physics and Chemistry of Solids, 1995, 56, 521-524.	1.9	48
265	High pressure phase transitions in aluminum phosphide. Solid State Communications, 1995, 95, 173-175.	0.9	15
266	Analysis of pressure-volume relations for NaCl crystal at high temperatures. Solid State Communications, 1995, 96, 417-420.	0.9	4
267	High-pressure synthesis, characterization, and equation of state of cubic C-BN solid solutions. Physical Review B, 1995, 51, 12149-12156.	1.1	236
268	High Pressure Phase of MgTe: Stable Structure at STP?. Physical Review Letters, 1995, 74, 5232-5235.	2.9	68
269	Pressure-induced phase transformations in AlAs: Comparison betweenab initiotheory and experiment. Physical Review B, 1995, 51, 5678-5681.	1.1	17
270	Electronic structure and total-energy calculations by a semi-self-consistent augmented-plane-wave method. Physical Review B, 1995, 51, 14048-14056.	1.1	1

#	Article	IF	Citations
271	Atomistic simulation of thermomechanical properties of Î²-SiC. Physical Review B, 1995, 52, 15150-15159.	1.1	105
272	bcc arsenic at 111 GPa: An x-ray structural study. Physical Review B, 1995, 51, 597-600.	1.1	39
273	Pressure evolution of the cinnabar phase of HgTe. Physical Review B, 1995, 51, 8731-8736.	1.1	56
274	Puzzling Results of Compressibility Measurements of Al _{5.1} Li ₃ Cu Quasi-Crystal. Europhysics Letters, 1995, 29, 19-23.	0.7	3
275	Compressibility of FeSi between 0 and 9 GPa, determined by high pressure time-of-flight neutron powder diffraction. Journal of Physics Condensed Matter, 1995, 7, L475-L479.	0.7	21
276	Phase transformation of BeSe and BeTe to the NiAs structure at high pressure. Physical Review B, 1995, 52, 7058-7064.	1.1	126
277	Static compression of Îµ-FeSi and an evaluation of reduced silicon as a deep Earth constituent. Geophysical Research Letters, 1995, 22, 445-448.	1.5	47
278	Compressional sound velocity, equation of state, and constitutive response of shock-compressed magnesium oxide. Journal of Geophysical Research, 1995, 100, 529-542.	3.3	99
279	Shear and compression waves in shocked calcium carbonate. Journal of Geophysical Research, 1995, 100, 1955-1980.	3.3	10
280	New High Pressure Crystal Structure and Equation of State of Cesium Hydride to 253 GPa. Physical Review Letters, 1995, 74, 2264-2267.	2.9	41
281	First-principles study of several hypothetical silica framework structures. Physical Review B, 1995, 52, 8064-8073.	1.1	113
282	A numerical investigation of the liquidâ€“vapor coexistence curve of silica. Journal of Chemical Physics, 1996, 104, 7633-7644.	1.2	116
283	Molecular dynamics simulations of compressible ions. Journal of Chemical Physics, 1996, 104, 8068-8081.	1.2	94
284	Anab InitioHartreeâ^'Fock Study of the Cubic and Tetragonal Phases of Bulk Tungsten Trioxide. Journal of the American Chemical Society, 1996, 118, 12174-12182.	6.6	120
285	Polarization dependence of Born effective charge and dielectric constant inKNbO3. Physical Review B, 1996, 54, 11161-11168.	1.1	54
286	Pressure-dependent properties of SiC polytypes. Physical Review B, 1996, 53, 13400-13413.	1.1	123
287	Physics of solids under strong compression. Reports on Progress in Physics, 1996, 59, 29-90.	8.1	252
288	The stability and equation of state of majoritic garnet synthesized from natural basalt at mantle conditions. Geophysical Research Letters, 1996, 23, 3377-3380.	1.5	18

#	Article	IF	Citations
289	Pressureâ€induced amorphization of covellite, CuS. Journal of Chemical Physics, 1996, 104, 11-16.	1.2	32
290	The fluorescence sideband method for obtaining acoustic velocities at high compressions: application to MgO and MgAl2O4. Physics and Chemistry of Minerals, 1996, 23, 25.	0.3	39
291	Thermal expansivity of lower mantle phases MgO and MgSiO3 perovskite at high pressure derived from vibrational spectroscopy. Physics of the Earth and Planetary Interiors, 1996, 98, 3-15.	0.7	73
292	Low-Compressibility Carbon Nitrides. Science, 1996, 271, 53-55.	6.0	1,210
293	Seismic Evidence for Partial Melt at the Base of Earth's Mantle. Science, 1996, 273, 1528-1530.	6.0	519
294	Polymorphs of Alumina Predicted by First Principles: Putting Pressure on the Ruby Pressure Scale. Science, 1996, 274, 1880-1882.	6.0	92
295	Ground-state properties and structural phase transformation of beryllium oxide. Journal of Physics Condensed Matter, 1996, 8, 3385-3390.	0.7	44
296	Pressure dependence of the lattice constant of diamond: Isotopic effects. JETP Letters, 1996, 63, 83-88.	0.4	10
297	Pressure dependence of hydrogen bonding in a novel H2Oî—¸H2 clathrate. Chemical Physics Letters, 1996, 257, 524-530.	1.2	63
298	Ground state properties and structural phase transformation of berylliumsulphide. Solid State Communications, 1996, 98, 741-743.	0.9	47
299	High pressure effect on the magnetic transition in heavy fermion systems CePd2Al3 and CePdAl. Physica B: Condensed Matter, 1996, 217, 97-101.	1.3	20
300	Structural, electronic and optical properties of carbon nitride. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1996, 209, 1-4.	2.6	43
301	Theoretical structural phase stability of BeO to 1 TPa. Physical Review B, 1996, 54, 8965-8968.	1.1	48
302	Pressure dependence of Born effective charges, dielectric constant, and lattice dynamics in SiC. Physical Review B, 1996, 53, 5430-5437.	1.1	59
303	Pressure-induced structural phase transitions in theAMnF4series (A=Cs, Rb, K) studied by synchrotron x-ray powder diffraction: Correlation between hydrostatic and chemical pressure. Physical Review B, 1996, 54, 7052-7061.	1.1	21
304	Nb4N3: Polymorphism in crystalline niobium nitrides. Physical Review B, 1996, 53, 12563-12565.	1.1	8
305	First-principles study on energetics ofc-BN(001) reconstructed surfaces. Physical Review B, 1996, 54, 5586-5603.	1.1	460
306	Anomalous compression in - an experimental and computational study. Journal of Physics Condensed Matter, 1997, 9, 5867-5874.	0.7	7

#	Article	IF	Citations
307	Equation of state ofMgAl2O4spinel to 65 GPa. Physical Review B, 1997, 56, 1-4.	1.1	95
308	IR spectroscopy of alkali halides at very high pressures: Calculation of equations of state and of the response of bulk moduli to theB1â˜’B2phase transition. Physical Review B, 1997, 56, 5835-5855.	1.1	64
309	Dynamic compression of an Feâ€“Crâ€“Ni alloy to 80 GPa. Journal of Applied Physics, 1997, 82, 4259-4269.	1.1	50
310	Evidence for â€œPartialâ€•(Sublattice) Amorphization in Co(OH)2. Physical Review Letters, 1997, 78, 1936-1939.	2.9	66
311	Tight-binding interatomic potentials based on total-energy calculation: Application to noble metals using molecular-dynamics simulation. Physical Review B, 1997, 55, 2150-2156.	1.1	70
312	Phase transformation of BeS and equation-of-state studies to 96 GPa. Physical Review B, 1997, 56, 14338-14343.	1.1	89
313	Equation of state of Î±-Si3N4s. Physical Review B, 1997, 55, 3456-3460.	1.1	51
314	Elastic constants of Mo/V superlattices. Physical Review B, 1997, 55, 10057-10063.	1.1	4
315	Theoretical study of a five-coordinated silica polymorph. Physical Review B, 1997, 56, 5797-5806.	1.1	68
316	Evaluation of the screened Korringa-Kohn-Rostoker method for accurate and large-scale electronic-structure calculations. Physical Review B, 1997, 55, 9400-9408.	1.1	63
317	Equation of state of polycrystalline Ni50Al50. Journal of Materials Research, 1997, 12, 3106-3108.	1.2	39
318	High Pressure - High Temperature Synthesis of Low-Compressibility Cubic C3N4. Materials Research Society Symposia Proceedings, 1997, 499, 303.	0.1	3
319	Structural Characterization of Crystalline Si-C-N Films. Materials Research Society Symposia Proceedings, 1997, 498, 301.	0.1	0
320	X-Ray Structural Study of Li3N at High Pressure. Materials Research Society Symposia Proceedings, 1997, 499, 133.	0.1	0
321	Progress in the Search for Metallic Hydrogen: 342 GPa. Materials Research Society Symposia Proceedings, 1997, 499, 341.	0.1	0
322	Novel Structure of MgSe in the Multimegabar Regime: Positional Parameter Determination. Materials Research Society Symposia Proceedings, 1997, 499, 429.	0.1	0
323	Synchrotron x-ray-diffraction study of Î±-cristobalite at high pressure and high temperature. High Pressure Research, 1997, 15, 307-319.	0.4	8
324	High-pressure phases of magnesium selenide and magnesium telluride. Physical Review B, 1997, 55, 775-779.	1.1	60

#	Article	IF	Citations
325	Evidence of a low compressibility carbon nitride with defect-zincblende structure. Journal of Applied Physics, 1997, 81, 2555-2559.	1.1	81
326	Ab initio calculations of the pressure-induced structural phase transitionsfor four II-VI compounds. Physical Review B, 1997, 55, 13025-13031.	1.1	191
327	Theoretical study of boron nitride modifications at hydrostatic pressures. Physical Review B, 1997, 55, 6203-6210.	1.1	131
328	Transition Metal Oxide Chemistry:â€‰ Electronic Structure Study of WO3, ReO3, and NaWO3. Journal of Physical Chemistry B, 1997, 101, 3945-3952.	1.2	107
329	Electrical resistivity of Fe3O4to 48 GPa: Compression-induced changes in electron hopping at mantle pressures. Journal of Geophysical Research, 1997, 102, 18139-18148.	3.3	43
330	Equation-of-state data for CsCl-type alkali halides. Journal of Physics Condensed Matter, 1997, 9, 5581-5592.	0.7	26
331	Structure, Bonding, and Geochemistry of Xenon at High Pressures. Science, 1997, 277, 930-933.	6.0	94
332	Constraints on core chemistry from the pressure dependence of the bulk modulus. Physics of the Earth and Planetary Interiors, 1997, 100, 49-59.	0.7	30
333	Thermal conductivity of corundum and periclase and implications for the lower mantle. Journal of Geophysical Research, 1997, 102, 2999-3008.	3.3	63
334	Single-crystal compression and crystal structure of clinopyroxene up to 10 GPa. American Mineralogist, 1997, 82, 245-258.	0.9	99
335	Equation of state of the rocksalt phase of IIIâ€“V nitrides to 72 GPa or higher. Journal of Physics and Chemistry of Solids, 1997, 58, 2093-2099.	1.9	134
336	Electronic, structural, and optical properties of crystalline yttria. Physical Review B, 1997, 56, 14993-15000.	1.1	139
337	A general equation of state for dense fluids. International Journal of Thermophysics, 1997, 18, 1197-1216.	1.0	17
338	High pressure X-ray diffraction study of Î²-Si3N4. Solid State Communications, 1997, 103, 107-112.	0.9	44
339	Structural and Electronic Properties of SrS, SrSe, and SrTe Under Pressure. Journal of Low Temperature Physics, 1998, 112, 211-226.	0.6	57
340	Solid hydrogen at 342â€‰GPa: no evidence for an alkali metal. Nature, 1998, 393, 46-49.	13.7	230
341	Abâ€Ìnitio Total Energy Calculation of Î±â€•and Î²â€Silicon Nitride and the Derivation of Effective Pair Potentials with Application to Lattice Dynamics. Journal of the American Ceramic Society, 1998, 81, 3189-3196.	1.9	81
342	Study of P-V-T relationship and thermodynamic properties for NaCl crystal. Journal of Physics and Chemistry of Solids, 1998, 59, 993-996.	1.9	7

#	Article	IF	Citations
343	Molecular dynamics simulation of high pressure phases of CuCl and CuBr. Journal of Physics and Chemistry of Solids, 1998, 59, 1293-1301.	1.9	35
344	Amorphization of Ca3(VO4)2at High Pressure. Journal of Solid State Chemistry, 1998, 139, 161-167.	1.4	16
345	High-pressure X-ray diffraction of Sr3(VO4)2 and Ba3(VO4)2. Physica B: Condensed Matter, 1998, 252, 268-273.	1.3	10
346	Surface atomic forces and multilayer relaxation of W(001), W(110) and Fe/W(110). Surface Science, 1998, 417, 151-158.	0.8	19
347	Determination of the partial molar volume of SiO2 in silicate liquids at elevated pressures and temperatures: a new experimental approach. Geochimica Et Cosmochimica Acta, 1998, 62, 2499-2508.	1.6	27
348	Calculation of thePâ^'Tphase diagram of Zr in different approximations for the exchange-correlation energy. Physical Review B, 1998, 57, 13485-13490.	1.1	51
349	Compression of klockmannite, CuSe. Journal of Chemical Physics, 1998, 109, 634-636.	1.2	9
350	Elastic moduli of tungsten to 15 Mbar, phase transition at 6.5 Mbar, and rheology to 6 Mbar. Physical Review B, 1998, 58, 2998-3002.	1.1	40
351	Structure and pressure variation of the anion polarizability and dependent properties in solid magnesium oxide. Molecular Physics, 1998, 95, 1-15.	0.8	8
352	The influence of yield strength on the non-hydrostatic compression of elastically anisotropic polycrystals. High Pressure Research, 1998, 16, 45-61.	0.4	3
353	Variable-cell-shape-based structural optimization applied to calcium nitrides. Physical Review B, 1998, 57, 7615-7620.	1.1	32
354	Equations of state for solids under strong compression. High Pressure Research, 1998, 16, 81-126.	0.4	106
355	High-pressure structural behaviour of silver(I) fluoride. Journal of Physics Condensed Matter, 1998, 10, 7945-7955.	0.7	19
356	Energetics of titanium nitrides of composition. Journal of Physics Condensed Matter, 1998, 10, 10223-10240.	0.7	6
357	Second-moment interatomic potential for Cu-Au alloys based on total-energy calculations and its application to molecular-dynamics simulations. Journal of Physics Condensed Matter, 1998, 10, 10979-10990.	0.7	28
358	Equation of state of wurtzitic boron nitride to 66 GPa. Applied Physics Letters, 1998, 72, 1691-1693.	1.5	59
359	Nonhydrostatic compression of elastically anisotropic polycrystals. I. Hydrostatic limits of 4:1 methanol-ethanol and paraffin oil. Physical Review B, 1998, 57, 3253-3263.	1.1	48
360	Prediction of structural parameters and physical properties ofCsHSO3up to 60 GPa. Physical Review B, 1998, 57, 4321-4326.	1.1	5

#	Article	IF	Citations
361	Total energy and magnetic moments in disorderedFexCu1â^'xalloys. Physical Review B, 1998, 57, 5213-5219.	1.1	86
362	Crystal structure of InBi under pressure up to 75 GPa. Physical Review B, 1998, 57, 4975-4978.	1.1	25
363	High pressure studies of the rhodiumâ€"hydrogen system in diamond anvil cell. Journal of Chemical Physics, 1998, 108, 2084-2087.	1.2	29
364	Analysis of lattice strains measured under nonhydrostatic pressure. Journal of Applied Physics, 1998, 83, 7567-7575.	1.1	335
365	Sevenfold Coordinated MgSe: Experimental Internal Atom Position Determination to 146 GPa, Diffraction Studies to 202 GPa, and Theoretical Studies to 500 GPa. Physical Review Letters, 1998, 81, 2723-2726.	2.9	39
366	Experimental confirmation of apâ^'pintraband gap inSr2FeO4. Physical Review B, 1998, 58, 10283-10287.	1.1	22
367	First principles calculations of structural properties of Î²-Si3â^'nCnN4 (n=0, 1, 2, 3). Journal of Applied Physics, 1998, 83, 1975-1978.	1.1	36
368	Ab Initio Electronic Band Structure Calculations for Calcium Monochalcogenides. International Journal of Modern Physics B, 1998, 12, 1709-1717.	1.0	39
369	Equation of State at High Pressure. , 1998, , 1-35.		3
370	A Fully Relativistic Full-Potential LCAO Method for Solids. Journal of the Physical Society of Japan, 1999, 68, 1982-1987.	0.7	31
371	Effects of temperature and composition on the bulk modulus of (Mg,Fe)O. American Mineralogist, 1999, 84, 272-276.	0.9	207
372	High pressure single crystal X-ray diffraction study on ruby up to 31 GPa. Zeitschrift Fur Kristallographie - Crystalline Materials, 1999, 214, 331-336.	0.4	24
373	Electronic structure of the bulk and layers of the alkaline earths (Be-Ba). Journal of Physics Condensed Matter, 1999, 11, 4291-4302.	0.7	6
374	Nonscalability and nontransferability in the electronic properties of the Y-Al-O system. Physical Review B, 1999, 59, 12815-12821.	1.1	112
375	Static compression of Ti3SiC2 to 61 GPa. Applied Physics Letters, 1999, 74, 3782-3784.	1.5	92
376	High-pressure studies of MgTe using first-principle electronic-structure calculations. Physical Review B, 1999, 60, 11846-11847.	1.1	17
377	Lattice strains in gold and rhenium under nonhydrostatic compression to 37 GPa. Physical Review B, 1999, 60, 15063-15073.	1.1	186
378	First-principles search for high-pressure phases ofGaAsO4. Physical Review B, 1999, 60, 3751-3756.	1.1	6

#	Article	IF	Citations
379	Experimental and theoretical study ofLi3Nat high pressure. Physical Review B, 1999, 59, 6083-6086.	1.1	21
380	Structural phase stability and electron-phonon coupling in lithium. Physical Review B, 1999, 59, 4028-4035.	1.1	46
381	STRUCTURAL PHASE STABILITY OF Ti3Al UNDER HIGH PRESSURE. International Journal of Modern Physics B, 1999, 13, 841-845.	1.0	6
382	Electronic band structure calculation and structural stability of high pressure phases of selenium. Solid State Communications, 1999, 109, 339-344.	0.9	9
383	Band structure calculation and structural stability of high pressure phases of EuSe. Solid State Communications, 1999, 112, 39-44.	0.9	17
384	Structural and electrical properties of NiAs-type compounds under pressure. Journal of Physics and Chemistry of Solids, 1999, 60, 167-179.	1.9	19
385	Model structures and properties of the electron density distribution for low quartz at pressure: a study of the SiO bond. Journal of Molecular Structure, 1999, 485-486, 13-25.	1.8	36
386	Atomistic study of zinc-blende BAs from molecular dynamics. Physics Letters, Section A: General, Atomic and Solid State Physics, 1999, 252, 71-76.	0.9	20
387	Structural transformations in a simple-hexagonal Hg-Sn alloy under pressure. Physical Review B, 1999, 59, 6058-6062.	1.1	16
388	Stability and Optical Properties of Î³-Gd2S3 at High Pressures. Journal of Solid State Chemistry, 1999, 148, 370-375.	1.4	7
389	Electronic structure calculations of Al-Cu alloys: Comparison with experimental results on Hume-Rothery phases. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1999, 79, 205-221.	0.6	19
390	Interatomic potentials for monoatomic metals from experimental data andab initiocalculations. Physical Review B, 1999, 59, 3393-3407.	1.1	1,231
391	Ionic layered PbFCl-type compounds under high pressure. Physical Review B, 1999, 59, 4011-4022.	1.1	47
392	The Miscibility of Copper Halides Using a Three-Body Potential. I. CuClxBr1â^'xCrystal. Molecular Simulation, 1999, 23, 127-142.	0.9	2
393	Relative stabilities, bulk moduli and electronic structure properties of different ultraâ€hard materials investigated within the local spin density functional approximation. Journal of Materials Chemistry, 1999, 9, 3151-3158.	6.7	36
394	Electronic and bonding properties of ANi2P2 (A=Ca, Sr, Ba). Journal of Alloys and Compounds, 1999, 288, 88-95.	2.8	26
395	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. Surface Science, 1999, 430, 213-222.	0.8	70
396	Quasicrystals under pressure: a comparison between Tiâ€“Zrâ€“Ni and Alâ€“Cuâ€“Fe icosahedral phases. Journal of Non-Crystalline Solids, 1999, 250-252, 844-848.	1.5	14

#	Article	IF	Citations
397	Electronic structure of yttrium aluminum garnet(Y3Al5O12). Physical Review B, 1999, 59, 10530-10535.	1.1	158
398	An equation of state applied to solid up to 1 TPa. Journal of Physics Condensed Matter, 1999, 11, 10375-10391.	0.7	27
399	Comparison of the Bulk and Surface Properties of Ceria and Zirconia by ab Initio Investigations. Journal of Physical Chemistry B, 1999, 103, 10158-10170.	1.2	145
400	First-principles study of elastic and thermal properties of refractory carbides and nitrides. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1999, 79, 839-858.	0.6	94
401	Elasticity, shear strength, and equation of state of molybdenum and gold from x-ray diffraction under nonhydrostatic compression to 24 GPa. Journal of Applied Physics, 1999, 86, 6729-6736.	1.1	129
402	Structural properties ofNaV2O5under high pressure. Physical Review B, 1999, 60, R6945-R6948.	1.1	31
403	Electronic structure, phase stability, and cohesive properties ofTi2XAl(X=Nb,V,Zr). Physical Review B, 1999, 60, 15683-15690.	1.1	41
404	Estimates of mantle relevant Clapeyron slopes in the MgSiO₃system from high-pressure spectroscopic data. American Mineralogist, 1999, 84, 233-244.	0.9	69
405	Crystal structures and compressibilities of synthetic 2M1 and 3T phengite micas. European Journal of Mineralogy, 2000, 12, 955-963.	0.4	63
406	The Crystal Structures of Thallium(I) Fluoride. Journal of Solid State Chemistry, 2000, 150, 266-275.	1.4	15
407	300-K Equation of State and High-Pressure Phase Stability of Al3BC3. Journal of Solid State Chemistry, 2000, 154, 254-256.	1.4	20
408	Reversible Antifluorite to Anticotunnite Phase Transition in Li2S at High Pressures. Journal of Solid State Chemistry, 2000, 154, 603-611.	1.4	80
409	Compressibility measurement of C 60 using synchrotron radiation. Solid State Communications, 2000, 114, 121-125.	0.9	32
410	The compressibility of nanocrystalline nickel. Solid State Communications, 2000, 115, 191-194.	0.9	55
411	High pressure band structures and structural stability of EuS. Solid State Communications, 2000, 115, 323-328.	0.9	18
412	Theoretical calculation of superconducting transition temperature in vanadium under pressure. Solid State Communications, 2000, 116, 401-404.	0.9	12
413	Structural and bonding properties of intermetallic compounds ARh2P2 (A=Ca, Sr, Ba). Solid State Communications, 2000, 116, 451-456.	0.9	6
414	High-pressure study on dioxolane silica sodalite (C3H6O2)2[Si12O24]â€”neutron and X-ray powder diffraction experiments. Solid State Communications, 2000, 113, 503-507.	0.9	15

#	Article	IF	Citations
415	Phase stability and EOS of orthorhombic high-pressure phase of NaI to 204 GPa. Journal of Physics and Chemistry of Solids, 2000, 61, 1883-1887.	1.9	3
416	High pressure optical and X-ray diffraction studies of two polymorphs of K(RE)P2Se6 (RE=Pr and Tb). Journal of Physics and Chemistry of Solids, 2000, 61, 123-134.	1.9	15
417	Electronic structure calculations of PbTe. Journal of Physics and Chemistry of Solids, 2000, 61, 1639-1645.	1.9	37
418	Atomistic study of zinc-blende CdS, CdSe, ZnS, and ZnSe from molecular dynamics. Materials Chemistry and Physics, 2000, 66, 10-16.	2.0	91
419	Graphite â† diamond transition under high pressure: A kinetics approach. Journal of Materials Science, 2000, 35, 6041-6054.	1.7	67
420	Electronic structure and bonding in titanium carbosulphide. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2000, 80, 379-394.	0.6	3
421	Tersoff Potential Parameters for Simulating Cubic Boron Carbonitrides. Japanese Journal of Applied Physics, 2000, 39, L48-L51.	0.8	156
422	In-situ high pressure X-ray diffraction of phase E to 15 GPa. American Mineralogist, 2000, 85, 765-769.	0.9	33
423	Structure type and bulk modulus of Fe₃S, a new iron-sulfur compound. American Mineralogist, 2000, 85, 1830-1833.	0.9	171
424	Accuracy of equation-of-state formulations. American Mineralogist, 2000, 85, 338-344.	0.9	160
425	First-principles investigations of transition metal dihydrides, TH2: T = Sc, Ti, V, Y, Zr, Nb; energetics and chemical bonding. Journal of Physics Condensed Matter, 2000, 12, 4535-4551.	0.7	48
426	The mixed P, T derivative of isothermal bulk modulus for solids. Journal of Applied Physics, 2000, 88, 6084-6085.	1.1	2
427	Analysis of dislocation mechanism for melting of elements: Pressure dependence. Journal of Applied Physics, 2000, 88, 6294-6301.	1.1	78
428	Effect of Defects on the Elastic Properties of WÃ¼stite. Physical Review Letters, 2000, 84, 507-510.	2.9	43
429	High-pressure stability of Ti-Zr-Ni quasicrystals. Physical Review B, 2000, 62, 8844-8848.	1.1	20
430	Energetic, vibrational, and electronic properties of silicon using a nonorthogonal tight-binding model. Physical Review B, 2000, 62, 4477-4487.	1.1	137
431	Occupation-number broadening schemes: Choice of â€œtemperatureâ€• Physical Review B, 2000, 61, 1654-1657.	1.1	19
432	Theoretical atomic volumes of the light actinides. Physical Review B, 2000, 61, 4644-4650.	1.1	104

#	Article	IF	Citations
433	Phase transitions of a simple hexagonalIn0.2Sn0.8alloy under high pressure. Physical Review B, 2000, 61, 5823-5826.	1.1	14
434	High-pressure structural study of UM2Al3(M = Pd, Ni): evidence for a pressure-induced electronic transition in UPd2Al3. Journal of Physics Condensed Matter, 2000, 12, 8801-8808.	0.7	5
435	Experimental and theoretical high pressure study of Î²-Cs2SO4. Zeitschrift Fur Kristallographie - Crystalline Materials, 2000, 215, 17-22.	0.4	0
436	Fullab initiogeometry optimization of all known crystalline phases ofSi3N4. Physical Review B, 2000, 61, 8696-8700.	1.1	82
437	Relative energetics and structural properties of zirconia using a self-consistent tight-binding model. Physical Review B, 2000, 61, 6617-6630.	1.1	82
438	Second-moment interatomic potential for aluminum derived from total-energy calculations and molecular dynamics application. Computational Materials Science, 2000, 17, 224-229.	1.4	17
439	Electronic and structural properties of BaTe. Computational Materials Science, 2000, 17, 81-87.	1.4	28
440	High pressure phase transformations in Î±-AlPO4: an x-ray diffraction investigation. Journal of Physics Condensed Matter, 2000, 12, 6683-6692.	0.7	19
441	High-pressure phase transformation of the silicon clathrate Si136. Journal of Physics Condensed Matter, 2000, 12, 4013-4020.	0.7	49
442	High-Pressure and High-Temperature Powder Diffraction. Reviews in Mineralogy and Geochemistry, 2000, 41, 521-557.	2.2	25
443	Theoretical study of the relative stability of structural phases in group-III nitrides at high pressures. Physical Review B, 2000, 62, 16612-16623.	1.1	196
444	Molecular Dynamics Study of Zinc-Blende GaN, AlN and InN. Molecular Simulation, 2000, 23, 327-341.	0.9	16
445	Structure and Properties of NaCl and the Suzuki Phase Na6CdCl8. Journal of Physical Chemistry B, 2000, 104, 1191-1197.	1.2	23
446	Density-functional study of bulk and surface properties of titanium nitride using different exchange-correlation functionals. Physical Review B, 2000, 62, 2899-2907.	1.1	386
447	Structural Properties of Ammonium Perchlorate Compressed to 5.6 GPa. Journal of Physical Chemistry A, 2000, 104, 11188-11193.	1.1	60
448	Electronic structure and bonding in garnet crystalsGd3Sc2Ga3O12,Gd3Sc2Al3O12,andGd3Ga3O12compared toY3Al3O12. Physical Review B, 2000, 61, 1817-1824.	1.1	85
449	Integrated Experimental and Computational Methods for Structure Determination and Characterization of a New, Highly Stable Cesium Silicotitanate Phase, Cs2TiSi6O15(SNL-A). Chemistry of Materials, 2000, 12, 3449-3458.	3.2	50
450	Equation of state and strength of natural majorite. Journal of Geophysical Research, 2000, 105, 5963-5971.	3.3	26

#	Article	IF	Citations
451	First-principles elastic constants and electronic structure ofÎ±â˜Pt2Siand PtSi. Physical Review B, 2001, 63, .	1.1	378
452	High pressure-high temperature synthesis and elasticity of the cubic nitride spinel Î³-Si3N4. Journal of Physics Condensed Matter, 2001, 13, 557-563.	0.7	86
453	Search for ultra-hard materials: theoretical characterisation of novel orthorhombic BC2N crystals. Solid State Sciences, 2001, 3, 943-957.	0.8	66
454	Lattice instabilities of cubic NiTi from first principles. Physical Review B, 2001, 65, .	1.1	68
455	Stability and equation of state of Fe3C to 73 GPa: Implications for carbon in the Earth's core. Geophysical Research Letters, 2001, 28, 1875-1878.	1.5	97
456	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. Physical Review B, 2001, 63, .	1.1	132
457	Vanadium oxides V2O5 and NaV2O5 under high pressures: Structural, vibrational, and electronic properties. Journal of Alloys and Compounds, 2001, 317-318, 103-108.	2.8	50
458	First-principles characterisation of new ternary heterodiamond BC2N phases. Computational Materials Science, 2001, 20, 107-119.	1.4	68
459	Static simulation of bulk and selected surfaces of anatase TiO2. Surface Science, 2001, 490, 116-124.	0.8	115
460	Systematics of elasticity:Ab initiostudy in B1-type alkaline earth oxides. Journal of Chemical Physics, 2001, 114, 10086-10093.	1.2	125
461	Equation of state of turbostratic boron nitride. High Pressure Research, 2001, 21, 115-120.	0.4	14
462	Ultralow Compressibility Silicate without Highly Coordinated Silicon. Physical Review Letters, 2001, 88, 015506.	2.9	59
463	Compression mechanism of cubic silica sodalite [Si12O24]: a first principles study of the Im3Ì…m to I4Ì…3m phase transition. Zeitschrift Fur Kristallographie - Crystalline Materials, 2001, 216, 495-500.	0.4	6
464	Strain Dependence of Solute Atom Energy in Aluminum-Rich Alloys. Materials Transactions, 2001, 42, 429-431.	0.4	2
465	Systematic ab initio study of the compressibility of silicate garnets. Acta Crystallographica Section B: Structural Science, 2001, 57, 163-177.	1.8	33
466	Calculated elastic and electronic properties of MgB2 at high pressures. Solid State Communications, 2001, 118, 279-282.	0.9	83
467	Electric field gradients in MgB2 synthesized at high pressure: 111Cd TDPAC study and ab initio calculation. Solid State Communications, 2001, 119, 153-158.	0.9	16
468	High-pressure phase transitions in AlSb. Journal of Physics and Chemistry of Solids, 2001, 62, 941-949.	1.9	8

#	Article	IF	Citations
469	Ab initio search of carbon nitrides, isoelectronic with diamond, likely to lead to new ultra hard materials. Comptes Rendus De L'Academie Des Sciences - Series IIc: Chemistry, 2001, 4, 255-272.	0.1	6
470	Tight-binding calculation of structural properties of bulk Cu3Au and its corresponding clusters. Superlattices and Microstructures, 2001, 30, 21-28.	1.4	8
471	Development of modified embedded atom potentials for the Cuâ€“Ag system. Superlattices and Microstructures, 2001, 30, 261-271.	1.4	11
472	The High Pressure Behaviour of SnS2: X-Ray Powder Diffraction and Quantum Mechanical Calculations up to 10 GPa. Physica Status Solidi (B): Basic Research, 2001, 223, 435-440.	0.7	19
473	Electronic Structure and Physical Properties of ABC2 (A = Zn, B = Si, Ge, Sn, and C = P, As) Ternary Pnictide Semiconductors. Physica Status Solidi (B): Basic Research, 2001, 226, 375-384.	0.7	17
474	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. Chemical Physics Letters, 2001, 338, 224-230.	1.2	35
475	Geometry Optimization and Ground-State Properties of Complex Ceramic Oxides. Journal of the American Ceramic Society, 2001, 84, 801-805.	1.9	21
476	High-pressure structural behaviour of heulandite. European Journal of Mineralogy, 2001, 13, 497-505.	0.4	51
477	Compression of synthetic hydroxylclinohumite [Mg9Si4O16(OH)2] and hydroxylchondrodite [Mg5Si2O8(OH)2]. American Mineralogist, 2001, 86, 990-996.	0.9	35
478	In situhigh-pressure x-ray diffraction study of icosahedral Al-Cu-TM (TM = V, Cr, Mn) alloys. Journal of Physics Condensed Matter, 2001, 13, 549-555.	0.7	9
479	Measurement and analysis of nonhydrostatic lattice strain component in niobium to 145 GPa under various fluid pressure-transmitting media. Journal of Applied Physics, 2001, 90, 3269-3275.	1.1	75
480	First-principles study of solute-dislocation interaction in aluminum-rich alloys. Physical Review B, 2001, 64, .	1.1	35
481	Nanocrystalline iron at high pressure. Journal of Applied Physics, 2001, 89, 4794-4796.	1.1	36
482	High-pressure band structure and structural stability of EuTe. Physical Review B, 2001, 64, .	1.1	24
483	Ultrahigh pressure equation of state of CaS to 1.5 Mbar. High Pressure Research, 2001, 21, 31-40.	0.4	1
484	Energetics of hydrogen impurities in aluminum and their effect on mechanical properties. Physical Review B, 2002, 65, .	1.1	75
485	X-ray diffraction patterns from samples in the laser-heated diamond anvil cell. Journal of Applied Physics, 2002, 91, 2769-2778.	1.1	15
486	First-principles-based thermodynamic description of solid copper using the tight-binding approach. Physical Review B, 2002, 65, .	1.1	20

#	Article	IF	Citations
487	Particle-size effect on the compressibility of nanocrystalline alumina. Physical Review B, 2002, 66, .	1.1	76
488	Block-diagonalization andf-electron effects in tight-binding theory. Physical Review B, 2002, 66, .	1.1	8
489	Equation of state of bismuth to 222 GPa and comparison of gold and platinum pressure scales to 145 GPa. Journal of Applied Physics, 2002, 92, 5892-5897.	1.1	108
490	Modeling the metal-semiconductor interaction: Analytical bond-order potential for platinum-carbon. Physical Review B, 2002, 65, .	1.1	144
491	Pressureâ€"volume relationship of Ta. Journal of Applied Physics, 2002, 91, 4143-4148.	1.1	33
492	Full-potential KKR calculations for MgO and divalent impurities in MgO. Physical Review B, 2002, 66, .	1.1	22
493	In situstructural properties of N2-,â€‰O2-, and air-clathrates by neutron diffraction. Journal of Chemical Physics, 2002, 117, 308-320.	1.2	126
494	Density-functional theory investigation of hardness, stability, and electron-energy-loss spectra of carbon nitrides withC11N4stoichiometry. Physical Review B, 2002, 65, .	1.1	95
495	Pressure-induced magnetic transitions in LaMn[sub 2]Si[sub 2]. Journal of Applied Physics, 2002, 91, 8126.	1.1	11
496	The high-pressure behaviour of 3R-NbS2. Zeitschrift Fur Kristallographie - Crystalline Materials, 2002, 217, 522-524.	0.4	6
497	Tight-binding description of the electronic structure and total energy of tin. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 2002, 82, 47-61.	0.6	10
498	Equations of state for barium in high-pressure phases. Journal of Physics Condensed Matter, 2002, 14, 5129-5134.	0.7	3
499	High-Pressure X-Ray Diffraction and Raman Scattering of LiTaO 3. Chinese Physics Letters, 2002, 19, 1666-1668.	1.3	11
500	Electronic structure of Al-Pd-Mn crystalline and quasicrystalline alloys. Journal of Physics Condensed Matter, 2002, 14, 87-102.	0.7	29
501	Tight-binding study of high-pressure phase transitions in titanium: Alpha to omega and beyond. Europhysics Letters, 2002, 60, 248-254.	0.7	28
502	Phase transitions under high pressure in binary Sn alloys (with In, Hg and Ga). Journal of Physics Condensed Matter, 2002, 14, 389-406.	0.7	9
503	Pressure-induced phase transition in LaAlO3. Journal of Physics Condensed Matter, 2002, 14, 3981-3991.	0.7	96
504	Lattice dynamics and elastic properties of corundum by the self-consistent atomic deformation method. Physical Review B, 2002, 66, .	1.1	13

#	Article	IF	Citations
505	Electronic structure and energetics of ordered titanium carbides of composition Ti2C. Journal of Physics Condensed Matter, 2002, 14, 4425-4444.	0.7	14
506	Modeling of compound semiconductors: Analytical bond-order potential for Ga, As, and GaAs. Physical Review B, 2002, 66, .	1.1	146
507	Thermal Expansion and Equation of State. , 2002, , 1-4.		3
508	Structure and elasticity of single-crystal (Mg,Fe)O and a new method of generating shear waves for gigahertz ultrasonic interferometry. Journal of Geophysical Research, 2002, 107, ECV 4-1.	3.3	149
509	Talc under tension and compression: Spinodal instability, elasticity, and structure. Journal of Geophysical Research, 2002, 107, ECV 2-1-ECV 2-10.	3.3	40
510	Iron-Nickel alloy in the Earth's core. Geophysical Research Letters, 2002, 29, 109-1-109-3.	1.5	51
511	Sodium under pressure:â€ƒbcc to fcc structural transition and pressure-volume relation to 100 GPa. Physical Review B, 2002, 65, .	1.1	114
512	Effective elastic stiffnesses of InAs under uniform strain. Journal of Applied Physics, 2002, 92, 3027-3033.	1.1	42
513	Thermomechanical model and temperature measurements for shocked ammonium perchlorate single crystals. Journal of Applied Physics, 2002, 91, 5650-5656.	1.1	16
514	Ab initio study of pressure effect on elastic properties of crystalline Au. Journal of Chemical Physics, 2002, 116, 2121-2124.	1.2	32
515	Molecular dynamics modeling of stishovite. Earth and Planetary Science Letters, 2002, 202, 147-157.	1.8	21
516	Experimental constraints on the chemical evolution of large icy satellites. Earth and Planetary Science Letters, 2002, 203, 399-412.	1.8	53
517	Compressibility of brownmillerite (Ca2Fe2O5): effect of vacancies on the elastic properties of perovskites. Physics of the Earth and Planetary Interiors, 2002, 129, 145-151.	0.7	38
518	Thermal equation of state of magnesiowÃ¼stite (Mg0.6Fe0.4)O. Physics of the Earth and Planetary Interiors, 2002, 129, 301-311.	0.7	57
519	Theoretical study of LaP and LaAs at high pressures. Journal of Alloys and Compounds, 2002, 336, 46-55.	2.8	44
520	Phase stability of the Hf-Nb system: From first-principles to CALPHAD. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2002, 26, 491-511.	0.7	35
521	Ab initio calculations of elastic constants and thermodynamic properties of bcc, fcc, and hcp Al crystals under pressure. Journal of Physics Condensed Matter, 2002, 14, 6989-7005.	0.7	627
522	Electronic Band Structure and Metallization of KI and RbI under High Pressure. Physica Status Solidi (B): Basic Research, 2002, 233, 339-350.	0.7	9

#	Article	IF	Citations
523	Electronic and structural properties of LaSb and LaBi. Physica B: Condensed Matter, 2002, 315, 64-73.	1.3	65
524	Effect of pressure on the superconducting transition temperature of Nbâ€“Zr and Tiâ€“V. Physica C: Superconductivity and Its Applications, 2002, 370, 108-112.	0.6	9
525	Effets chimiques et magnÃ©tovolumiques compÃ©titifs dans les nitrures dâ€™insertion. Comptes Rendus Chimie, 2002, 5, 539-546.	0.2	6
526	Klockmannite, CuSe: structure, properties and phase stability from ab initio modeling. Acta Crystallographica Section B: Structural Science, 2002, 58, 437-447.	1.8	40
527	Pressure-induced structural and magnetic phase transition in ferromagnetic CrTe. Journal of Magnetism and Magnetic Materials, 2002, 250, 353-363.	1.0	11
528	Precise measurement of equation-of-state and elastic properties for GaN up to 16GPa. Solid State Communications, 2002, 121, 555-559.	0.9	19
529	FCCâ€“HCP phase boundary in lead. Solid State Communications, 2002, 122, 125-127.	0.9	50
530	Equation of state of CeCu2Ge2 at cryogenic temperature. Solid State Communications, 2002, 123, 113-116.	0.9	35
531	Structural phase stability and superconductivity of LaN. Solid State Communications, 2002, 124, 97-102.	0.9	38
532	Electronic structure calculations of lead chalcogenides PbS, PbSe, PbTe. Journal of Physics and Chemistry of Solids, 2002, 63, 833-841.	1.9	143
533	Behavior of Micas at High-Pressure and High-Temperature. Reviews in Mineralogy and Geochemistry, 2002, 46, 99-116.	2.2	35
534	Theory for structure and bulk modulus determination. Physical Review B, 2003, 68, .	1.1	42
535	New isothermal equation of state of solids applied to high pressures. Pramana - Journal of Physics, 2003, 61, 753-757.	0.9	8
536	Static compression of ?-Fe2O3: linear incompressibility of lattice parameters and high-pressure transformations. Physics and Chemistry of Minerals, 2003, 30, 582-588.	0.3	30
537	New density measurements on carbonate liquids and the partial molar volume of the CaCO 3 component. Contributions To Mineralogy and Petrology, 2003, 146, 370-381.	1.2	52
538	A model study for the breaking of N2 from CNx within DFT. Solid State Sciences, 2003, 5, 701-703.	1.5	26
539	Structure and electronic properties of new model dinitride systems: a density-functional study of CN2, SiN2, and GeN2. Chemical Physics Letters, 2003, 373, 636-641.	1.2	44
540	First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure. Physica B: Condensed Matter, 2003, 339, 208-215.	1.3	92

#	Article	IF	Citations
541	Theoretical studies on the high pressure phases of Lanthanum monochalcogenides. Journal of Physics and Chemistry of Solids, 2003, 64, 15-26.	1.9	26
542	Pressure dependence of T C of the layered superconductor Y 2 C 2 I 2 : lattice versus electronic effects. Journal of Solid State Chemistry, 2003, 171, 367-370.	1.4	6
543	Interatomic potential for Pd and molecular-dynamics simulation of diffusion in Pd/Pd(111) system. Thin Solid Films, 2003, 428, 40-46.	0.8	13
544	New insights on high-pressure behaviour of microporous materials from X-ray single-crystal data. Microporous and Mesoporous Materials, 2003, 61, 105-115.	2.2	39
545	Structure and stability of Î±- and Î²-Ti2Se. Electron diffractionversusdensity-functional theory calculations. Acta Crystallographica Section A: Foundations and Advances, 2003, 59, 18-21.	0.3	10
546	On the elastic properties of InAs under hydrostatic pressure. Physica Status Solidi (B): Basic Research, 2003, 235, 437-440.	0.7	7
547	Electronic structure calculationsof magnesium chalcogenides MgS and MgSe. Physica Status Solidi (B): Basic Research, 2003, 240, 565-573.	0.7	56
548	Electronic Structure and Bulk Properties of Î²â€SiAlONs. Journal of the American Ceramic Society, 2003, 86, 1162-1167.	1.9	13
549	High-pressure X-ray diffraction study on Î±-PbF2. Journal of Physics and Chemistry of Solids, 2003, 64, 919-925.	1.9	21
550	In search of new candidates for ultra-hard materials: the ternary BC3N3 stoichiometry. Journal of Physics and Chemistry of Solids, 2003, 64, 1539-1545.	1.9	15
551	Applicability of three-parameter equation of state of solids: compatibility with first principles approaches and application to solids. Journal of Physics Condensed Matter, 2003, 15, 1643-1663.	0.7	6
552	Ab initiostudy of anthracene under high pressure. Physical Review B, 2003, 67, .	1.1	65
553	Electronic, optical, and structural properties of oligophenylene molecular crystals under high pressure: Anab initioinvestigation. Physical Review B, 2003, 67, .	1.1	37
554	CubicHf3N4andZr3N4:A class of hard materials. Physical Review B, 2003, 68, .	1.1	294
555	Equation of state of stishovite and interpretation of SiO2shock-compression data. Journal of Geophysical Research, 2003, 108, ECV 5-1-ECV 5-7.	3.3	30
556	The equation of state of CsCl-structured FeSi to 40 GPa: Implications for silicon in the Earth's core. Geophysical Research Letters, 2003, 30, 14-1-14-4.	1.5	59
557	Static compression of iron-silicon alloys: Implications for silicon in the Earth's core. Journal of Geophysical Research, 2003, 108, .	3.3	73
558	Sound velocities of iron-nickel and iron-silicon alloys at high pressures. Geophysical Research Letters, 2003, 30, .	1.5	107

#	Article	IF	Citations
559	High-pressure alloying of potassium and iron: Radioactivity in the Earth's core?. Geophysical Research Letters, 2003, 30, n/a-n/a.	1.5	45
560	First-principles prediction of theP-V-Tequation of state of gold and the 660-km discontinuity in Earth's mantle. Journal of Geophysical Research, 2003, 108, .	3.3	209
561	Electronic structure of ionic PbFCl-type compounds under pressure. Journal of Physics Condensed Matter, 2003, 15, 1677-1683.	0.7	11
562	Elasticity and rheology of platinum under high pressure and nonhydrostatic stress. Physical Review B, 2003, 68, .	1.1	36
563	Elasticity and strength of hydrous ringwoodite at high pressure. Earth and Planetary Science Letters, 2003, 214, 645-654.	1.8	66
564	Second-moment interatomic potential for Al, Ni and Niâ€“Al alloys, and molecular dynamics application. Computational Materials Science, 2003, 27, 191-198.	1.4	36
565	High-pressure structural phase transitions in magnesium fluoride studied by electronic structure calculations. Journal of Alloys and Compounds, 2003, 352, 60-65.	2.8	32
566	Pressure induced structural phase transitions and metallization of BaF2. Journal of Alloys and Compounds, 2003, 359, 66-72.	2.8	48
567	Elastic Properties of Zinc-blende G a N, A l N and I n N from Molecular Dynamics. Molecular Simulation, 2003, 29, 201-209.	0.9	40
568	Scheelite CaWO4at high pressures. Journal of Physics Condensed Matter, 2003, 15, 7261-7270.	0.7	39
569	Structure and bulk modulus of M2AlC (M=Ti, V, and Cr). Applied Physics Letters, 2003, 83, 899-901.	1.5	189
570	Equation of state and phonon frequency calculations of diamond at high pressures. Physical Review B, 2003, 68, .	1.1	82
571	Experimental and Theoretical Study of Deviations from Vegard's Law in the SnxGe1-x System. Chemistry of Materials, 2003, 15, 2511-2519.	3.2	82
572	High-pressure structure and equation of state study of nitrosonium nitrate from synchrotron x-ray diffraction. Journal of Chemical Physics, 2003, 118, 8350-8356.	1.2	20
573	Ab initio 0 K isotherm for crystalline 1,1-diamino-2,2-dinitroethylene. Journal of Chemical Physics, 2003, 118, 11073-11078.	1.2	22
574	Theoretical investigation of the solubility in(MxM2â^'xâ€²)AlC(MandMâ€²=Ti,V,Cr). Physical Review B, 2003, 68, .	1.1	87
575	High-pressure x-ray diffraction studies of the nanostructured transparent vitroceramic mediumK2Oâ^'SiO2â^'Ga2O3. Physical Review B, 2003, 68, .	1.1	34
576	First principles calculations of pressure-induced structural phase transition of Co. Advances in Quantum Chemistry, 2003, 42, 199-207.	0.4	4

#	Article	IF	Citations
577	Stability of magnesiowustite in Earth's lower mantle. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 4405-4408.	3.3	62
578	Chain-length-dependent intermolecular packing in polyphenylenes: a high pressure study. Journal of Physics Condensed Matter, 2003, 15, 3375-3389.	0.7	41
579	Equation of state of stishovite to lower mantle pressures. American Mineralogist, 2003, 88, 301-307.	0.9	123
580	Equation of state and compressibility of phlogopite by in-situ high-pressure X-ray powder diffraction. European Journal of Mineralogy, 2003, 15, 455-463.	0.4	24
581	The fusion curve of albite revisited and the compressibility of NaAlSi₃O₈liquid with pressure. American Mineralogist, 2003, 88, 109-120.	0.9	32
582	A standard-free pressure calibration using simultaneous XRD and elastic property measurements in a multi-anvil device. European Journal of Mineralogy, 2003, 15, 865-873.	0.4	23
583	The pseudo-binary mercury chalcogenide alloy HgSe0.7S0.3at high pressure: a mechanism for the zinc blende to cinnabar reconstructive phase transition. Journal of Physics Condensed Matter, 2003, 15, 2339-2349.	0.7	4
585	Molecular Dynamics Simulation of Germanium Nanoparticles. Materials Research Society Symposia Proceedings, 2003, 769, 6151.	0.1	1
586	New condensed matter probes for diamond anvil cell technology. Journal of Physics Condensed Matter, 2004, 16, S1071-S1086.	0.7	6
587	High-pressure and high-temperature powder diffraction on molybdenum diphosphide, MoP2. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, 309-313.	0.4	6
588	Thermoelastic and texture behavior of aluminum at high pressure and high temperature investigated byin situneutron diffraction. Journal of Applied Physics, 2004, 95, 4645-4650.	1.1	23
589	Lack of the critical pressure for weakening of size-induced stiffness in 3Câ€“SiC nanocrystals under hydrostatic compression. Applied Physics Letters, 2004, 85, 1973-1975.	1.5	31
590	Equation of state and structural changes in diaminodinitroethylene under compression. Journal of Chemical Physics, 2004, 120, 8060-8066.	1.2	64
591	Bonding and classification of nanolayered ternary carbides. Physical Review B, 2004, 70, .	1.1	212
592	High-pressure x-ray diffraction and Raman spectroscopy ofHfV2O7. Physical Review B, 2004, 70, .	1.1	16
593	Rumpled relaxation and surface core-level shift in PbS(001). Physical Review B, 2004, 70, .	1.1	8
595	Hardness, elasticity, and fracture toughness of polycrystalline spinel germanium nitride and tin nitride. Journal of Materials Research, 2004, 19, 1392-1399.	1.2	28
596	Second-moment interatomic potential for gold and its application to molecular-dynamics simulations. Journal of Physics Condensed Matter, 2004, 16, 8399-8407.	0.7	22

#	Article	IF	Citations
597	LiSrAlF6with the LiBaCrF6-type structure. Journal of Physics Condensed Matter, 2004, 16, 3005-3013.	0.7	7
598	The crystal structures of pressure-induced LiSrAlF6-II and LiCaAlF6-II. Journal of Physics Condensed Matter, 2004, 16, 1033-1043.	0.7	9
599	Single-crystal elasticity of andradite garnet to 11 GPa. Journal of Physics Condensed Matter, 2004, 16, S1041-S1052.	0.7	25
600	Electronic Structure and Bonding of Î²â€SiAlON. Journal of the American Ceramic Society, 2000, 83, 780-786.	1.9	38
601	Elastic Moduli and Hardness of Cubic Silicon Nitride. Journal of the American Ceramic Society, 2002, 85, 86-90.	1.9	146
602	Anomalous Dynamical Charge Change Behavior of Nanocrystalline 3C-SiC upon Compression. Journal of the American Ceramic Society, 2004, 87, 2291-2293.	1.9	6
603	First principles search of hard materials within the Siî—¸Cî—¸N ternary system. Solid State Sciences, 2004, 6, 315-323.	1.5	18
604	Phonon Density of States and Elastic Properties of Fe-based Materials under Compression. Hyperfine Interactions, 2004, 153, 3-15.	0.2	7
605	Structural properties of the zircon- and scheelite-type phases ofYVO4at high pressure. Physical Review B, 2004, 70, .	1.1	108
606	Compression of Zr2InC to 52GPa. Applied Physics Letters, 2004, 85, 1514-1516.	1.5	65
607	Potential new candidates for hard materials within the ternary XC3N3 (XÂ=ÂB, Al, Ga) stoichiometry. Comptes Rendus Chimie, 2004, 7, 529-535.	0.2	6
608	Study of -Al2O3 and the role of Y in YAlO3 and Y3Al5O12 by first principles electronic structure calculations. Physica B: Condensed Matter, 2004, 353, 192-200.	1.3	12
609	Structural and electronic properties of PbTiO3 slabs: a DFT periodic study. Surface Science, 2004, 552, 149-159.	0.8	62
610	Interplay of Electronic Structure and Bulk Properties in 2D and 3D Ternary Carbonitrides from First Principles. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2004, 630, 2587-2598.	0.6	9
611	Electronic band structure and chemical bonding in the new antiperovskites AsNMg3 and SbNMg3. Journal of Solid State Chemistry, 2004, 177, 61-64.	1.4	29
612	The hydrogen concentration dependence of the unit-cell volume in RMn2Hx (R = Y, Gd, Tb and Dy). Physica Status Solidi A, 2004, 201, 1458-1462.	1.7	4
613	High-pressure stability and structural properties of CdS and CdSe. Physica Status Solidi (B): Basic Research, 2004, 241, 101-107.	0.7	55
614	Electronic and structural properties of strontium chalcogenides SrS, SrSe and SrTe. Physica Status Solidi (B): Basic Research, 2004, 241, 2529-2537.	0.7	43

#	Article	IF	Citations
615	Ab initio study of the electronic structure of some B2 intermetallic compounds. Physica B: Condensed Matter, 2004, 348, 206-212.	1.3	31
616	Density functional approach to study structural properties and electric field gradients in rare earth materials. Physica B: Condensed Matter, 2004, 349, 76-83.	1.3	23
617	An isothermal equation of state for solids. Physica B: Condensed Matter, 2004, 350, 375-388.	1.3	6
618	Analysis of a Pâ€“Vâ€“T relationship for MgO. Physica B: Condensed Matter, 2004, 352, 164-171.	1.3	4
619	High pressure X-ray diffraction study of Fe2B. Solid State Communications, 2004, 129, 573-575.	0.9	12
620	Ab initio calculations and experimental determination of the structure of Cr2AlC. Solid State Communications, 2004, 130, 445-449.	0.9	179
621	Equation of state of silicon nitride carbodiimide Si2CN4. Solid State Communications, 2004, 132, 573-576.	0.9	6
622	Strength of magnesium oxide under high pressure: evidence for the grain-size dependence. Solid State Communications, 2004, 132, 795-798.	0.9	45
623	High-pressure crystal structure studies of Fe, Ru and Os. Journal of Physics and Chemistry of Solids, 2004, 65, 1565-1571.	1.9	9
624	X-ray diffraction from solids under nonhydrostatic compressionâ€”some recent studies. Journal of Physics and Chemistry of Solids, 2004, 65, 1589-1596.	1.9	58
625	Calculation of bulk modulus for highly anisotropic materials. Physics Letters, Section A: General, Atomic and Solid State Physics, 2004, 326, 442-448.	0.9	25
626	High-pressure X-ray diffraction studies on Î²-Ni(OH)2. Physica B: Condensed Matter, 2004, 349, 245-250.	1.3	11
627	Pressure induced phase transition and amorphization of Na3ONO2. Physical Chemistry Chemical Physics, 2004, 6, 881.	1.3	14
628	A comparison of volume compressions of silver and gold up to 150 GPa. Journal of Applied Physics, 2004, 95, 4767-4771.	1.1	39
629	Subduction Factory 3: An Excel worksheet and macro for calculating the densities, seismic wave speeds, and H2O contents of minerals and rocks at pressure and temperature. Geochemistry, Geophysics, Geosystems, 2004, 5, n/a-n/a.	1.0	246
630	Single-crystal elasticity of grossular- and almandine-rich garnets to 11 GPa by Brillouin scattering. Journal of Geophysical Research, 2004, 109, .	3.3	56
631	Compression of Ti3Si0.5Ge0.5C2 to 53 GPa. Applied Physics Letters, 2004, 84, 2799-2801.	1.5	57
632	Pressure-induced structural phase transition in the IVâ€“VI semiconductor SnS. Journal of Physics Condensed Matter, 2004, 16, 3545-3554.	0.7	62

#	Article	IF	Citations
633	B1-to-B2phase transition of transition-metal monoxideCdOunder strong compression. Physical Review B, 2004, 70, .	1.1	72
634	Constraining the equation of state of fluid H2O to 80 GPa using the melting curve, bulk modulus, and thermal expansivity of Ice VII. Geochimica Et Cosmochimica Acta, 2004, 68, 2781-2790.	1.6	110
635	Equations of state of the high-pressure phases of a natural peridotite and implications for the Earth's lower mantle. Earth and Planetary Science Letters, 2004, 223, 381-393.	1.8	70
636	Limits to resolution in composition and density in ultra high-pressure experiments on natural mantle-rock samples. Physics of the Earth and Planetary Interiors, 2004, 143-144, 241-253.	0.7	5
637	Non-collinear magnetism in iron at high pressures. Physics of the Earth and Planetary Interiors, 2004, 143-144, 445-453.	0.7	31
638	High pressure study of Î²-UH3 crystallographic and electronic structure. Journal of Alloys and Compounds, 2004, 370, 59-64.	2.8	18
639	Ab initio study of the electronic structure of rhodium based intermetallic compounds under pressure. Journal of Alloys and Compounds, 2004, 379, 8-15.	2.8	31
640	The Performance of Hybrid Density Functionals in Solid State Chemistry. Structure and Bonding, 2004, , 171-232.	1.0	171
641	Ab initiostudy of M2AlN (M = Ti,V,Cr). Journal of Physics Condensed Matter, 2005, 17, L15-L19.	0.7	30
642	Theoretical investigation of the electronic structure and structural phase stability of CeGa2 under pressure. Physica B: Condensed Matter, 2005, 355, 59-63.	1.3	9
643	Effects of high pressure on stability of the nanocrystalline LiAlSi2O6 phase of a glassâ€“ceramic composite: A synchrotron X-ray diffraction study. Physica B: Condensed Matter, 2005, 365, 155-162.	1.3	14
644	Equation of state of aluminum carbide Al4C3. Solid State Communications, 2005, 133, 385-388.	0.9	37
645	Electronic structure of Sc2AC (A=Al, Ga, In, Tl). Solid State Communications, 2005, 133, 381-383.	0.9	25
646	Equation of state of aluminum silicon carbide Î±-Al4SiC4. Solid State Communications, 2005, 135, 87-89.	0.9	11
647	Investigations of pressure induced structural phase transformations in pentaerythritol. Solid State Communications, 2005, 136, 56-61.	0.9	2
648	A combined first-principles and experimental study of the lattice site preference of Pt in B2 NiAl. Acta Materialia, 2005, 53, 2101-2109.	3.8	71
649	First-principles study of constitutional point defects in B2 NiAl using special quasirandom structures. Acta Materialia, 2005, 53, 2643-2652.	3.8	42
650	Phase stability in the Feâ€“Ni system: Investigation by first-principles calculations and atomistic simulations. Acta Materialia, 2005, 53, 4029-4041.	3.8	262

#	Article	IF	Citations
651	Crystal structure of the Chevrel phaseSnMo6S8at high pressure. Physical Review B, 2005, 72, .	1.1	3
652	Investigation of structural transformations in pyridine nitrate at low temperatures and high pressures. Crystallography Reports, 2005, 50, 78-84.	0.1	12
653	Band Structure and the Magnetic and Elastic Properties of SrFeO[sub 3] and LaFeO[sub 3] Perovskites. Physics of the Solid State, 2005, 47, 2082.	0.2	74
654	Elastic properties and 2D icosahedral bonding in borides of hexagonal WC type. Scripta Materialia, 2005, 52, 29-31.	2.6	6
655	Electronic structure, lattice constant, optical and mechanical properties for NaCl-structured Tiâ€“Alâ€“N by density functional theory. Physica B: Condensed Matter, 2005, 358, 77-85.	1.3	6
656	Study of electronic structure and elastic properties of transition metal and actinide carbides. Physica B: Condensed Matter, 2005, 367, 6-18.	1.3	37
657	Synchrotron X-ray diffraction and absorption studies of CeM2X2 (M=Cu, Ni and X=Si, Ge) at high pressure. Solid State Communications, 2005, 134, 747-751.	0.9	7
658	A theoretical analysis of the TiO2/Sn doped (110) surface properties. Surface Science, 2005, 580, 71-79.	0.8	42
659	Elastic properties and chemical bonding in fluoritelike Be2B, AlBeB, MgBeB, and NaBeB. Journal of Structural Chemistry, 2005, 46, 535-537.	0.3	7
660	High Pressure Study of HfNi Crystallographic and Electronic Structure. Hyperfine Interactions, 2005, 159, 357-362.	0.2	0
661	Calibration based on a primary pressure scale in a multi-anvil device. , 2005, , 427-449.		3
662	Total energies. Springer Series in Solid-state Sciences, 2005, , 253-274.	0.3	0
663	Nitrogen-Containing Molecular Systems at High Pressures and Temperature. , 2005, , 189-222.		2
664	Electronic structure and structural stability of ThGa2under pressure: anab initiostudy. Philosophical Magazine Letters, 2005, 85, 27-32.	0.5	9
665	Sound Velocities of Hot Dense Iron: Birch's Law Revisited. Science, 2005, 308, 1892-1894.	6.0	149
666	Sound Velocity and Release Behaviour of Shock-Compressed LY12 Al. Chinese Physics Letters, 2005, 22, 1742-1745.	1.3	10
667	Influence of pressure on the structure and electronic properties of the layered superconductor Y2C2I2. Journal of Physics Condensed Matter, 2005, 17, S3121-S3130.	0.7	7
668	Electronic properties of barium chalcogenides from first-principles calculations: Tailoring wide-band-gap II-VI semiconductors. Physical Review B, 2005, 71, .	1.1	55

#	Article	IF	Citations
669	First-principles investigation on chemical bonding and bulk modulus of the ternary carbideZr2Al3C5. Physical Review B, 2005, 72, .	1.1	14
670	Structural properties of the sesquicarbide superconductorLa2C3at high pressure. Physical Review B, 2005, 72, .	1.1	15
671	Structure and bonding ofM2SbP(M=Ti,Zr,Hf). Physical Review B, 2005, 71, .	1.1	29
672	High-pressure structural study of the scheelite tungstatesCaWO4andSrWO4. Physical Review B, 2005, 72, .	1.1	159
673	STUDY OF THE ELECTRONIC STRUCTURE AND PHYSICAL PROPERTIES OF THE IRIDIUM BASED INTERMETALLIC COMPOUNDS UNDER PRESSURE. International Journal of Modern Physics B, 2005, 19, 4587-4604.	1.0	12
674	Theoretical investigation of the bonding and solubility in Nb2â^'xWxAlC. Journal of Physics Condensed Matter, 2005, 17, 6047-6056.	0.7	9
675	The performance of hybrid density functionals in solid state chemistry: the case of BaTiO3. Molecular Physics, 2005, 103, 2483-2496.	0.8	141
676	A high-pressure X-ray diffraction study of iron nitrides: Implications for Earth's core. Journal of Geophysical Research, 2005, 110, .	3.3	67
677	Structural Refinement of the High-Pressure Phase of Aluminum Trihydroxide:Â In-Situ High-Pressure Angle Dispersive Synchrotron X-ray Diffraction and Theoretical Studies. Journal of Physical Chemistry B, 2005, 109, 8857-8860.	1.2	22
678	Ab Initio All-Electron Periodic Hartreeâ^'Fock Study of Hydrostatic Compression of Pentaerythritol Tetranitrate. Journal of Physical Chemistry B, 2005, 109, 13668-13675.	1.2	14
679	Thermal equation of state for Pt. Physical Review B, 2005, 72, .	1.1	21
680	Strength, elasticity, and equation of state of the nanocrystalline cubic silicon nitrideÎ³â^'Si3N4to68GPa. Physical Review B, 2005, 72, .	1.1	43
681	Pressure and temperature dependence of elastic wave velocity of MgSiO3 perovskite and the composition of the lower mantle. Physics of the Earth and Planetary Interiors, 2005, 151, 143-154.	0.7	99
682	Designing meaningful density functional theory calculations in materials scienceâ€"a primer. Modelling and Simulation in Materials Science and Engineering, 2005, 13, R1-R31.	0.8	342
683	STRUCTURAL PHASE TRANSITION INDUCED BY PRESSURE IN THE ORDERED ALLOY FeRh. International Journal of Modern Physics B, 2005, 19, 3389-3395.	1.0	5
684	Octahedral tilting evolution and phase transition in orthorhombic NaMgF3perovskite under pressure. Geophysical Research Letters, 2005, 32, n/a-n/a.	1.5	46
685	Temperature dependence of the first pressure derivative of the isothermal bulk modulus for solid materials at zero pressure: Application to MgO. Journal of Geophysical Research, 2005, 110, .	3.3	6
686	Effect of pressure on the structural properties and Raman modes ofLiCoO2. Physical Review B, 2005, 72, .	1.1	48

#	Article	IF	Citations
687	Theoretical investigation of the bonding and elastic properties of nanolayered ternary nitrides. Physical Review B, 2005, 71, .	1.1	173
688	Progress in the realization of a practical pressure scale for the range 1â€“300ÂGPa. High Pressure Research, 2005, 25, 87-99.	0.4	37
689	Ancient subduction, mantle eclogite, and the 300 km seismic discontinuity. Geology, 2005, 33, 1.	2.0	66
690	Rietveld refinement study of the pressure dependence of the internal structural parameteruin the wurtzite phase of ZnO. Physical Review B, 2005, 71, .	1.1	71
691	Scaling law for high pressure isotherms of solids. High Pressure Research, 2005, 25, 267-276.	0.4	12
692	First-principles thermoelasticity of transition metals at high pressure: Tantalum prototype in the quasiharmonic limit. Physical Review B, 2006, 74, .	1.1	53
693	Atomistic calculation of elastic moduli in strained silicon. Semiconductor Science and Technology, 2006, 21, 906-911.	1.0	85
694	Equation of state of scheelite-structured ZrGeO4and HfGeO4. Journal of Physics Condensed Matter, 2006, 18, 8241-8250.	0.7	12
695	Compression behavior ofM2AlC(M=Ti, V, Cr, Nb, and Ta) phases to above50GPa. Physical Review B, 2006, 73, .	1.1	162
696	Semiempirical van der Waals correction to the density functional description of solids and molecular structures. Physical Review B, 2006, 73, .	1.1	707
697	Ab initiostudy of metal-organic framework-5Zn4O(1,4â^'benzenedicarboxylate)3: An assessment of mechanical and spectroscopic properties. Physical Review B, 2006, 73, .	1.1	83
698	Crystal structure and equation of state of MgSiO3perovskite. Geophysical Research Letters, 2006, 33, .	1.5	41
699	Thermal equation of state of Fe3S and implications for sulfur in Earth's core. Journal of Geophysical Research, 2006, 111, n/a-n/a.	3.3	63
700	The effect of pressure on the structure and volume of ferromagnesian post-perovskite. Geophysical Research Letters, 2006, 33, .	1.5	24
701	First-principles study of intrinsic point defects in ZnO: Role of band structure, volume relaxation, and finite-size effects. Physical Review B, 2006, 73, .	1.1	463
702	TIN-BASED GROUP IV SEMICONDUCTORS: New Platforms for Opto- and Microelectronics on Silicon. Annual Review of Materials Research, 2006, 36, 497-554.	4.3	231
703	Analytic bond-order potential for atomistic simulations of zinc oxide. Journal of Physics Condensed Matter, 2006, 18, 6585-6605.	0.7	68
704	Carbon Sequestration via Aqueous Olivine Mineral Carbonation:â€‰ Role of Passivating Layer Formation. Environmental Science & Technology, 2006, 40, 4802-4808.	4.6	291

#	Article	IF	Citations
705	Electronic structures of and composition gaps among the ternary carbidesTi2MC. Physical Review B, 2006, 74, .	1.1	146
706	Ab initioinvestigation on the phase stability of Ti3SiC2, Ti3Si0.5Ge0.5C2, and Ti3GeC2at high pressures. High Pressure Research, 2006, 26, 127-130.	0.4	4
707	Pressure-Induced Chemical Decomposition and Structural Changes of Boric Acid. Journal of Physical Chemistry B, 2006, 110, 13858-13865.	1.2	14
708	Solid ammonia at high pressure: A single-crystal x-ray diffraction study to123GPa. Physical Review B, 2006, 73, .	1.1	49
709	Pressure-Induced Phase Transition in BaTiO 3 Nanocrystals. Chinese Physics Letters, 2006, 23, 1249-1252.	1.3	6
710	First-principles calculations of ground-state and high-pressure phase of magnesium telluride. Computational Materials Science, 2006, 37, 603-606.	1.4	7
711	Effect of transition metal additives on electronic structure and elastic properties of TiAl andTi3Al. Physical Review B, 2006, 74, .	1.1	58
712	Experimental study of the NaClâ€“H2O system up to 28GPa: Implications for ice-rich planetary bodies. Physics of the Earth and Planetary Interiors, 2006, 155, 152-162.	0.7	35
713	Structural geomimetism: A conceptual framework for devising new materials from first principlesâ˜†. Progress in Solid State Chemistry, 2006, 34, 21-66.	3.9	8
714	Effects of Pt on the elastic properties of B2 NiAl: A combined first-principles and experimental study. Acta Materialia, 2006, 54, 2361-2369.	3.8	30
715	OsB2 and RuB2, ultra-incompressible, hard materials: First-principles electronic structure calculations. Chemical Physics Letters, 2006, 425, 311-314.	1.2	93
716	Equation of state for solids with high accuracy and satisfying the limitation condition at high pressure. Physica B: Condensed Matter, 2006, 371, 257-271.	1.3	14
717	Electronic structure and lattice dynamics of CaPd3B studied by first-principles methods. Physics Letters, Section A: General, Atomic and Solid State Physics, 2006, 356, 251-254.	0.9	4
718	High pressure study of structural and electronic properties of magnesium telluride. Journal of Physics and Chemistry of Solids, 2006, 67, 1668-1673.	1.9	10
719	Crystal structure and high-pressure properties of Î³-Mo2N determined by neutron powder diffraction and X-ray diffraction. Journal of Solid State Chemistry, 2006, 179, 1762-1767.	1.4	61
720	Pressure-induced polymorphism in Al3BC3: A first-principles study. Journal of Solid State Chemistry, 2006, 179, 2739-2743.	1.4	7
721	High-pressure studies of SrNi3(P2O7)2 pyrophosphate by Raman spectroscopy and X-ray diffraction. Journal of Molecular Structure, 2006, 794, 334-340.	1.8	14
722	Ab initio study of Nb2SC and Nb2S2C: Differences in coupling between the S and Nbâ€“C layers. Solid State Communications, 2006, 137, 306-309.	0.9	19

#	Article	IF	Citations
723	Equation of state of cubic hafnium(IV) nitride having Th3P4 -type structure. Solid State Communications, 2006, 139, 255-258.	0.9	29
724	An infrared spectroscopic study of NH4Br â€"ammonium bromide to 55ÂGPa. Solid State Communications, 2006, 140, 202-207.	0.9	14
725	High pressure phase transition and band structures of different phases in CeO2. Solid State Communications, 2006, 140, 313-317.	0.9	24
726	Band structure and high pressure study of Rh3Sc, Rh3Y and Rh3La. European Physical Journal B, 2006, 49, 67-75.	0.6	15
727	Ab-initio calculation of stability and structural properties of cadmium chalcogenides CdS, CdSe, and CdTe under high pressure. European Physical Journal D, 2006, 56, 409-418.	0.4	19
728	Elastic properties and stability of coexisting 3T and 2M 1 phengite polytypes. Physics and Chemistry of Minerals, 2006, 32, 670-678.	0.3	24
729	First principles study of structural, electronic and optical properties of KCl crystal. Chemical Physics, 2006, 330, 1-8.	0.9	10
730	High pressure X-ray diffraction study of CdAl2Se4 and Raman study of AAl2Se4 (A=Hg, Zn) and CdAl2X4 (X=Se, S). Journal of Physics and Chemistry of Solids, 2006, 67, 1660-1667.	1.9	40
731	High-pressure structure of LaSr2Mn2O7 bilayer manganite. Journal of Physics and Chemistry of Solids, 2006, 67, 2046-2050.	1.9	10
732	X-ray high-pressure study of Ti2AlN and Ti2AlC. Journal of Physics and Chemistry of Solids, 2006, 67, 2091-2094.	1.9	107
733	Pressure induced structural phase transition in SnS â€" An ab initio study. Bulletin of Materials Science, 2006, 29, 25-28.	0.8	10
734	Phase stability of Ti3SiC2 at elevated temperatures. Scripta Materialia, 2006, 54, 105-107.	2.6	43
735	Grain size dependence of the bulk modulus of nanocrystalline nickel. Scripta Materialia, 2006, 55, 473-476.	2.6	47
736	Effect of Anneal on the Release Behaviour of LY12-Al Alloy. Chinese Physics Letters, 2006, 23, 1265-1268.	1.3	7
737	Electronic structure and elastic properties of Yn+1Co3n+5B2n(). Journal of Physics Condensed Matter, 2006, 18, 4071-4076.	0.7	5
738	Nonhydrostatic compression of gold powder to 60 GPa in a diamond anvil cell: estimation of compressive strength from x-ray diffraction data. Journal of Physics Condensed Matter, 2006, 18, S969-S978.	0.7	30
739	First-principles study of osmium under high pressure. Journal of Physics Condensed Matter, 2006, 18, 8749-8759.	0.7	26
740	Single-crystal elasticity of brucite, Mg(OH)2, to 15 GPa by Brillouin scattering. American Mineralogist, 2006, 91, 1893-1900.	0.9	56

#	Article	IF	Citations
741	High-pressure proton disorder in brucite. American Mineralogist, 2006, 91, 127-134.	0.9	75
742	First-Principles Study of Orthorhombic Perovskites MgSiO 3 up to 120 GPa and Its Geophysical Implications. Chinese Physics Letters, 2006, 23, 2334-2337.	1.3	5
743	Applicability of isothermal unrealistic two-parameter equations of state for solids. Journal of Physics Condensed Matter, 2006, 18, 10481-10508.	0.7	6
744	Crystallization of water in a dynamic diamond-anvil cell: Evidence for ice VII-like local order in supercompressed water. Physical Review B, 2006, 74, .	1.1	52
745	Accurate Equation of State of AlPdMn up to 35ÂGPa and Pressure Effect on the Frozen-In Phason Strain. Physical Review Letters, 2006, 96, 105501.	2.9	5
746	High-pressure Raman and x-ray study of the spin-frustrated pyrochloreGd2Ti2O7. Physical Review B, 2006, 74, .	1.1	68
747	High-pressure equation of state for Nb with a helium-pressure medium: Powder x-ray diffraction experiments. Physical Review B, 2006, 73, .	1.1	67
748	First-principles study of migration mechanisms and diffusion of oxygen in zinc oxide. Physical Review B, 2006, 73, .	1.1	133
749	Ab initiocalculation of the electronic structure and spectroscopic properties of spinelÎ³â^'Sn3N4. Physical Review B, 2006, 73, .	1.1	49
750	First-principles prediction of the mechanical properties and electronic structure of ternary aluminum carbideZr3Al3C5. Physical Review B, 2006, 73, .	1.1	67
751	TEMPERATURE EFFECT ON THERMOMECHANICAL PROPERTIES OF BERYLLIUM CHALCOGENIDES BeS, BeSe AND BeTe. Modern Physics Letters B, 2006, 20, 49-61.	1.0	17
752	Achieving high-density states through shock-wave loading of precompressed samples. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9172-9177.	3.3	103
753	Calculated structural, elastic and electronic properties of SiX2O4(X = Mg, Zn, Cd) compounds under pressure. Modelling and Simulation in Materials Science and Engineering, 2007, 15, 787-798.	0.8	12
754	First-principles study of the elastic and thermodynamic properties of CaSiO3perovskite. Journal of Physics Condensed Matter, 2007, 19, 246103.	0.7	7
755	Theory and Practice â€“ Techniques for Measuring High P/T Elasticity. , 2007, , 269-291.		3
756	Thermal expansion of iron-rich alloys and implications for the Earth's core. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9162-9167.	3.3	39
757	The albite fusion curve re-examined: New experiments and the high-pressure density and compressibility of high albite and NaAlSi3O8 liquid. American Mineralogist, 2007, 92, 1573-1585.	0.9	46
758	P-V and T-V Equations of State of natural biotite: An in-situ high-pressure and high-temperature powder diffraction study, combined with Mossbauer spectroscopy. American Mineralogist, 2007, 92, 1158-1164.	0.9	21

#	Article	IF	Citations
759	Ab initioand classical molecular dynamics of neon melting at high pressure. Physical Review B, 2007, 75, .	1.1	17
760	Susceptibility studies of the weak itinerant ferromagnet<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">Ru</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>under high pressure to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"	1.1	35
761	Mechanical and electronic properties of superhard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Re</mml:mi><mml:msub><mml:mi mathvariant="normal">B</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2007, 76, .	1.1	122
762	High-pressure structural studies of dysprosium using angle-dispersive x-ray diffraction. Physical Review B, 2007, 75, .	1.1	17
763	Comment on â€œPressure-volume equation of state of the high-pressure<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>B</mml:mi><mml:mn>2</mml:mn></mml:mrow></mml:math>phase of NaClâ€• Physical Review B, 2007, 76, .	1.1	3
764	Compressibility measurements and phonon spectra of hexagonal transition-metal nitrides at high pressure:ÎµâˆTaN,Îˆâˆ'MoN, andCr2N. Physical Review B, 2007, 75, .	1.1	60
765	Electronic structure, elastic properties, surface energies, and work functions ofNiGeandPtGewithin the framework of density-functional theory for various surface terminations. Physical Review B, 2007, 75, .	1.1	23
766	Pressure-induced structural phase transition inNaAlH4. Physical Review B, 2007, 75, .	1.1	23
767	Ab initiocalculations of elastic properties of compressed Pt. Physical Review B, 2007, 76, .	1.1	35
768	Ab initiostudies of solid bromine under high pressure. Physical Review B, 2007, 76, .	1.1	35
769	Phase stability and shear softening inCaSiO3perovskite at high pressure. Physical Review B, 2007, 75, .	1.1	74
770	Structural stability and magnetism of FeN from first principles. Physical Review B, 2007, 75, .	1.1	43
771	Systematic study on the pressure dependence of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>M</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Al</mml:mi><mml:mi mathvariant="normal">C</mml:mi></mml:mrow></mml:math>phases<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
777	The effect of electronic orbital interactions on p-type doping tendency in ZnO series: First-principles calculations. Chinese Physics B, 2007, 16, 3815-3819.	1.3	2
779	Ab initio calculations of the elastic properties of ferropericlase Mg1â^'xFexO (). Physics of the Earth and Planetary Interiors, 2007, 164, 177-185.	0.7	11
780	A computer simulation study of natural silicate melts. Part II: High pressure properties. Geochimica Et Cosmochimica Acta, 2007, 71, 4538-4556.	1.6	128
781	Ab initio studies of the electronic structure of the quaternary system LiBC4N4. Journal of Alloys and Compounds, 2007, 427, 61-66.	2.8	6
782	Pressure induced phase transition in Fe0.47NbS2 studied by powder X-ray diffraction. Journal of Alloys and Compounds, 2007, 429, 82-86.	2.8	12
783	Infrared spectrum and compressibility of Ti3GeC2 to 51GPa. Journal of Alloys and Compounds, 2007, 433, 265-268.	2.8	45
784	Band structure calculation and high-pressure transition in praseodymium oxide. Journal of Alloys and Compounds, 2007, 436, 56-60.	2.8	11
785	Correlation between composition and structure in boracites. Journal of Physics Condensed Matter, 2007, 19, 275207.	0.7	6
786	Pressure scales and hydrostaticity. High Pressure Research, 2007, 27, 465-472.	0.4	26
787	Band structure of indium oxide: Indirect versus direct band gap. Physical Review B, 2007, 75, .	1.1	180
788	Phase stability and elastic properties of Tan+1AlCn(n= 1â€“3) at high pressure and elevated temperature. Journal of Physics Condensed Matter, 2007, 19, 136207.	0.7	39
789	On the compression behaviour of (Ti0.5,V0.5)2AlC and (Ti0.5,Nb0.5)2AlC to quasi-hydrostatic pressures above 50 GPa. Journal of Physics Condensed Matter, 2007, 19, 246215.	0.7	26
790	On the compression behavior of Cr₂GeC and V₂GeC up to quasi-hydrostatic pressures of 50 GPa. Journal of Physics Condensed Matter, 2007, 19, 456218.	0.7	40
791	Melting of transition metals at high pressure and the influence of liquid frustration: The late metals Cu, Ni, and Fe. Physical Review B, 2007, 76, .	1.1	40
792	Phenomenological Hugoniot curves for transition metals up to 1 TPa. Journal of Physics Condensed Matter, 2007, 19, 476218.	0.7	9
793	Melting curve of tantalum from first principles. Physical Review B, 2007, 75, .	1.1	99
794	Anomalous compression behavior in lanthanum/cerium-based metallic glass under high pressure. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 13565-13568.	3.3	86
795	Calculations of the superconducting properties of scandium under high pressure. Physical Review B, 2007, 76, .	1.1	15

#	Article	IF	Citations
796	Structural distortions inAlF3: A test for density-functional methods. Physical Review B, 2007, 75, .	1.1	3
797	Shape and Thermodynamic Stability of Pyrite FeS₂ Nanocrystals and Nanorods. Journal of Physical Chemistry C, 2007, 111, 11742-11746.	1.5	52
798	Equation of state of cubic boron nitride at high pressures and temperatures. Physical Review B, 2007, 75, .	1.1	81
799	Classical molecular dynamical simulations of high pressure behavior of alpha cristobalite (SiO₂). Journal of Physics Condensed Matter, 2007, 19, 456201.	0.7	11
800	Equation of state and high-pressure stability of Fe3P-schreibersite: Implications for phosphorus storage in planetary cores. Geophysical Research Letters, 2007, 34, .	1.5	39
801	First-Principles Investigation of Dense B₄C₃. Journal of Physical Chemistry C, 2007, 111, 13679-13683.	1.5	11
802	Equations of state of MgO, Au, Pt, NaCl-B1, and NaCl-B2: Internally consistent high-temperature pressure scales. High Pressure Research, 2007, 27, 431-446.	0.4	232
803	Thermodynamics of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>L</mml:mi><mml:msub><mml:mn>1</mml:mn><mml:mn>0</mml:mn></mml:msub></mml:mr in FePt nanoparticles studied by Monte Carlo simulations based on an analytic bond-order potential. Physical Review B, 2007, 76, .	1.1	67
804	First principles study of structural phase transition of YSb and ScSb compounds. Solid State Communications, 2007, 141, 359-364.	0.9	18
805	Thermal stability of superhard Tiâ€“Bâ€“N coatings. Surface and Coatings Technology, 2007, 201, 6148-6153.	2.2	59
806	Determination of the thermal stability and isothermal bulk modulus of the ZrO2 polymorphs at room temperature by molecular dynamics with a semi-empirical quantum-chemical model. Ceramics International, 2007, 33, 705-709.	2.3	21
807	Energetic balance and kinetics for the decomposition of supersaturated Ti1â^'xAlxN. Acta Materialia, 2007, 55, 1441-1446.	3.8	106
808	Thermal stability of Ti3SiC2 thin films. Acta Materialia, 2007, 55, 1479-1488.	3.8	198
809	Theoretical elastic stiffness, structure stability and thermal conductivity of La2Zr2O7 pyrochlore. Acta Materialia, 2007, 55, 2949-2957.	3.8	127
810	Structural and electronic properties of CaS Crystal: A density functional theory investigation. Physica B: Condensed Matter, 2007, 391, 193-198.	1.3	32
811	Electronic structure and ground-state properties of alkali-metal oxidesâ€“Li2O, Na2O, K2O and Rb2O: A first-principles study. Physica B: Condensed Matter, 2007, 396, 124-131.	1.3	29
812	Anisotropic elastic behaviour and structural evolution of zeolite phillipsite at high pressure: A synchrotron powder diffraction study. Microporous and Mesoporous Materials, 2007, 105, 239-250.	2.2	27
813	Single crystal X-ray diffraction study of a mixed-valence gold compound, Cs2AuIAuIIICl6 under high pressures up to 18GPa: Pressure-induced phase transition coupled with gold valence transition. Journal of Solid State Chemistry, 2007, 180, 1353-1364.	1.4	24

#	Article	IF	Citations
814	First-principles calculations of structural, elastic, electronic and optical properties of the antiperovskite AsNMg3. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 371, 337-343.	0.9	80
815	Electronic structure calculations of europium chalcogenides EuS and EuSe. Physica Status Solidi (B): Basic Research, 2007, 244, 1988-1996.	0.7	14
816	First-principles study of electronic structure and ground-state properties of alkali-metal sulfides â€“ Li2S, Na2S, K2S and Rb2S. Physica Status Solidi (B): Basic Research, 2007, 244, 1337-1346.	0.7	59
817	Effect of pressure on the structural properties and electronic band structure of GaSe. Physica Status Solidi (B): Basic Research, 2007, 244, 244-255.	0.7	33
818	High pressure structure of Tb2Ti2O7 pyrochlore at cryogenic temperatures. Physica Status Solidi (B): Basic Research, 2007, 244, 266-269.	0.7	12
819	Equation of state of nanocrystalline BaTiO3 up to 52 GPa at room temperature. Physica Status Solidi (B): Basic Research, 2007, 244, 290-294.	0.7	4
820	Ab initio electronic band structure calculations of halfâ€metallic c alcium pnictides. Physica Status Solidi (B): Basic Research, 2007, 244, 4643-4650.	0.7	3
821	Six-fold-coordinated phosphorus by oxygen in AlPO4 quartz homeotype under high pressure. Nature Materials, 2007, 6, 698-702.	13.3	64
822	Ab initio investigation of the electronic structure and the magnetic trends within equiatomic FeN. Journal of Magnetism and Magnetic Materials, 2007, 312, 298-304.	1.0	11
823	New aspects of the energetics of ordered Ti2C and Ti2N. Journal of Physics Condensed Matter, 2007, 19, 196226.	0.7	16
824	Structural and elastic properties of Zr2AlX and Ti2AlX (X = C and N) under pressure effect. European Physical Journal B, 2007, 56, 209-215.	0.6	73
825	Do carbonate liquids become denser than silicate liquids at pressure? Constraints from the fusion curve of K2CO3 to 3.2ÂGPa. Contributions To Mineralogy and Petrology, 2007, 153, 55-66.	1.2	33
826	The correlation between the electronic structure and elastic properties of nanolaminates. Jom, 2007, 59, 60-64.	0.9	71
827	HighPâ€“T Nano-Mechanics of Polycrystalline Nickel. Nanoscale Research Letters, 2007, 2, 476-91.	3.1	9
828	Ab initio study of pressure-induced magnetic transition in manganese pnictides. Journal of Magnetism and Magnetic Materials, 2007, 309, 251-255.	1.0	9
829	Impurity effects on the phase transformations and equations of state of zirconium metals. Journal of Physics and Chemistry of Solids, 2007, 68, 2297-2302.	1.9	26
830	Phase stabilities of monoclinic oxoborates LaB3O6 and GdB3O6 in C121 and I12/a1 phaseâ€”Energetics and chemical bonds derived from first-principles calculations. Journal of Solid State Chemistry, 2007, 180, 2763-2774.	1.4	3
831	High pressure structural studies on SrRuO3. Journal of Physics and Chemistry of Solids, 2008, 69, 2237-2239.	1.9	8

#	Article	IF	Citations
832	High-pressure modifications of CaZn2, SrZn2, SrAl2, and BaAl2: Implications for Laves phase structural trends. Journal of Solid State Chemistry, 2008, 181, 3016-3023.	1.4	22
833	The effect of oxygen vacancies and aluminium substitution on the high-pressure properties of brownmillerite-structured Ca2Fe2â^'x Al x O5. Physics and Chemistry of Minerals, 2008, 35, 493-504.	0.3	11
834	Firstâ€principles study of phase transition of tin and lead under high pressure. Physica Status Solidi (B): Basic Research, 2008, 245, 53-57.	0.7	17
835	Pressure effects in lutetium yttrium oxyorthosilicate single crystals. Journal of Raman Spectroscopy, 2008, 39, 1268-1275.	1.2	18
836	First principles study of structural, elastic, electronic and optical properties of the cubic perovskite BaHfO3. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 4527-4531.	0.9	59
837	First-principles study on electronic structure and elastic properties of Ti2SC. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 5220-5223.	0.9	35
838	Structural, electronic and elastic properties of M2SC (M=Ti, Zr, Hf) compounds. Physics Letters, Section A: General, Atomic and Solid State Physics, 2008, 372, 6448-6452.	0.9	46
839	Pressure effects on the structural and electronic properties of ABX4 scintillating crystals. Progress in Materials Science, 2008, 53, 711-773.	16.0	316
840	Theoretical study of melting curves on Ta, Mo, and W at high pressures. Physica B: Condensed Matter, 2008, 403, 2065-2070.	1.3	14
841	Prediction study of structural and elastic properties under pressure effect of M2SnC (M=Ti, Zr, Nb,) Tj ETQq1 1 0.784314 rgBT /Overlock	1.3	55
842	High-pressure X-ray diffraction study of SrMoO4 and pressure-induced structural changes. Journal of Solid State Chemistry, 2008, 181, 355-364.	1.4	94
843	Cation-dependent anomalous compression of gallosilicate zeolites with CGS topology: A high-pressure synchrotron powder diffraction study. Journal of Solid State Chemistry, 2008, 181, 730-734.	1.4	2
844	Pressure-induced zircon-type to scheelite-type phase transitions in YbPO4 and LuPO4. Journal of Solid State Chemistry, 2008, 181, 2633-2638.	1.4	56
845	In situ observations of temperature- and pressure-induced phase transitions in TiH2: Angle-dispersive and synchrotron energy-dispersive X-ray diffraction studies. Journal of Physics and Chemistry of Solids, 2008, 69, 2240-2244.	1.9	11
846	High-pressure structural integrity and structural transformations of glass-derived nanocomposites: A review. Journal of Physics and Chemistry of Solids, 2008, 69, 2268-2273.	1.9	7
847	First principles study of barium chalcogenides. Journal of Physics and Chemistry of Solids, 2008, 69, 2924-2927.	1.9	37
848	Density functional study of structures and mechanical properties of Y-doped Î±-SiAlONs. Journal of the European Ceramic Society, 2008, 28, 995-1002.	2.8	14
849	High-pressure effects on boron nitride multi-walled nanotubes: An X-ray diffraction study. Chemical Physics Letters, 2008, 466, 205-208.	1.2	6

#	Article	IF	Citations
850	Structure, elastic properties and phase stability of Cr1â€“xAlxN. Acta Materialia, 2008, 56, 2469-2475.	3.8	109
851	Theoretical investigation of typical fcc precipitates in Mg-based alloys. Acta Materialia, 2008, 56, 3353-3357.	3.8	43
852	Stability of Tiâ€“Bâ€“N solid solutions and the formation of nc-TiN/a-BN nanocomposites studied by combined ab initio and thermodynamic calculations. Acta Materialia, 2008, 56, 4440-4449.	3.8	40
853	A model for evolution of shape changing precipitates in multicomponent systems. Acta Materialia, 2008, 56, 4896-4904.	3.8	24
854	Synchrotron X-ray diffraction study of ZnTe at high pressure. Solid State Communications, 2008, 145, 374-378.	0.9	13
855	First-principles study of structural and elastic properties of Sc2AC (A=Al, Ga, In, Tl). Solid State Communications, 2008, 146, 175-180.	0.9	36
856	Electronic structure and mechanical properties of osmium borides, carbides and nitrides from first principles. Solid State Communications, 2008, 146, 450-453.	0.9	45
857	Effect of dopants on the structure and properties of Ge2Sb2Te5 studied by Ab initio calculations. Solid State Communications, 2008, 148, 113-116.	0.9	23
858	Structural and electronic properties of M2InC (M = Ti, Zr, and Hf). Solid State Communications, 2008, 148, 459-463.	0.9	27
859	Phase stabilities of self-organized nc-TiN/a-Si3N4 nanocomposites and of Ti1â^'xSixNy solid solutions studied by ab initio calculation and thermodynamic modeling. Thin Solid Films, 2008, 516, 2264-2275.	0.8	73
860	Electronic topological transition and phase transition in rhodium and iridium based inter metallic compounds. Physica B: Condensed Matter, 2008, 403, 2530-2541.	1.3	3
861	First principles electronic and thermal properties of some AlRE intermetallics. Physica B: Condensed Matter, 2008, 403, 3615-3622.	1.3	27
862	Pressure-induced electronic and structural phase transformation properties in half-metallic PmN: A first-principles approach. Physica B: Condensed Matter, 2008, 403, 4333-4337.	1.3	21
863	Ab initio investigation of perovskite and post-perovskite CaPtO3. Chemical Physics, 2008, 352, 92-96.	0.9	6
864	First-principles investigations of structural, electronic and magnetic properties of cubic LaMnO3. Materials Science in Semiconductor Processing, 2008, 11, 81-86.	1.9	11
865	Electronic band-edge properties of rock salt PbY and SnY (Y= S, Se, and Te). Optical Materials, 2008, 30, 1451-1460.	1.7	11
866	Pressure-induced structural evolution and elastic behaviour of Na6Cs2Ga6Ge6O24Â·Ge(OH)6 variant of cancrinite: A synchrotron powder diffraction study. Microporous and Mesoporous Materials, 2008, 116, 51-58.	2.2	10
867	High-pressure study of the Sr2CoWO6 ordered double perovskite tungstate oxide. Journal of Molecular Structure, 2008, 888, 244-252.	1.8	29

#	Article	IF	Citations
868	First principles study of structural, magnetic and electronic properties of half-metallic CrO2 under pressure. European Physical Journal B, 2008, 61, 131-139.	0.6	36
869	Molybdenum at High Pressure and Temperature: Melting from Another Solid Phase. Physical Review Letters, 2008, 100, 135701.	2.9	127
870	Effects of sample preparation on the mechanical properties of AlMgB₁₄. High Pressure Research, 2008, 28, 63-68.	0.4	22
871	Electronic and structural properties of NaZnX (X = P, As, Sb): anab initiostudy. Journal of Physics Condensed Matter, 2008, 20, 085220.	0.7	23
872	Ruby under pressure. High Pressure Research, 2008, 28, 75-126.	0.4	367
873	Magneto-elastic effects in compressed cobalt from first-principles. Physical Review B, 2008, 77, .	1.1	21
874	Pressure-temperature stability studies of FeOOH using X-ray diffraction. American Mineralogist, 2008, 93, 1882-1885.	0.9	69
875	Structural stability ofFe5Si3andNi2Sistudied by high-pressure x-ray diffraction andab initiototal-energy calculations. Physical Review B, 2008, 77, .	1.1	51
876	Decomposition of lanthanum hafnate at high pressures. Physical Review B, 2008, 77, .	1.1	40
877	Combined Raman scattering andab initioinvestigation of pressure-induced structural phase transitions in the scintillator<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZnWO</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2008, 78, .	1.1	83
878	Theoretical study of the structural, elastic and electronic properties of the GeX₂O₄(X= Mg, Zn, Cd) compounds under pressure. Modelling and Simulation in Materials Science and Engineering, 2008, 16, 055007.	0.8	30
879	Study of Ti2SC under compression up to 47GPa. Journal of Alloys and Compounds, 2008, 448, L1-L4.	2.8	57
880	Single-crystal elasticity of diaspore, AlOOH, to 12GPa by Brillouin scattering. Physics of the Earth and Planetary Interiors, 2008, 170, 221-228.	0.7	13
881	Temperature induced immiscibility in the NaClâ€“H2O system at high pressure. Physics of the Earth and Planetary Interiors, 2008, 170, 107-114.	0.7	12
882	Phase transitions and isothermal equations of state of epsilon hexanitrohexaazaisowurtzitane (CL-20). Journal of Applied Physics, 2008, 104, .	1.1	33
883	PHASE STABILITY OF EPSILON AND GAMMA HNIW (CL-20) AT HIGH-PRESSURE AND TEMPERATURE. AIP Conference Proceedings, 2008, , .	0.3	5
884	Anomalous high-pressure behavior of amorphous selenium from synchrotron x-ray diffraction and microtomography. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 13229-13234.	3.3	50
885	First-principle calculations of elastic and electronic properties of the filled skutterudite CeFe4P12. Computational Materials Science, 2008, 43, 1022-1026.	1.4	20

#	Article	IF	Citations
886	Elastic constants and high pressure structural transitions in yttrium pnictides. Computational Materials Science, 2008, 43, 1112-1116.	1.4	25
887	Electronic structure, elasticity and hardness of diborides of zirconium and hafnium: First principles calculations. Computational Materials Science, 2008, 44, 411-421.	1.4	134
888	Electronic Energy Band Structure of the Double Perovskite Ba₂MnWO₆. Journal of Physical Chemistry B, 2008, 112, 6742-6746.	1.2	16
889	P-V equation of state for Fe2P and pressure-induced phase transition in Fe3P. High Pressure Research, 2008, 28, 375-384.	0.4	16
890	Phase diagram studies on iron and nickel silicides: high-pressure experiments andab initiocalculations. Journal of Physics: Conference Series, 2008, 121, 022013.	0.3	2
891	Melting curve and Hugoniot of molybdenum up to 400 GPa byab initiosimulations. Journal of Physics: Conference Series, 2008, 121, 012009.	0.3	11
892	Elastic, electronic and optical properties of the filled tetrahedral semiconductor LiCdP. Semiconductor Science and Technology, 2008, 23, 105024.	1.0	6
893	Phase Transition and Compressibility in Silicon Nanowires. Nano Letters, 2008, 8, 2891-2895.	4.5	49
894	Characterization of the High-Pressure Structural Transition and Thermodynamic Properties in Sodium Chloride: A Computational Investigation on the Basis of the Density Functional Theory. Journal of Physical Chemistry B, 2008, 112, 13898-13905.	1.2	9
895	Equations of State and High-Pressure Phases of Explosives. , 2009, , 99-126.		5
896	Structural and elastic properties under pressure effect of Hf₂AlN and Hf₂AlC. High Pressure Research, 2008, 28, 45-53.	0.4	14
897	Pressure-temperature studies of talc plus water using X-ray diffraction. American Mineralogist, 2008, 93, 1043-1050.	0.9	10
898	High pressure structural behavior and synthesis of Zr2SC. Journal of Physics Condensed Matter, 2008, 20, 135211.	0.7	26
899	CALCULATED STRUCTURAL AND ELASTIC PROPERTIES OF M₂InC(M=Sc, Ti,) Tj ETQq1 1 0.784314 rgBT /Ov Physics Letters B, 2008, 22, 2063-2076.	1.0	42
900	Mechanical stability of TiO₂polymorphs under pressure:ab initiocalculations. Journal of Physics Condensed Matter, 2008, 20, 345218.	0.7	19
901	NANOLAYERED MAX PHASES FROM ab initio CALCULATIONS. International Journal of Modern Physics B, 2008, 22, 4495-4499.	1.0	7
902	Theoretical investigation of phase transition properties in strontium chalcogenides using potential model. Phase Transitions, 2008, 81, 403-411.	0.6	8
903	Theoretical Prediction for Structural Stabilities and Optical Properties of SrS, SrSe and SrTe under High Pressure. Chinese Physics Letters, 2008, 25, 1807-1810.	1.3	34

#	Article	IF	Citations
904	Improving the charge density normalization in Korringaâ€“Kohnâ€“Rostoker Green-function calculations. Journal of Physics Condensed Matter, 2008, 20, 035220.	0.7	19
905	Structural and mechanical properties of Mg₁₇Al₁₂and Mg₂₄Y₅from first-principles calculations. Journal Physics D: Applied Physics, 2008, 41, 195408.	1.3	65
906	Elastic properties of Sr_{n+1}Ti_nO_{3n+1}phases (n= 1â€“3, infty). Journal of Physics Condensed Matter, 2008, 20, 055224.	0.7	21
907	Ab-initio melting curve and principal Hugoniot of tantalum. Journal of Physics: Conference Series, 2008, 121, 012010.	0.3	4
908	Theoretical study of structural parameters and energy gap composition dependence of Ga_{1â^'x}B_xN alloys. Semiconductor Science and Technology, 2008, 23, 125036.	1.0	11
909	Structure of the ternary carbide Ti₃SnC₂fromab initiocalculations. Journal of Physics Condensed Matter, 2008, 20, 085211.	0.7	16
910	Phase stability and elastic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>X</mml:mi><mml:msub><mml:mrow><mml:mtext>MgB</mml:mtext></mml:mrow><mml:mrow		
	byab initiocalculations<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
922	High-pressure high-temperature synthesis of novel binary and ternary nitride phases of group 4 and 14 elements. Journal of Physics: Conference Series, 2008, 121, 062003.	0.3	3
923	Structural phase transitions of sodium nitride at high pressure. Physical Review B, 2009, 79, .	1.1	30
924	Limits to Poissonâ€™s ratio in isotropic materials. Physical Review B, 2009, 80, .	1.1	143
925	Low-temperature and high-pressure Raman and x-ray studies of pyrochlore<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Tb</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Phonon anomalies and possible phase transition. Physical Review B, 2009, 79, .	1.1	34
926	Experimental and theoretical investigation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ThGeO</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml: high pressure. Physical Review B, 2009, 80, .	1.1	40
927	Carbon nitride:Ab initioinvestigation of carbon-rich phases. Physical Review B, 2009, 80, .	1.1	48
928	Electronic structure, stability, and mechanism of the decohesion and shear of interfaces in superhard nanocomposites and heterostructures. Physical Review B, 2009, 79, .	1.1	69
929	Structure of Carbon Dioxide Phase IV: Breakdown of the Intermediate Bonding State Scenario. Physical Review Letters, 2009, 103, 185701.	2.9	52
930	Pressure-induced lattice collapse in the tetragonal phase of single-crystalline<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mrow><mml:mn>1.05</mml Physical Review B, 2009, 80, .	1.1	29
931	Impact of the crystal structure ofHfO2on the transport properties of modelHfO2/Si/HfO2silicon-on-insulator field-effect transistors: A combined DFT-scattering theory approach. Physical Review B, 2009, 79, .	1.1	5
932	High-pressure phases, vibrational properties, and electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Ne</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mo>(</mml:mo><mml:mrow xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>Ar</mml:mtext><mml:msub><mml:mrow><mml:mrow><mml:mm Physical Review B, 2009, 80, .	1.1	59
933	Solid phases of phosphorus carbide: Anab initiostudy. Physical Review B, 2009, 79, .	1.1	37
934	Analysis of nonhydrostatic high-pressure diffraction data (cubic system): Assessment of various assumptions in the theory. Journal of Applied Physics, 2009, 106, .	1.1	34
935	First-principles study of structural, thermodynamic, elastic, and magnetic properties of Cr2GeC under pressure and temperature. Journal of Applied Physics, 2009, 106, .	1.1	37
936	High-pressure powder x-ray diffraction experiments andab initiocalculation of Ti3AlC2. Journal of Applied Physics, 2009, 106, .	1.1	15
937	Phase stability of YbVO4 under pressure: In situ x-ray and Raman spectroscopic investigations. Journal of Applied Physics, 2009, 106, .	1.1	35
938	PRESSURE-RELATED PHASE STABILITY OF MgSiO3and(Mg0.75, Fe0.25)SiO3 AT LOWER MANTLE CONDITION. International Journal of Modern Physics B, 2009, 23, 3323-3329.	1.0	2
939	Synthesis and elastic properties of V₂AlC thin films by magnetron sputtering from elemental targets. Journal Physics D: Applied Physics, 2009, 42, 185408.	1.3	30

#	Article	IF	Citations
940	Steric effect on the M site of nanolaminate compounds M₂SnC (M = Ti, Zr, Hf and Nb). Journal of Physics Condensed Matter, 2009, 21, 045404.	0.7	22
941	Equation of state and structure of prehnite to 9.8 GPa. European Journal of Mineralogy, 2009, 21, 561-570.	0.4	8
942	Anharmonic OH vibrations in brucite: Small pressure-induced redshift in the range 0-22 GPa. American Mineralogist, 2009, 94, 1687-1697.	0.9	19
943	Ab initiocalculations of the structure and mechanical properties of vanadium oxides. Journal of Physics Condensed Matter, 2009, 21, 145404.	0.7	45
944	Pressure-induced phase transformations in cubic Gd2O3. Journal of Applied Physics, 2009, 106, .	1.1	40
945	Hexagonal Ti2SC with high hardness and brittleness: a first-principles study. Scripta Materialia, 2009, 61, 576-579.	2.6	38
946	Structural, elastic, electronic and optical properties of the cubic perovskite BiAlO3. Solid State Sciences, 2009, 11, 556-561.	1.5	31
947	First-principle study of hydrogen stability within TiCo3. Solid State Sciences, 2009, 11, 894-899.	1.5	4
948	Electronic structure and chemical bonding properties of UO2F2 from first principles. Solid State Sciences, 2009, 11, 1380-1385.	1.5	5
949	First-principles investigation of the binary AB2 type Laves phase in Mgâ€“Alâ€“Ca alloy: Electronic structure and elastic properties. Solid State Sciences, 2009, 11, 1400-1407.	1.5	100
950	X-ray/neutron diffraction studies and ab initio electronic structure of CeMgNi4 and its hydride. Solid State Sciences, 2009, 11, 1971-1978.	1.5	35
951	Structural, electronic and elastic properties of MAX phases M2GaN (M=Ti, V and Cr). Solid State Sciences, 2009, 11, 1875-1881.	1.5	34
952	DFT calculations on the electronic structures of BiOX (X = F, Cl, Br, I) photocatalysts with and without semicore Bi 5d states. Journal of Computational Chemistry, 2009, 30, 183-190.	1.5	152
953	Firstâ€principles calculations on the energetics, electronic structures and magnetism of SrFeO₂. Journal of Computational Chemistry, 2009, 30, 2684-2693.	1.5	5
954	The bulk modulus of SmFeAs(O0.93F0.07). Physica C: Superconductivity and Its Applications, 2009, 469, 782-784.	0.6	16
955	Structural and elastic properties under pressure effect of the cubic antiperovskite compounds ANCa3 (A=P, As, Sb, and Bi). Physics Letters, Section A: General, Atomic and Solid State Physics, 2009, 373, 1777-1781.	0.9	31
956	First principles studies of SnTiO3 perovskite as potential environmentally benign ferroelectric material. Chemical Physics, 2009, 355, 43-49.	0.9	74
957	X-ray diffraction and infrared spectroscopy of monazite-structured CaSO4 at high pressures: Implications for shocked anhydrite. Journal of Physics and Chemistry of Solids, 2009, 70, 134-141.	1.9	23

#	Article	IF	Citations
958	Theoretical study of the phonon properties of SrS. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2009, 162, 116-119.	1.7	21
959	Calculated structural, electronic and elastic properties of M2GeC (M=Ti, V, Cr, Zr, Nb, Mo, Hf, Ta and) Tj ETQq1 1 0.784314 rgBT /Ove	1.1	66
960	New Ternary Silicide LiRh₂Si₂ â€“ Structure and Bonding Peculiarities. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2009, 635, 1894-1903.	0.6	15
961	Firstâ€principles study on the boron antimony compound. Physica Status Solidi (B): Basic Research, 2009, 246, 119-123.	0.7	23
962	First principles calculations of Alâ€rich RE (RE = Ho, Er, Tm and Yb) intermetallic compounds. Physica Status Solidi (B): Basic Research, 2009, 246, 1206-1214.	0.7	10
963	Firstâ€principles calculations of structural, elastic and electronic properties of Ni₂MnZ (Z) Tj ETQq1 1 0.784314 rgBT /Ov	0.7	86
964	Bonding properties and bulk modulus of M₄AlC₃ (M = V, Nb, and Ta) studied by firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 1039-1043.	0.7	17
965	Structural changes in nanocrystalline mackinawite (FeS) at high pressure. Journal of Applied Crystallography, 2009, 42, 15-21.	1.9	28
966	Self-consistent thermodynamic description of silicate liquids, with application to shock melting of MgO periclase and MgSiO₃perovskite. Geophysical Journal International, 2009, 178, 162-179.	1.0	130
967	Theoretical prediction of the structural and electronic properties of pseudocubic X3As4 (X=C, Si, Ge) Tj ETQq1 1 0.784314 rgBT /Ove	1.3	5
968	Structural transition of Li3N under high pressure: A first-principles study. Solid State Communications, 2009, 149, 612-615.	0.9	14
969	Structural, elastic and electronic properties of XNCa3 (X = Ge, Sn and Pb) compounds. Solid State Communications, 2009, 149, 619-624.	0.9	28
970	First-principles study of crystal structures of under pressure. Solid State Communications, 2009, 149, 1342-1346.	0.9	1
971	On the compression behavior of Ti2InC, (Ti0.5, Zr0.5)2InC, and M2SnC (, Nb, Hf) to quasi-hydrostatic pressures up to 50 GPa. Solid State Communications, 2009, 149, 1978-1983.	0.9	27
972	Structural studies on Na0.75CoO2 thermoelectric material at high pressures. Solid State Communications, 2009, 149, 1712-1716.	0.9	5
973	Elastic properties of mono- and polycrystalline (and Lu) under pressure effect. Solid State Communications, 2009, 149, 1658-1662.	0.9	10
974	Static compressibility, thermal expansion and elastic anisotropy of single crystals. Solid State Communications, 2009, 149, 2110-2114.	0.9	12
975	Prediction study of the structural, elastic, electronic and optical properties of the antiperovskite. Solid State Communications, 2009, 149, 2002-2006.	0.9	19

#	Article	IF	Citations
976	First-principles study of structural, elastic, electronic and optical properties of SrMO3 (M=Ti and Sn). Solid State Communications, 2009, 149, 2244-2249.	0.9	21
977	300-K equation of state of rhombohedral boron subnitride,. Solid State Communications, 2009, 149, 2169-2171.	0.9	29
978	The properties of the Pt6/BaO(100) interface and NO adsorption at the interface. Surface Science, 2009, 603, 2413-2421.	0.8	1
979	Energetics of point defects in TiC. Journal of the European Ceramic Society, 2009, 29, 773-777.	2.8	25
980	Intercalation of Al into MC (M= Ti, V, Cr). Journal of the European Ceramic Society, 2009, 29, 2885-2891.	2.8	11
981	Elastic, electronic and optical properties of the filled tetrahedral semiconductor Î±-LiCdAs. Materials Science in Semiconductor Processing, 2009, 12, 198-205.	1.9	5
982	Structural and thermodynamic properties of the cubic perovskite BiAlO3. Physica B: Condensed Matter, 2009, 404, 3534-3538.	1.3	24
983	Theoretical investigation on structural, magnetic and electronic properties of ferromagnetic GdN under pressure. Journal of Magnetism and Magnetic Materials, 2009, 321, 607-612.	1.0	21
984	Compression behaviour of nitridocarbidosilicates studied with X-ray diffraction and ab initio calculations. Journal of Physics and Chemistry of Solids, 2009, 70, 97-106.	1.9	7
985	Study of structural stabilities and optical properties of HgTe under high pressure. Journal of Physics and Chemistry of Solids, 2009, 70, 433-438.	1.9	5
986	FP-LMTO calculations of elastic and electronic properties of the filled skutterudite CeRu4P12. Journal of Physics and Chemistry of Solids, 2009, 70, 622-626.	1.9	20
987	Electronic band structure of from first principles. Journal of Solid State Chemistry, 2009, 182, 2678-2684.	1.4	11
988	First principles studies of ZrNi and ZrNiH3. Chemical Physics Letters, 2009, 473, 61-65.	1.2	24
989	X-ray diffraction studies and equation of state of methane at 202GPa. Chemical Physics Letters, 2009, 473, 72-74.	1.2	43
990	Electronic structure and lattice anisotropy of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si18.gif" display="inline" overflow="scroll"><mml:mrow><mml:mtext>Cd</mml:mtext><mml:mo stretchy="false">(</mml:mo><mml:msub><mml:mrow><mml:mtext>UO</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:m	1.2	3
991	Chemical Physics Letters, 2009, 476, 213-217. Structural, elastic, electronic, optical and thermal properties of c-SiGe2N4. European Physical Journal B, 2009, 71, 185-194.	0.6	11
992	High-pressure structural investigation of several zircon-type orthovanadates. Physical Review B, 2009, 79, .	1.1	90
993	Density-functional study of the thermodynamic properties and the pressureâ€“temperature phase diagram of Ti. Physical Review B, 2009, 80, .	1.1	94

#	Article	IF	Citations
994	Structural, electronic and elastic properties of Ti2TlC, Zr2TlC and Hf2TlC. Open Physics, 2009, 7, .	0.8	5
995	Phase transitions in wolframite-type<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CdWO</mml:mtext></mml:mrow><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> high pressure studied by Raman spectroscopy and density-functional theory. Physical Review B, 2009, 79, .	1.1	64
996	High-Pressure Investigation on Calcium Borohydride. Journal of Physical Chemistry C, 2009, 113, 15087-15090.	1.5	23
997	FIRST-PRINCIPLES STUDY OF ELECTRONIC STRUCTURE AND GROUND-STATE PROPERTIES OF ALKALI-METAL SELENIDES AND TELLURIDES (M₂A)[M: Li, Na, K; A: Se, Te]. International Journal of Modern Physics B, 2009, 23, 5027-5037.	1.0	24
998	Structure and elasticity of serpentine at high-pressure. Earth and Planetary Science Letters, 2009, 279, 11-19.	1.8	86
999	Bottom-up versus top-down solidification of the cores of small solar system bodies: Constraints on paradoxical cores. Earth and Planetary Science Letters, 2009, 284, 564-569.	1.8	69
1000	Detecting deeply subducted crust from the elasticity of hollandite. Earth and Planetary Science Letters, 2009, 288, 349-358.	1.8	41
1001	First-principles study of zinc-blende to rocksalt phase transition in BP and BAs. Computational Materials Science, 2009, 44, 1386-1389.	1.4	24
1002	Prediction study of the structural, elastic and electronic properties of ANSr3 (A=As, Sb and Bi). Computational Materials Science, 2009, 46, 881-886.	1.4	22
1003	Structural stabilities, electronic and optical properties of CaF2 under high pressure: A first-principles study. Computational Materials Science, 2009, 47, 41-45.	1.4	18
1004	Theoretical study of mechanical, electronic, chemical bonding and optical properties of Ti2SnC, Zr2SnC, Hf2SnC and Nb2SnC. Computational Materials Science, 2009, 47, 491-500.	1.4	95
1005	Quantum size effects in Pb/Si(111) thin films from density functional calculations. Computational Materials Science, 2009, 47, 584-592.	1.4	18
1006	Pressure-induced structural phase transition in the Bechgaard-Fabre salts. Synthetic Metals, 2009, 159, 2097-2100.	2.1	8
1007	Elasticity of stishovite and acoustic mode softening under high pressure by Brillouin scattering. Physics of the Earth and Planetary Interiors, 2009, 172, 235-240.	0.7	49
1008	Ab initio study of the phase stability and mechanical properties of 5d transition metal nitrides MN2. Journal of Alloys and Compounds, 2009, 472, 425-428.	2.8	17
1009	Structural and electronic properties of ZnO under high pressure. Journal of Alloys and Compounds, 2009, 476, 306-310.	2.8	42
1010	Synthesis and properties of oxygen-bearing c-Zr3N4 and c-Hf3N4. Journal of Alloys and Compounds, 2009, 480, 46-49.	2.8	15
1011	Theoretical investigation of zincblende AlSb and GaSb compounds. Journal of Alloys and Compounds, 2009, 478, 653-656.	2.8	14

#	Article	IF	Citations
1012	Elastic stability, electronic structure and optical properties of PtN2 with pyrite and fluorite structures. Journal of Alloys and Compounds, 2009, 478, 297-302.	2.8	7
1013	High-pressure structural, electronic and optical properties of KMgF3: A first-principles study. Journal of Alloys and Compounds, 2009, 484, 597-600.	2.8	21
1014	Structural phase transition, elastic properties and electronic properties of chalcopyrite CuAlX2 (X=S,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.8	45
1015	FP-APW+lo calculations of the electronic and optical properties of alkali metal sulfides under pressure. Journal of Physics Condensed Matter, 2009, 21, 095404.	0.7	32
1016	Size-dependent elasticity of nanocrystalline titania. Physical Review B, 2009, 79, .	1.1	53
1017	Elasticity of phaseâ€X at high pressure. Geophysical Research Letters, 2009, 36, .	1.5	20
1018	Effect of high pressure on multiferroic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BiFeO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:m Physical Review B, 2009, 79, .	1.1	149
1019	Ab initiorefinement of the thermal equation of state for bcc tantalum: the effect of bonding on anharmonicity. Journal of Physics Condensed Matter, 2009, 21, 095408.	0.7	29
1020	Magnetic phase transition in CoO under high pressure: A challenge for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mtext>LSDA</mml:mtext><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math Physical Review B, 2009, 79, .	1.1	23
1021	First-principles study of structural and bonding properties of vanadium carbide and niobium carbide. Physica Scripta, 2009, 80, 055601.	1.2	13
1022	Post-spinel transformations and equation of state in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>ZnGa</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:m Determination at high pressure byin situx-ray diffraction. Physical Review B, 2009, 79, .	1.1	77
1023	Phase stability of AlYB₁₄sputtered thin films. Journal of Physics Condensed Matter, 2009, 21, 355006.	0.7	8
1024	Interatomic Potential for Platinum and Self-Diffusion on Pt(111) Surface by Molecular-Dynamics Simulation. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 335-344.	0.5	1
1025	Superhard diamondlike<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>BC</mml:mtext></mml:mrow><mml:mn>5</mml:mn></mml:msub></mml:mrow></mml:math> A first-principles investigation. Physical Review B, 2009, 80, .	1.1	24
1026	First-Principles Study of Structural Stabilities, Electronic and Optical Properties of SrF ₂ under High Pressure. Chinese Physics Letters, 2009, 26, 077103.	1.3	11
1027	Theoretical investigation of half metallicity in Fe/Co/Ni doped ZnSe material systems. Journal of Applied Physics, 2009, 106, .	1.1	36
1028	Ab initiostudy of structural, elastic, and high-pressure properties of rubidium halides RbX (X =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.6	8
1029	Structural phase transitions in RbBH4 under compression. Journal of Alloys and Compounds, 2009, 476, 5-8.	2.8	16

#	Article	IF	Citations
1030	Equilibrium structure of Î´-Bi₂O₃from first principles. Journal of Physics Condensed Matter, 2009, 21, 175403.	0.7	18
1031	Nanocrystalline tungsten carbide: As incompressible as diamond. Applied Physics Letters, 2009, 95, .	1.5	41
1032	Evidence for a low-compressibility carbon nitride polymorph elaborated at ambient pressure and mild temperature. Diamond and Related Materials, 2009, 18, 627-631.	1.8	11
1033	Structural Characterization Combined with the First Principles Simulations of Barium/Strontium Cobaltite/Ferrite as Promising Material for Solid Oxide Fuel Cells Cathodes and High-Temperature Oxygen Permeation Membranes. ACS Applied Materials & Interfaces, 2009, 1, 1512-1519.	4.0	50
1034	In situ Raman spectroscopy of MgSiO3 enstatite up to 1550 K. American Mineralogist, 2009, 94, 1638-1646.	0.9	25
1035	ISOTHERMAL EQUATIONS OF STATE OF LLM-105. , 2009, , .		3
1036	High pressure behaviour of heavy rare earth mono antimonides. Journal of Physics: Conference Series, 2010, 215, 012114.	0.3	5
1037	Compressibility of cubic vanadium mononitride. Europhysics Letters, 2010, 92, 66001.	0.7	14
1038	First-principles study of zinc-blende to rocksalt phase transition in BN. Open Physics, 2010, 8, 628-633.	0.8	6
1039	Thermal expansion and elasticity of PdFe3N within the quasiharmonic approximation. European Physical Journal B, 2010, 77, 401-406.	0.6	21
1040	Strength effects in diamond under shock compression from 0.1 to 1 TPa. Physical Review B, 2010, 81, .	1.1	87
1041	High-pressure stability and compressibility of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>A</mml:mi><mml:msub><mml:mrow><mml:mtext>PO</mml:mtext></mml:mrow><mml:mn	1.1	123
1042	Revie The pressure-volume-temperature equation of state of MgO derived from shock Hugoniot data and its application as a pressure scale. Journal of Applied Physics, 2010, 107, 113518.	1.1	22
1043	Crystal Structures and Thermodynamic Investigations of LiK(BH₄)₂, KBH₄, and NaBH₄ from First-Principles Calculations. Journal of Physical Chemistry C, 2010, 114, 678-686.	1.5	56
1044	Intermetallic hydrides: A review with ab initio aspects. Progress in Solid State Chemistry, 2010, 38, 1-37.	3.9	80
1045	YNi and its hydrides: Phase stabilities, electronic structures and chemical bonding properties from first principles. Chemical Physics, 2010, 377, 109-114.	0.9	4
1046	Ab-initio investigations of the electronic properties of bulk wurtzite Beryllia and its derived nanofilms. Physics Letters, Section A: General, Atomic and Solid State Physics, 2010, 374, 3977-3981.	0.9	5
1047	Compression of silver in a diamond anvil cell: Pressure dependences of strength and grain size from X-ray diffraction data. Journal of Physics and Chemistry of Solids, 2010, 71, 1088-1093.	1.9	5

#	Article	IF	Citations
1048	New high-pressure phase of HfTiO4 and ZrTiO4 ceramics. Materials Research Bulletin, 2010, 45, 1732-1735.	2.7	28
1049	Influence of Nb on the phase stability of Tiâ€“Alâ€“N. Scripta Materialia, 2010, 63, 807-810.	2.6	44
1050	Nanoscale twinning-induced elastic strengthening in silicon carbide nanowires. Scripta Materialia, 2010, 63, 981-984.	2.6	33
1051	DFT study of hydrogen instability and magnetovolume effects in CeNi. Solid State Sciences, 2010, 12, 59-64.	1.5	9
1052	DFT study of electronic and magnetic structure of perovskite and post-perovskite CaRhO3. Solid State Sciences, 2010, 12, 373-378.	1.5	15
1053	First-principles study of structural, elastic, electronic and optical properties of perovskites XCaH3 (X=Cs and Rb) under pressure. Solid State Sciences, 2010, 12, 587-596.	1.5	22
1054	Structural, elastic, electronic and thermal properties of the cubic perovskite-type BaSnO3. Solid State Sciences, 2010, 12, 630-636.	1.5	49
1055	AMoO4 (AÂ=ÂMg, Ni) molybdates: Phase stabilities, electronic structures and chemical bonding properties from first principles. Solid State Sciences, 2010, 12, 1779-1785.	1.5	37
1056	Phase stability and mechanical properties of rhenium borides by firstâ€principles calculations. Journal of Computational Chemistry, 2010, 31, 1904-1910.	1.5	29
1057	A high-pressure cubic-to-tetragonal phase-transition in melanophlogite, a SiO2 clathrate phase. Microporous and Mesoporous Materials, 2010, 129, 267-273.	2.2	11
1058	First-principles study on phase stability and compression behavior of Ti2SC and Ti2AlC. Physica B: Condensed Matter, 2010, 405, 720-723.	1.3	22
1059	Structural and electronic properties of Er-monopnictides under high pressure. Physica B: Condensed Matter, 2010, 405, 2245-2250.	1.3	14
1060	Pressure-induced structural phase transition and electronic properties of actinide nitrides: Ab initio calculations. Physica B: Condensed Matter, 2010, 405, 3106-3112.	1.3	11
1061	First-principles study on electronic structure and elastic properties of hexagonal Zr2Sc. Physica B: Condensed Matter, 2010, 405, 4294-4298.	1.3	45
1062	On a universal relation for defect data in solids. Physica B: Condensed Matter, 2010, 405, 4320-4322.	1.3	2
1063	Potential existence of post-perovskite nitrides; DFT studies of ThTaN3. Journal of Solid State Chemistry, 2010, 183, 994-999.	1.4	14
1064	Ab-initio calculations of Co-based diluted magnetic semiconductors Cd1âˆ'xCoxX (X=S, Se, Te). Journal of Magnetism and Magnetic Materials, 2010, 322, 3214-3222.	1.0	102
1065	Structural stability of metal hydrides, alanates and borohydrides of alkali and alkali- earth elements: A review. International Journal of Hydrogen Energy, 2010, 35, 5454-5470.	3.8	168

#	Article	IF	Citations
1066	Stability of the hydrides REMgNi4H4 (REÂ=ÂY, Gd) from first principles. International Journal of Hydrogen Energy, 2010, 35, 7858-7865.	3.8	20
1067	Structural stability and optical properties of AlN explored by ab initio calculations. Physica B: Condensed Matter, 2010, 405, 555-558.	1.3	14
1068	Structural, elastic and electronic properties of new antiperovskite-type superconductor from first-principles. Physica B: Condensed Matter, 2010, 405, 1562-1570.	1.3	25
1069	Phase stability, electronic and elastic properties of ScN. Physica B: Condensed Matter, 2010, 405, 2599-2603.	1.3	25
1070	Full-potential calculation of the structural, elastic, electronic and magnetic properties of XFeO3 (X=Sr and Ba) perovskite. Physica B: Condensed Matter, 2010, 405, 3515-3519.	1.3	64
1071	Ab initio study of structural, elastic, electronic and optical properties of spinel SnMg2O4. Physica B: Condensed Matter, 2010, 405, 4079-4085.	1.3	24
1072	Elastic and electronic properties of ScMn2 from first-principles calculations. Physica B: Condensed Matter, 2010, 405, 4812-4817.	1.3	10
1073	First-principles calculations of structural, elastic, electronic and optical properties of XO (X=Ca, Sr) Tj ETQq1 1 0.784314 rgBT /Overlo 92-101.	1.9	27
1074	X-ray diffraction study of -Ca3(PO4)2 at high pressure. Solid State Communications, 2010, 150, 443-445.	0.9	15
1075	A study of the phase transitions, electronic structures and optical properties of under high pressure. Solid State Communications, 2010, 150, 620-624.	0.9	40
1076	The melting curve of perovskite under lower mantle pressures. Solid State Communications, 2010, 150, 590-593.	0.9	9
1077	Theoretical investigations of the physical properties of tetragonal CaSiO3 perovskite. Solid State Communications, 2010, 150, 943-948.	0.9	21
1078	Ab initio investigation of the structural, elastic and electronic properties of the anti-perovskite TlNCa3. Solid State Communications, 2010, 150, 932-937.	0.9	11
1079	Origin of incompressibility and hardness from electronic and mechanical properties of hard material ruthenium diboride. Solid State Communications, 2010, 150, 1095-1098.	0.9	11
1080	Inverse-perovskite oxides with , Ge, Sn, Pb: Structural, elastic and thermal properties. Solid State Communications, 2010, 150, 1995-2000.	0.9	12
1081	Experimental and computational study on the effect of yttrium on the phase stability of sputtered Crâ€“Alâ€“Yâ€“N hard coatings. Acta Materialia, 2010, 58, 2708-2715.	3.8	59
1082	First-principles calculations of the elastic, phonon and thermodynamic properties of Al12Mg17. Acta Materialia, 2010, 58, 4012-4018.	3.8	103
1083	Lattice anisotropy, electronic and chemical structures of uranyl carbonate, UO2CO3, from first principles. Chemical Physics, 2010, 372, 46-50.	0.9	6

#	Article	IF	Citations
1084	Potential existence of postperovskite nitrofluorides: In silico LaZrN2F. Chemical Physics Letters, 2010, 498, 77-80.	1.2	3
1085	Electronic properties of pseudocubic IVâ€“V compounds with 3:4 stoichiometry: Chemical trends. Chemical Physics Letters, 2010, 501, 47-53.	1.2	14
1086	The Highâ€Pressure Characterization of Energetic Materials: Diaminotetrazolium Nitrate (HDATâ€NO₃). Propellants, Explosives, Pyrotechnics, 2010, 35, 24-30.	1.0	5
1087	The Highâ€Pressure Characterization of Energetic Materials: 2â€Methylâ€5â€Nitraminoâ€2Hâ€Tetrazole. Propellants, Explosives, Pyrotechnics, 2010, 35, 550-554.	1.0	3
1088	High-pressure structural and electronic properties of InN. Physica Status Solidi (B): Basic Research, 2010, 247, 313-317.	0.7	6
1089	Density functional calculations of the electronic structure and optical properties of magnesium oxide. Physica Status Solidi (B): Basic Research, 2010, 247, 157-162.	0.7	11
1090	Structural stabilities and electronic and elastic properties of CdO: A first-principles study. Physica Status Solidi (B): Basic Research, 2010, 247, 2202-2206.	0.7	10
1091	Diffusion of platinum adatoms and dimers on Pt(111) surface by molecularâ€dynamics simulation. International Journal of Quantum Chemistry, 2010, 110, 202-209.	1.0	8
1092	Thermodynamics of the Earth's Mantle. Reviews in Mineralogy and Geochemistry, 2010, 71, 465-484.	2.2	19
1093	Stress state of diamond and gold under nonhydrostatic compression to 360 GPa. Journal of Applied Physics, 2010, 108, 063521.	1.1	18
1094	Electronic mechanism for toughness enhancement in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
1102	High-pressure x-ray diffraction study of bulk and nanocrystalline PbMoO4. Journal of Applied Physics, 2010, 108, 073518.	1.1	29
1103	High-pressure phase transitions and compressibility of wolframite-type tungstates. Journal of Applied Physics, 2010, 107, .	1.1	66
1104	First-principles study of phase transition and elastic properties of ScSb and YSb compounds. Phase Transitions, 2010, 83, 450-456.	0.6	3
1105	STRUCTURAL PHASE TRANSITIONS AND MECHANICAL PROPERTIES OF OsO2 UNDER HIGH PRESSURE. International Journal of Modern Physics B, 2010, 24, 4269-4279.	1.0	4
1106	First-principles investigations on structural and elastic properties of CaX (X=S, Se and Te) under high pressure. High Pressure Research, 2010, 30, 310-317.	0.4	20
1107	High pressure study and electronic structure of the super-alloy Hflr₃. Journal of Physics: Conference Series, 2010, 215, 012012.	0.3	3
1108	The influence of hydrogen contamination on the structural stability of CoSn under compression. Journal of Physics Condensed Matter, 2010, 22, 435501.	0.7	3
1109	Equation of state and anharmonicity of carbon dioxide phase I up to 12 GPa and 800 K. Journal of Chemical Physics, 2010, 133, 144501.	1.2	24
1110	Evidence for the existence of a PbCO₃-II phase from high pressure X-ray measurements. Zeitschrift FÃ¼r Kristallographie, 2010, 225, 146-152.	1.1	10
1111	Study of electronic and structural properties of half metallic rare earth mononitrides. Journal of Physics: Conference Series, 2010, 215, 012113.	0.3	2
1112	First-principles study of structural, elastic, electronic and optical properties of perovskites hydrides XLiH₃ (X = Ba and Sr) under pressure. EPJ Applied Physics, 2010, 51, 20302.	0.3	13
1113	Coulomb-potential-dependent decohesion of MagnÃ©li phases. Journal of Physics Condensed Matter, 2010, 22, 292203.	0.7	20
1114	Elasticity, strength, and refractive index of argon at high pressures. Physical Review B, 2010, 81, .	1.1	28
1115	High-pressure x-ray diffraction andab initiostudy of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ni</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Pd</mml:mtext></mml:mrow><mml:mn>2</mml:mn></m. Physical Review B, 2010, 82, .	1.1	91
1116	First-principles study of the mechanical and optical properties of amorphous hydrogenated silicon and silicon-rich silicon oxide. Physical Review B, 2010, 81, .	1.1	24
1117	Deconfinement transition and dimensional crossover in the Bechgaard-Fabre salts: Pressure- and temperature-dependent optical investigations. Physical Review B, 2010, 81, .	1.1	35
1118	Lattice Dynamics and Thermodynamics of Molybdenum from First-Principles Calculations. Journal of Physical Chemistry B, 2010, 114, 298-310.	1.2	39
1119	Synchrotron X-ray Diffraction and Infrared Spectroscopy Studies of C₆₀H₁₈ under High Pressure. Journal of Physical Chemistry Letters, 2010, 1, 714-719.	2.1	8

#	Article	IF	Citations
1120	Siâ^'Ge-based Oxynitrides: From Molecules to Solids. Chemistry of Materials, 2010, 22, 3884-3899.	3.2	9
1121	Structural, elastic, electronic and thermal properties of M2SbP (M = Ti, Zr and Hf). Philosophical Magazine, 2010, 90, 1623-1638.	0.7	0
1122	Pressure-Induced Decomposition of Indium Hydroxide. Journal of the American Chemical Society, 2010, 132, 12674-12678.	6.6	9
1123	Force-matched embedded-atom method potential for niobium. Physical Review B, 2010, 81, .	1.1	120
1124	Structural, electronic and thermo-elastic properties of Cu6Sn5 and Cu5Zn8 intermetallic compounds: First-principles investigation. Intermetallics, 2010, 18, 922-928.	1.8	40
1125	Ab-initio determination of X-ray structure factors and the Compton profiles of CdO. Journal of Alloys and Compounds, 2010, 501, 136-142.	2.8	8
1126	First-principles study of the structural, elastic and electronic properties of the anti-perovskites SnBSc3 and PbBSc3. Journal of Alloys and Compounds, 2010, 504, 296-302.	2.8	15
1127	First-principles study of elastic and electronic properties of MgZn2 and ScZn2 phases in Mgâ€"Scâ€"Zn alloy. Journal of Alloys and Compounds, 2010, 506, 412-417.	2.8	135
1128	First-principles study of spin-polarized electronic band structures in ferromagnetic Zn1â^'xTMxS (TM=Fe, Co and Ni). Journal of Alloys and Compounds, 2010, 508, 245-250.	2.8	50
1129	High-pressure behavior of otavite (CdCO3). Journal of Alloys and Compounds, 2010, 508, 251-257.	2.8	28
1130	Structure, thermodynamics, and diffusion in CaAl2Si2O8 liquid from first-principles molecular dynamics. Geochimica Et Cosmochimica Acta, 2010, 74, 5657-5671.	1.6	59
1131	High-pressure phase relations in the composition of albite NaAlSi3O8 constrained by an ab initio and quasi-harmonic Debye model, and their implications. Earth and Planetary Science Letters, 2010, 298, 427-433.	1.8	18
1132	First principles studies of phase stability, electronic and elastic properties in BBi compound. Computational Materials Science, 2010, 47, 968-972.	1.4	27
1133	First-principles investigations on electronic and elastic properties of YX (X=N, P, As and Sb) under high pressure. Computational Materials Science, 2010, 48, 59-64.	1.4	25
1134	First-principles thermodynamics from phonon and Debye model: Application to Ni and Ni3Al. Computational Materials Science, 2010, 47, 1040-1048.	1.4	357
1135	Structural stabilities, electronic and elastic properties for LaSb: A first-principles study. Computational Materials Science, 2010, 47, 1060-1063.	1.4	3
1136	Structural, elastic and electronic properties of the hexagonal anti-perovskites SbNBa3 and BiNBa3. Computational Materials Science, 2010, 48, 711-718.	1.4	22
1137	Electronic and structural properties of Î³-Be3N2 by LCAO method. Computational Materials Science, 2010, 49, S268-S271.	1.4	3

#	Article	IF	Citations
1138	Theoretical prediction of the elastic, electronic and optical properties of the filled tetrahedral semiconductor Î±-LiMgSb. Computational Materials Science, 2010, 49, 64-69.	1.4	19
1139	Theoretical study of electronic, magnetic and structural properties of Mo and W based group V (N, P,) Tj ETQq1 1 0.784314 rgBT /Ove	1.4	26
1140	First-principles study of structural stabilities, electronic and elastic properties of BaF2 under high pressure. Computational Materials Science, 2010, 49, 530-534.	1.4	12
1141	First-principles study on the structural stabilities, electronic and elastic properties for zirconium under pressure. Computational Materials Science, 2010, 50, 179-183.	1.4	20
1142	Pâ¿¢Vâ¿¢T relation of MgO derived by simultaneous elastic wave velocity and in situ X-ray measurements: A new pressure scale for the mantle transition region. Physics of the Earth and Planetary Interiors, 2010, 183, 196-211.	0.7	113
1143	The isothermal equation of state of CaPtO3 post-perovskite to 40GPa. Physics of the Earth and Planetary Interiors, 2010, 182, 113-118.	0.7	12
1144	Equation of state (EOS) and collapse of magnetism in iron-rich meteorites at high pressure by first-principles calculations. Physics of the Earth and Planetary Interiors, 2010, 182, 175-178.	0.7	5
1145	Pressure-induced phase transition in defect Chalcopyrites HgAl2Se4 and CdAl2S4. Journal of Physics and Chemistry of Solids, 2010, 71, 832-835.	1.9	33
1146	A simple thermodynamic description of the combined Einstein and elastic models. Journal of Physics Condensed Matter, 2010, 22, 425401.	0.7	8
1147	Pressure-induced phase transition in cubic Lu2O3. Journal of Applied Physics, 2010, 108, .	1.1	39
1148	First-Principles Prediction on the High-Pressure Structures of Transition Metal Diborides (TMB₂, TM = Sc, Ti, Y, Zr). Inorganic Chemistry, 2010, 49, 6859-6864.	1.9	41
1149	Ab initiothermodynamics beyond the quasiharmonic approximation: W as a prototype. Physical Review B, 2010, 81, .	1.1	20
1150	First-principles investigations on electronic, elastic and optical properties of XC (X=Si, Ge, and Sn) under high pressure. Journal of Applied Physics, 2010, 108, .	1.1	78
1151	Compressibility of cubic white, orthorhombic black, rhombohedral black, and simple cubic black phosphorus. Physical Review B, 2010, 82, .	1.1	36
1152	Phase stability and mechanical properties of tungsten borides from first principles calculations. Physical Chemistry Chemical Physics, 2010, 12, 13158.	1.3	126
1153	INVESTIGATION OF STRUCTURAL PHASE TRANSFORMATION IN HALF METALLIC FERROMAGNETIC EuN UNDER PRESSURE. International Journal of Modern Physics B, 2011, 25, 851-862.	1.0	2
1154	Phase transformation of Ho2O3 at high pressure. Journal of Applied Physics, 2011, 110, .	1.1	36
1155	High-pressure synchrotron X-ray diffraction study of the pyrochlores: Ho₂Ti₂O₇, Y₂Ti₂O₇and Tb₂Ti₂O₇. High Pressure Research, 2011, 31, 219-227.	0.4	22

#	Article	IF	Citations
1156	Pressure-induced structural phase transition and electronic properties of RESb (REâ€‰=â€‰Ho, Er and Tm) compounds:ab initiocalculations. Phase Transitions, 2011, 84, 603-612.	0.6	7
1157	Pressure-Induced Phase Transitions of C₇₀ Nanotubes. Journal of Physical Chemistry C, 2011, 115, 8918-8922.	1.5	31
1158	Elasticity and anisotropy of Fe3C at high pressures. American Mineralogist, 2011, 96, 1530-1536.	0.9	44
1159	Ab initiostudy of Heusler alloys Co₂XY (Xâ€‰=â€‰Cr, Mn, Fe; Yâ€‰=â€‰Al,â€‰Ga) under high pressure. Philosophical Magazine Letters, 2011, 91, 545-553.	0.5	44
1160	Superhard phases of B2O: An isoelectronic compound of diamond. Diamond and Related Materials, 2011, 20, 501-504.	1.8	16
1161	Tungsten tetraboride, an inexpensive superhard material. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10958-10962.	3.3	299
1162	First-principles calculations of structural and electronic properties of Ta-doped Si clusters, wires, and bulk systems. Physical Review B, 2011, 83, .	1.1	27
1163	First-principles investigation of the electronic, elastic and thermodynamic properties of VC under high pressure. Chinese Physics B, 2011, 20, 047103.	0.7	14
1164	Anomalous sound velocities in polycrystalline MgO under non-hydrostatic compression. Geophysical Research Letters, 2011, 38, n/a-n/a.	1.5	10
1165	Trench parallel anisotropy and large delay times: Elasticity and anisotropy of antigorite at high pressures. Geophysical Research Letters, 2011, 38, .	1.5	65
1166	Mid-mantle anisotropy: Elasticity of aluminous phases in subducted MORB. Geophysical Research Letters, 2011, 38, n/a-n/a.	1.5	22
1167	Pressure-induced structural transitions in europium to 92 GPa. Physical Review B, 2011, 83, .	1.1	33
1168	Direct observation of the influence of the As-Fe-As angle on the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>T</mml:mi><mml:mrow><mml:mi>c</mml:mi></mml:mrow></mml:msub></mml:m superconducting SmFeAsO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:m	1.1	28
1169	Compressibility of Fe_{1.087}Te: a high pressure X-ray diffraction study. High Pressure Research, 2011, 31, 603-610.	0.4	7
1170	Phase-field-crystal methodology for modeling of structural transformations. Physical Review E, 2011, 83, 031601.	0.8	107
1171	Thermo-physical properties of LiH at high pressures by ab initio calculations. Journal of Applied Physics, 2011, 109, 103515.	1.1	16
1172	First-principles investigation of electronic, vibrational, elastic, and structural properties of ThN and UN up to 100 GPa. Physical Review B, 2011, 84, .	1.1	46
1173	High-pressure structural phase transitions and mechanical properties of calcite rock. Computational Materials Science, 2011, 50, 852-857.	1.4	28

#	Article	IF	Citations
1174	Ab initio calculation of vibrational and thermodynamic properties of SrX (S, Se, Te) in the B1 (NaCl) and B2 (CsCl) structures. Computational Materials Science, 2011, 50, 1701-1710.	1.4	36
1175	Study of structural, elastic and electronic properties of GdX (X=Bi, Sb) compounds using LSDA and LSDA+U approach. Computational Materials Science, 2011, 50, 1965-1972.	1.4	10
1176	Dependence of pressure on elastic, electronic and optical properties of CeO2 and ThO2: A first principles study. Computational Materials Science, 2011, 50, 2280-2286.	1.4	36
1177	Study of the hydrostatic pressure on orthorhombic IVâ€“VI compounds including many-body effects. Computational Materials Science, 2011, 50, 2872-2879.	1.4	40
1178	Ab initio study of AlCu2M (M=Sc, Ti and Cr) ternary compounds under pressures. Computational Materials Science, 2011, 50, 2930-2937.	1.4	21
1179	First-principles calculations of mechanical and thermodynamic properties of YAlO3. Computational Materials Science, 2011, 50, 3056-3062.	1.4	38
1180	Structural, electronic, elastic and thermodynamic properties of AlSi2RE (RE=La, Ce, Pr and Nd) from first-principle calculations. Computational Materials Science, 2011, 50, 3303-3310.	1.4	11
1181	Equations of state in solids: Fitting theoretical data, possibly including noise and jumps. Computational and Theoretical Chemistry, 2011, 975, 111-115.	1.1	13
1182	Stability of the C14 Laves phase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si11.gif" display="inline" overflow="scroll"><mml:msub><mml:mrow><mml:mstyle mathvariant="normal"><mml:mi>(Fe,Si)</mml:mi></mml:mstyle></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si12.gif" display="inline" overflow="scroll"><mml:mstyle mathvariant="normal"><mml:mi>Mo</mml:mi></mml:mstyle></mml:math> from ab initio calculations. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 492-498.	0.7	11
1183	Structural, elastic and electronic properties of Mg(Cu1â^'xZnx)2 alloys calculated by first-principles. Journal of Alloys and Compounds, 2011, 509, 2885-2890.	2.8	22
1184	Density functional study of the structural, electronic, elastic and thermodynamic properties of ACRu3 (AÂ=ÂV, Nb and Ta) compounds. Intermetallics, 2011, 19, 476-485.	1.8	24
1185	Phase stability of Heusler compound Co2FeSi under pressure: An in-situ x-ray diffraction investigation. Journal of Applied Physics, 2011, 110, .	1.1	11
1186	High-pressure equation of state properties of bismuth oxide. Journal of Applied Physics, 2011, 110, .	1.1	14
1187	FIRST PRINCIPLES STUDY OF THE STRUCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF Ti₂InC and Ti₂InN. Modern Physics Letters B, 2011, 25, 747-761.	1.0	16
1188	Novel Pressure-Induced Structural Transformations of Inorganic Nanowires. , 0, , .		0
1189	Compressibility of CaMnO₃: A study using a large-volume diffraction press. Powder Diffraction, 2011, 26, 262-266.	0.4	8
1190	Thermodynamics of mantle minerals - II. Phase equilibria. Geophysical Journal International, 2011, 184, 1180-1213.	1.0	475
1191	Structural, elastic, electronic, optical and thermodynamic properties of KMgH3. Solid State Sciences, 2011, 13, 647-652.	1.5	12

#	Article	IF	Citations
1192	Ab initio investigations of the perovskite and K2NiF4 phases in the Csâ€“Caâ€“H system. Solid State Sciences, 2011, 13, 569-573.	1.5	3
1193	Ab initio investigations of the Ca2IrO4-type structure as a â€œpost-K2NiF4â€• Case study of Na2OsO4. Solid State Sciences, 2011, 13, 1396-1400.	1.5	8
1194	Theoretical prediction of the structural, elastic, electronic and optical properties of Zr3N4 and Hf3N4 compounds. Solid State Sciences, 2011, 13, 1414-1419.	1.5	16
1195	Band parameters of Î±-LiBeN semiconductor from density functional calculations. Superlattices and Microstructures, 2011, 50, 319-330.	1.4	2
1196	A pressure-induced amorphous phase transition in magnesium-substituted -tricalcium phosphate. Solid State Communications, 2011, 151, 1609-1611.	0.9	7
1197	First-principles studies on Ti3Si0.5Ge0.5C2 under pressure. Solid State Communications, 2011, 151, 1564-1567.	0.9	2
1198	First-principles calculations of structural and thermodynamic properties of Y 3Al5O12. Solid State Communications, 2011, 151, 1559-1563.	0.9	13
1199	Anisotropic behavior of energetic materials at elevated pressure and temperature. Journal of Loss Prevention in the Process Industries, 2011, 24, 805-805.	1.7	2
1200	Î³â€²-ZnFe3N thin films: A proposal for a moderately ductile, corrosion-protective coating on steel. Scripta Materialia, 2011, 65, 380-383.	2.6	8
1201	Extending the rule of mixture to the sub unit-cell level. Scripta Materialia, 2011, 65, 735-738.	2.6	12
1202	First-principles investigations on electronic, elastic and thermodynamic properties of ZrC and ZrN under high pressure. Materials Chemistry and Physics, 2011, 129, 99-104.	2.0	57
1203	Determination of the bulk modulus of hydroxycancrinite, a possible zeolitic precursor in geopolymers, by high-pressure synchrotron X-ray diffraction. Cement and Concrete Composites, 2011, 33, 1014-1019.	4.6	19
1204	The effect of crystallite size and stress condition on the equation of state of nanocrystalline MgO. Journal of Applied Physics, 2011, 110, .	1.1	14
1205	In situ high-pressure synchrotron x-ray diffraction study of CeVO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>and TbVO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>up to 50 GPa. Physical Review B, 2011, 84, .	1.1	62
1206	Pressure-induced phase transitions in AgClO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2011, 84, .	1.1	21
1207	High-pressure x-ray diffraction study of CdMoO4 and EuMoO4. Journal of Applied Physics, 2011, 109, 043510-043510-5.	1.1	30
1208	Optimizing the composition and properties of nanostructural coatings for cutting tools on the basis of the electron-density functional. Russian Engineering Research, 2011, 31, 458-464.	0.2	6
1209	Pressure effect on crystal structure and superconductivity of La_{0.8}Th_{0.2}FeAsO. Physica Status Solidi - Rapid Research Letters, 2011, 5, 208-210.	1.2	0

#	Article	IF	Citations
1210	The Gruneisen parameter for silver azide. Russian Physics Journal, 2011, 54, 765-772.	0.2	2
1211	Ab initio study of ultra-incompressible ternary BeCN2 polymorph. Journal of Physics and Chemistry of Solids, 2011, 72, 667-672.	1.9	12
1212	Supertoughening in B1 transition metal nitride alloys by increased valence electron concentration. Acta Materialia, 2011, 59, 2121-2134.	3.8	166
1213	Structural and electronic properties of bulk GaP and AlP and their superlattices. Superlattices and Microstructures, 2011, 49, 132-143.	1.4	18
1214	Inverted equations of state for solids under high pressures. Indian Journal of Physics, 2011, 85, 1341-1366.	0.9	13
1215	Theoretical Study of Electronic Structure and Thermoelectric Properties of Doped CuAlO2. Journal of Electronic Materials, 2011, 40, 987-991.	1.0	13
1216	Cr-Doped IIIâ€“V Nitrides: Potential Candidates for Spintronics. Journal of Electronic Materials, 2011, 40, 1428-1436.	1.0	43
1217	Thermoelastic properties and crystal structure of CaPtO₃post-perovskite from 0 to 9â€…GPa and from 2Âto 973â€…K. Journal of Applied Crystallography, 2011, 44, 999-1016.	1.9	10
1218	High-pressure experimental study on Rb₂S: antifluorite to Ni₂In-type phase transitions. Acta Crystallographica Section B: Structural Science, 2011, 67, 109-115.	1.8	38
1219	Xâ€ray diffraction of cubic Gd₂O₃/Er under high pressure. Physica Status Solidi (B): Basic Research, 2011, 248, 1123-1127.	0.7	18
1220	Electronic structure, effective masses, mechanical and thermoâ€acoustic properties of cubic HfO₂ under pressure. Physica Status Solidi (B): Basic Research, 2011, 248, 950-955.	0.7	6
1221	Structural and mechanical properties of dolomite rock under high pressure conditions: A firstâ€principles study. Physica Status Solidi (B): Basic Research, 2011, 248, 1894-1900.	0.7	18
1222	First principles study of structural, elastic, electronic and optical properties of Nb₂N and Ta₂N compounds. Physica Status Solidi (B): Basic Research, 2011, 248, 2787-2792.	0.7	13
1223	The High-Pressure Characterization of Energetic Materials: 1,4-Dimethyl-5-Aminotetrazolium 5-Nitrotetrazolate. Propellants, Explosives, Pyrotechnics, 2011, 36, 446-450.	1.0	5
1224	Bulk modulus of basic sodalite, Na8[AlSiO4]6(OH)2Â·2H2O, a possible zeolitic precursor in coal-fly-ash-based geopolymers. Cement and Concrete Research, 2011, 41, 107-112.	4.6	29
1225	Pressure induced reactions amongst calcium aluminate hydrate phases. Cement and Concrete Research, 2011, 41, 571-578.	4.6	37
1226	Gibbs2: A new version of the quasi-harmonic model code. I. Robust treatment of the static data. Computer Physics Communications, 2011, 182, 1708-1720.	3.0	299
1227	First principles study of Ca2PtO4 in K2NiF4 and â€˜post-K2NiF4â€™ type structures. Chemical Physics Letters, 2011, 503, 49-52.	1.2	2

#	Article	IF	Citations
1228	Electronic structure and equation of state of PdO2 from ab initio. Chemical Physics Letters, 2011, 508, 215-218.	1.2	21
1229	Electronic and thermodynamic properties of B2-FeSi from first principles. Physica B: Condensed Matter, 2011, 406, 363-367.	1.3	16
1230	Electronic and thermal properties of B2-type AlRE intermetallic compounds: A first principles study. Physica B: Condensed Matter, 2011, 406, 449-455.	1.3	10
1231	First-principles study on alloying stability, electronic structure, and mechanical properties of Al-based intermetallics. Physica B: Condensed Matter, 2011, 406, 1149-1153.	1.3	26
1232	First-principles study of the structural, elastic, electronic and optical properties of the monoclinic BiScO3. Physica B: Condensed Matter, 2011, 406, 2028-2032.	1.3	14
1233	First-principles study of structural stability, electronic and elastic properties of ZrC compounds. Physica B: Condensed Matter, 2011, 406, 2750-2754.	1.3	34
1234	Structural parameters, electronic structures, elastic stiffness and thermal properties of M2PC (M=V,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.3	15
1235	Pressure induced structural phase transition and electronic properties of actinide monophospides: Ab-initio calculations. Physica B: Condensed Matter, 2011, 406, 3175-3179.	1.3	6
1236	Electronic structure of (BP)n/(BAs)n (001) superlattices. Physica B: Condensed Matter, 2011, 406, 3247-3255.	1.3	22
1237	Half metallic Co2TiGeâ€"a theoretical and experimental investigation. Journal of Magnetism and Magnetic Materials, 2011, 323, 22-27.	1.0	21
1238	Half-metallic ferromagnetism in (C, Si, Ge, Sn and Pb)-doped I2â€"VI compounds: An ab initio study. Journal of Physics and Chemistry of Solids, 2011, 72, 227-232.	1.9	7
1239	High pressure investigation on double perovskite Ba2MgWO6. Journal of Physics and Chemistry of Solids, 2011, 72, 609-612.	1.9	25
1240	Structural transition of Ti3SiC2 under high hydrostatic pressure: A first-principles study. Journal of Physics and Chemistry of Solids, 2011, 72, 740-743.	1.9	3
1241	Ground state and lattice dynamical study of ionic conductors CaF2, SrF2 and BaF2 using density functional theory. Journal of Physics and Chemistry of Solids, 2011, 72, 934-939.	1.9	20
1242	Effect of high hydrostatic pressure on structural stability of Ti3GeC2: A first-principles investigation. Journal of Solid State Chemistry, 2011, 184, 786-789.	1.4	8
1243	Theoretical investigation of new type of ternary magnesium alloys AMgNi4 (A=Y, La, Ce, Pr and Nd). Physica B: Condensed Matter, 2011, 406, 1330-1335.	1.3	20
1244	High-pressure phase transitions of Mg2Ge and Mg2Sn: First-principles calculations. Physica B: Condensed Matter, 2011, 406, 1789-1794.	1.3	20
1245	First-principles study of structural, electronic and elastic properties of single crystal CuZr. Physica B: Condensed Matter, 2011, 406, 3389-3391.	1.3	8

#	Article	IF	Citations
1246	Theoretical study of the structural, elastic, electronic and thermal properties of the MAX phase Nb2SiC. Solid State Communications, 2011, 151, 382-387.	0.9	15
1247	First-principles studies of the electronic and elastic properties of Ti2GeC. Solid State Communications, 2011, 151, 491-494.	0.9	7
1248	Half-metallic ferromagnetism in I2â€“VI compounds with non-magnetic dopants. Solid State Communications, 2011, 151, 1169-1174.	0.9	5
1249	Prediction study of the elastic and thermodynamic properties of the newly discovered tetragonal SrPd2Ge2 phase. Solid State Communications, 2011, 151, 976-981.	0.9	2
1250	First-principles study on the crystal, electronic structure and mechanical properties of hexagonal Al3RE (RE = La, Ce, Pr, Nd, Sm, Gd) intermetallic compounds. Solid State Communications, 2011, 151, 1135-1140.	0.9	17
1251	Structure and mechanical properties of TiAlNâ€“WNx thin films. Surface and Coatings Technology, 2011, 205, 4821-4827.	2.2	47
1252	Elastic Tensor and Thermodynamic Property of Magnesium Silicate Perovskite from First-principles Calculations. Chinese Journal of Chemical Physics, 2011, 24, 703-710.	0.6	11
1253	Study of the structural, elastic and electronic properties of ordered Ca(Mg1â^'xLix)2alloys from first-principles calculations. Physica Scripta, 2011, 84, 055603.	1.2	4
1254	Anisotropic exchange interaction between nonmagnetic europium cations in Eu<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>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2011, 84, .	1.1	22
1255	Comparative in situ X-ray diffraction study of San Carlos olivine: Influence of water on the 410 km seismic velocity jump in Earth's mantle. American Mineralogist, 2011, 96, 697-702.	0.9	10
1256	Thermodynamic and mechanical stabilities of Î³â€²-Ir3(Al,W). Journal of Applied Physics, 2011, 109, 023504.	1.1	14
1257	Experimental and theoretical study of structural properties and phase transitions in YAsO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>and YCrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>	1.1	43
1258	Structural and thermodynamic properties of compressed palladium:Ab initioand molecular dynamics study. Physical Review B, 2011, 83, .	1.1	38
1259	AB INITIO ELECTRONIC STRUCTURE CALCULATIONS OF HALF-METALLIC FERROMAGNETISM IN CALCIUM CHALCOGENIDES DOPED WITH B, C AND N. Modern Physics Letters B, 2011, 25, 1537-1548.	1.0	10
1260	Equations of state of 2,6-diamino-3,5-dinitropyrazine-1-oxide. Journal of Applied Physics, 2011, 110, .	1.1	30
1261	Treatment of first-principles data for predictive quasiharmonic thermodynamics of solids: The case of MgO. Physical Review B, 2011, 84, .	1.1	39
1262	Effects of hydrostatic pressure on the electrical properties of hexagonal Ge2Sb2Te5: Experimental and theoretical approaches. Applied Physics Letters, 2011, 98, .	1.5	10
1263	Strength and elasticity of niobium under high pressure. Journal of Applied Physics, 2011, 109, 113539.	1.1	29

#	Article	IF	Citations
1264	Ab initio investigation of structural, electronic, mechanical, and thermodynamic properties of AlSc2 intermetallic compound under pressure. Journal of Applied Physics, 2011, 110, 033533.	1.1	16
1265	New accurate elastic parameters for the forsterite-fayalite solid solution. American Mineralogist, 2011, 96, 1742-1747.	0.9	33
1266	Elastic and Electronic Properties of Mg₂Ca and Mg₂Y Phases. Advanced Materials Research, 0, 233-235, 2231-2238.	0.3	3
1267	Phase field modeling of twinning in indentation of transparent crystals. Modelling and Simulation in Materials Science and Engineering, 2011, 19, 085005.	0.8	51
1268	A first-principles study of the phase transition from Holl-I to Holl-II in the composition KAlSi3O8. American Mineralogist, 2011, 96, 974-982.	0.9	14
1269	Ab initio study of the electronic structure and elastic properties of Al 5 C 3 N. Chinese Physics B, 2011, 20, 126201.	0.7	5
1270	High Pressure X-Ray Diffraction Study of a Grossularâ€"Andradite Solid Solution and the Bulk Modulus Variation along this Solid Solution. Chinese Physics Letters, 2011, 28, 076101.	1.3	9
1271	First-Principles Calculations of Structural, Elastic and Electronic Properties of Tetragonal HfO ₂ under Pressure. Communications in Theoretical Physics, 2011, 56, 779-784.	1.1	7
1272	First-Principles Investigations on Electronic, Elastic and Thermodynamic Properties of VN under High Pressure. Advanced Materials Research, 2012, 550-553, 2805-2809.	0.3	2
1273	Correlation between superconductivity and structural properties under high pressure of iron pnictide superconductor Ce_{0.6}Y_{0.4}FeAsO_{0.8}F_{0.2}. Applied Physics Letters, 2012, 100, 052601.	1.5	2
1274	Elasticity and high-pressure structure of arsenoflorencite-(La): insights into the high-pressure behaviour of the alunite supergroup. Mineralogical Magazine, 2012, 76, 975-985.	0.6	3
1275	Vibrational and elastic properties of ferromagnesite across the electronic spin-pairing transition of iron. American Mineralogist, 2012, 97, 583-591.	0.9	64
1276	STRUCTURAL PHASE TRANSITION, ELASTIC AND ELECTRONIC PROPERTIES OF CuXSe2(X = In, Ga) CHALCOPYRITE. Surface Review and Letters, 2012, 19, 1250021.	0.5	4
1277	The effects of composition upon the high-pressure behaviour of amphiboles: compression of gedrite to 7 GPa and a comparison with anthophyllite and proto-amphibole. Mineralogical Magazine, 2012, 76, 987-995.	0.6	9
1278	Pressure induced phase transition in defect chalcopyrite compounds. Journal of Physics: Conference Series, 2012, 377, 012024.	0.3	0
1279	Structural and chemical properties of the nitrogen-rich energetic material triaminoguanidinium 1-methyl-5-nitriminotetrazolate under pressure. Journal of Chemical Physics, 2012, 137, 054501.	1.2	15
1280	Study of phase transition and cohesive energy in MgO. Journal of Physics: Conference Series, 2012, 377, 012067.	0.3	8
1281	High pressure transport, structural, and first principles investigations on the fluorite structured intermetallic, PtAl2. Journal of Applied Physics, 2012, 111, .	1.1	2

#	Anharmonic phonons of NaZr<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>(PO<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 747 Td (xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mml:	IF	Citations
1282		1.1	43
1283	New high-pressure phase and equation of state of Ce2Zr2O8. Journal of Applied Physics, 2012, 111, .	1.1	23
1284	Simultaneous sound velocity and density measurements of NaCl at high temperatures and pressures: Application as a primary pressure standard. American Mineralogist, 2012, 97, 1670-1675.	0.9	48
1285	Pressure-induced structural change of intermediate-range order in poly(4-methyl-1-pentene) melt. Physical Review E, 2012, 85, 021807.	0.8	21
1286	First-principles study of B1 to B2 phase transition in PbS. Journal of Physics: Conference Series, 2012, 377, 012068.	0.3	5
1287	Strength of solid helium under high pressure. Journal of Physics: Conference Series, 2012, 377, 012007.	0.3	9
1288	Strength of rhenium from x-ray diffraction experiments under nonhydrostatic compression to 250 GPa. Journal of Physics: Conference Series, 2012, 377, 012008.	0.3	12
1289	A new probabilistic tool for the determination and optimization of multiphase equation of state parameters: Application to tin. EPJ Web of Conferences, 2012, 26, 04024.	0.1	1
1290	Structural and electronic properties of Cd-rich lanthanide intermetallics. Journal of Physics: Conference Series, 2012, 377, 012081.	0.3	4
1291	High - pressure synchrotron x-ray diffraction study of RMnO₃(R = Eu, Gd, Tb and Dy) upto 50 GPa. Journal of Physics: Conference Series, 2012, 377, 012025.	0.3	9
1292	Energetics, equation of state, and elasticity of NAL phase: Potential host for alkali and aluminum in the lower mantle. Geophysical Research Letters, 2012, 39, .	1.5	19
1293	Mechanism of Morphology Transformation of Tetragonal Phase LaVO₄ Nanocrystals Controlled by Surface Chemistry: Experimental and Theoretical Insights. Crystal Growth and Design, 2012, 12, 5042-5050.	1.4	22
1294	Dynamical stability and phase transition of ZrC under pressure. Phase Transitions, 2012, 85, 1060-1069.	0.6	14
1295	Effects of surface chemistry on the morphology transformation of ZnWO₄nanocrystals: investigated from experiment and theoretical calculations. CrystEngComm, 2012, 14, 920-928.	1.3	14
1296	High Pressure Structural Studies on Rare-Earth Sesquioxides. Journal of Physics: Conference Series, 2012, 377, 012015.	0.3	19
1297	Phase transformation in hexagonal ErMnO3 under high pressure. Journal of Applied Physics, 2012, 112, 113512.	1.1	13
1298	First-principles investigation of structural and electronic properties of MgCu2 Laves phase under pressure. Intermetallics, 2012, 31, 257-263.	1.8	97
1299	First-principles study on the structure, elastic and electronic properties of hexagonal HfPtAl under pressure. Solid State Communications, 2012, 152, 462-465.	0.9	0

#	Article	IF	Citations
1300	Derivation of the isothermal equation of state of carbon monoxide to 50GPa. Chemical Physics Letters, 2012, 546, 86-89.	1.2	0
1301	Phase stability, elastic, electronic, thermal and optical properties of Ti3Al1â^'xSixC2 (0â‰¤xâ‰¤1): First principle study. Physica B: Condensed Matter, 2012, 407, 4221-4228.	1.3	38
1302	First principles investigations of the electronic structure and chemical bonding of U3Si2C2 â€“ A uranium silicideâ€“carbide with the rare [SiC] unit. Chemical Physics Letters, 2012, 550, 88-93.	1.2	5
1303	Influence of magnetic ordering on the elastic properties of PdFe3N. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2012, 30, .	0.9	4
1304	Compressibility and structural stability of nanoparticulate goethite. RSC Advances, 2012, 2, 6768.	1.7	6
1305	Pressure-induced phase transition study of magnesiochromite (MgCr2O4) by Raman spectroscopy and X-ray diffraction. Physics of the Earth and Planetary Interiors, 2012, 196-197, 75-82.	0.7	50
1306	Ab initio study of some fundamental properties of the M3X (M=Cr, V; X=Si, Ge) compounds. Physica B: Condensed Matter, 2012, 407, 3591-3595.	1.3	4
1307	First-principles investigation of the ternary scandium based inverse-perovskite carbides Sc3AC (AÂ=ÂAl,) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	22
1308	Pressure-dependent structure, mechanical and thermodynamic properties of tetragonal AsTiZr arsenide: A density functional theory study. Solid State Communications, 2012, 152, 1694-1699.	0.9	1
1309	Intercomparison of pressure standards (Au, Pt, Mo, MgO, NaCl and Ne) to 2.5 Mbar. Journal of Geophysical Research, 2012, 117, .	3.3	61
1310	An X-ray diffraction study of pressure-induced phase transitions in Bi2MoO6. Journal of Solid State Chemistry, 2012, 194, 15-18.	1.4	10
1311	Structural, electronic and mechanical properties of RuO2 from first-principles calculations. Materials Science in Semiconductor Processing, 2012, 15, 331-339.	1.9	25
1312	Dimorphic LaPdSn and ErAgSn â€“ A first principles study. Intermetallics, 2012, 20, 33-38.	1.8	5
1313	First principles study of structural, electronic and elastic properties of cubic and orthorhombic RhSi. Intermetallics, 2012, 26, 150-156.	1.8	26
1314	Compressibility and structural stability of CeN from experiment and theory. The B1â€“B2 transition. Journal of Alloys and Compounds, 2012, 533, 29-32.	2.8	18
1315	The elasticity of lawsonite at high pressure and the origin of low velocity layers in subduction zones. Earth and Planetary Science Letters, 2012, 349-350, 116-125.	1.8	35
1316	First-principles thermal equation of state of tungsten carbide. Computational Materials Science, 2012, 59, 41-47.	1.4	16
1317	Ab initio study of the effect of Zr content on elastic and electronic properties of L12â€“Al3(Sc1â^'xZrx) alloys. Computational Materials Science, 2012, 59, 87-93.	1.4	22

#	Article	IF	Citations
1318	First-principles investigations on the crystal, electronic structure and mechanical properties of AlCr2 compound at varying pressures. Computational Materials Science, 2012, 61, 140-144.	1.4	4
1319	Elastic, thermodynamic, electronic and optical properties of U2Ti. Computational Materials Science, 2012, 63, 256-260.	1.4	18
1320	Structural, elastic, electronic, chemical bonding and thermodynamic properties of CaMg2N2 and SrMg2N2: First-principles calculations. Computational Materials Science, 2012, 53, 204-213.	1.4	12
1321	First-principles study of phase transition and elastic properties of XBi (X=Ce, Pr) compounds. Computational Materials Science, 2012, 53, 75-78.	1.4	2
1322	On the electronic nature of silicon and germanium based oxynitrides and their related mechanical, optical and vibrational properties as obtained from DFT and DFPT. Computational Materials Science, 2012, 53, 158-168.	1.4	9
1323	Theory study of structural parameters, elastic stiffness, electronic structures and lattice dynamics of RBRh3 (R=Sc, Y, La and Lu). Computational Materials Science, 2012, 54, 336-344.	1.4	4
1324	The structure, elastic, electronic properties and Debye temperature of M2AlC (MV, Nb and Ta) under pressure from first-principles. Computational Materials Science, 2012, 54, 16-22.	1.4	39
1325	Half-metallic ferromagnetism in alkaline earth selenides by first principles calculations. Computational Materials Science, 2012, 54, 219-226.	1.4	15
1326	Pressure dependence of structural, electronic, elastic and thermodynamic behaviors of AlY2: A first principles study. Computational Materials Science, 2012, 58, 17-23.	1.4	8
1327	Structural, electronic, elastic and thermodynamic properties of CaAl2Zn2 compound under different pressures. Computational Materials Science, 2012, 59, 33-40.	1.4	3
1328	The electronic and optical properties of the fluoroperovskite BaXF3 (X=Li, Na, K, and Rb) compounds. Computational Materials Science, 2012, 59, 6-13.	1.4	51
1329	First-Principles Calculations of Clean and Defected ZnO Surfaces. Journal of Physical Chemistry C, 2012, 116, 21391-21400.	1.5	33
1330	Crystal structure and electronic properties of the new structure dinitrideâ€“nitride N₂MN (M: Cu, Ag). Physica Status Solidi (B): Basic Research, 2012, 249, 2096-2107.	0.7	3
1331	First-principles study of the crystal structure and equation of state of naphthaline and anthracene. Journal of Structural Chemistry, 2012, 53, 417-423.	0.3	12
1332	First-principles study of elastic and structural properties of Zr3Al3C5. European Physical Journal B, 2012, 85, 1.	0.6	5
1333	Rare earth rhodium borides RRh3B (R = Y, Zr, and Nb): mechanical, thermal and optical properties. European Physical Journal B, 2012, 85, 1.	0.6	20
1334	Effect of nanostructuration on compressibility of cubic BN. Journal of Superhard Materials, 2012, 34, 336-338.	0.5	6
1335	From soft to superhard: Fifty years of experiments on cold-compressed graphite. Journal of Superhard Materials, 2012, 34, 360-370.	0.5	22

#	Article	IF	Citations
1336	Firstâ€principles study of highâ€pressure elasticity of CFâ€•and CTâ€structure MgAl₂O₄. Geophysical Research Letters, 2012, 39, .	1.5	2
1337	Multiâ€technique equation of state for Fe₂SiO₄melt and the density of Feâ€bearing silicate melts from 0 to 161 GPa. Journal of Geophysical Research, 2012, 117, .	3.3	76
1338	MAX phases Nb2AC (A=S, Sn): An ab initio study. Computational Materials Science, 2012, 65, 365-371.	1.4	22
1339	Ab initio investigations of structural, elastic and electronic properties of ZnSiP2: Pressure effect. Computational Materials Science, 2012, 65, 520-527.	1.4	29
1340	The low velocity layer in subduction zone: Structure and elasticity of glaucophane at high pressures. Physics of the Earth and Planetary Interiors, 2012, 208-209, 50-58.	0.7	26
1341	Hybrid density functional study of the structural, bonding, and electronic properties of bismuth vanadate. Physical Review B, 2012, 86, .	1.1	55
1342	High-pressure physical properties of magnesium silicate post-perovskite from ab initio calculations. Bulletin of Materials Science, 2012, 35, 665-672.	0.8	4
1343	Extreme Conditions. , 2012, , 413-471.		0
1344	Structural Stability and Compressibility Study for ZnO Nanobelts under High Pressure. Journal of Physical Chemistry C, 2012, 116, 2074-2079.	1.5	23
1345	Polymorphism and Formation Mechanism of Nanobipods in Manganese Sulfide Nanocrystals Induced by Temperature or Pressure. Journal of Physical Chemistry C, 2012, 116, 3292-3297.	1.5	48
1346	Complex high-pressure polymorphism of barium tungstate. Physical Review B, 2012, 86, .	1.1	66
1347	Elastic property and intrinsic hardness of novel superhard ternary nitrides (CSi2N4 and SiC2N4). Physica B: Condensed Matter, 2012, 407, 4323-4332.	1.3	3
1348	Quantum mechanically guided design of Co₄₃Fe₂₀Ta_{5.5}X_{31.5}(X=B, Si, P, S) metallic glasses. Journal of Physics Condensed Matter, 2012, 24, 175402.	0.7	5
1349	Elastic and electronic properties of tI26-type Mg₁₂RE (RE = Ce, Pr and Nd) phases. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 035018.	0.8	50
1350	First-principle investigations of structural stability of beryllium under high pressure. Journal of Applied Physics, 2012, 112, 023519.	1.1	12
1351	Theoretical investigation of halfâ€metallicity in Co/Ni substituted AlN. International Journal of Quantum Chemistry, 2012, 112, 882-888.	1.0	15
1352	Effects of pressure on the structure and lattice dynamics of TmPO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>: Experiments and calculations. Physical Review B, 2012, 85, .	1.1	32
1353	Effects of high-pressure on the structural, vibrational, and electronic properties of monazite-type PbCrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	1.1	63

#	Article	IF	Citations
1354	Crystal structure of graphite under room-temperature compression and decompression. Scientific Reports, 2012, 2, 520.	1.6	158
1355	Melting of cubic boron nitride at extreme pressures. Journal of Physics Condensed Matter, 2012, 24, 055401.	0.7	6
1356	Pressure-induced structural change in orthorhombic perovskite GdMnO₃. Journal of Physics Condensed Matter, 2012, 24, 115402.	0.7	24
1357	Origin of the nitrogen over- and understoichiometry in Ti_{0.5}Al_{0.5}N thin films. Journal of Physics Condensed Matter, 2012, 24, 155401.	0.7	45
1358	Constraints on the phase diagram of molybdenum from first-principles free-energy calculations. Physical Review B, 2012, 85, .	1.1	55
1359	Ab initiobased empirical potential used to study the mechanical properties of molybdenum. Physical Review B, 2012, 85, .	1.1	71
1360	Analysis of high derivative thermoelastic properties of MgO. Indian Journal of Physics, 2012, 86, 259-265.	0.9	3
1361	HgO at high pressures: the transition to the NaCl structure (HgO-III) and the equation of state of tetragonal HgO-II. Physics and Chemistry of Minerals, 2012, 39, 269-275.	0.3	3
1362	Elastic properties of Î³â€²-Fe4N probed by nanoindentation and ab initio calculation. Acta Materialia, 2012, 60, 2054-2060.	3.8	44
1363	Tantalum-doped hydroxyapatite thin films: Synthesis and characterization. Acta Materialia, 2012, 60, 3435-3443.	3.8	25
1364	High pressure study of low compressibility tetracalcium aluminum carbonate hydrates 3CaOÂ·Al2O3Â·CaCO3Â·11H2O. Cement and Concrete Research, 2012, 42, 105-110.	4.6	64
1365	Experimental determination of bulk modulus of 14Ã… tobermorite using high pressure synchrotron X-ray diffraction. Cement and Concrete Research, 2012, 42, 397-403.	4.6	67
1366	Elastic Properties of Tricalcium Aluminate from Highâ€Pressure Experiments and Firstâ€Principles Calculations. Journal of the American Ceramic Society, 2012, 95, 2972-2978.	1.9	32
1367	Density, elastic and magnetic properties of Coâ€“Feâ€“Taâ€“Si metallic glasses by theory and experiment. Scripta Materialia, 2012, 66, 765-768.	2.6	15
1368	Theoretical investigations of the physical properties of zircon-type YVO4. Journal of Solid State Chemistry, 2012, 185, 42-48.	1.4	31
1369	Electronic structure and chemical bonding of Î±- and Î²-CeIr2Si2 intermediate valence compounds. Journal of Solid State Chemistry, 2012, 186, 81-86.	1.4	5
1370	Structural phase transitions of SrF2 at high pressure. Journal of Solid State Chemistry, 2012, 186, 231-234.	1.4	13
1371	Mechanical properties and work function of L21 structure AlCu2X (X=Ti, Mn, Zr, or Hf) intermetallics. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2012, 545, 13-19.	2.6	11

#	Article	IF	Citations
1372	Elastic, electronic and thermal properties of YSZ from first principles. Solid State Sciences, 2012, 14, 106-110.	1.5	22
1373	Elastic properties and electronic structures of typical Alâ€“Ce structures from first-principles calculations. Solid State Sciences, 2012, 14, 555-561.	1.5	41
1374	Compressibility of NaMnSi2O6: The role of electronic isovalency for the validity of bulk-modulusâ€“volume relationship. Solid State Sciences, 2012, 14, 1036-1039.	1.5	3
1375	The predominance of the rutile phase of SnO2 : First principles study. Solid State Communications, 2012, 152, 349-353.	0.9	6
1376	Theoretical investigation on first-principles electronic and thermal properties of some CdRE intermetallics. Physica B: Condensed Matter, 2012, 407, 198-203.	1.3	6
1377	Ab initio study of lattice dynamics and thermal equation of state of Ni. Physica B: Condensed Matter, 2012, 407, 330-334.	1.3	7
1378	Crystal structure, electronic and elastic properties for novel Hf3AlN and Zr3AlN ceramics explored by first principles studies. Physica B: Condensed Matter, 2012, 407, 547-550.	1.3	6
1379	Mechanical properties and hardness of new carbon-rich superhard C11N4 from first-principles investigations. Physica B: Condensed Matter, 2012, 407, 2282-2288.	1.3	24
1380	Structural, elastic and thermodynamic properties under pressure and temperature effects of MgIn2S4 and CdIn2S4. Physica B: Condensed Matter, 2012, 407, 2295-2300.	1.3	17
1381	Evidence of Coulomb correction and spinâ€“orbit coupling in rare-earth dioxides CeO2, PrO2 and TbO2: An ab initio study. Journal of Magnetism and Magnetic Materials, 2012, 324, 1397-1405.	1.0	35
1382	Pressure induced structural phase transitionsâ€”A review. Open Chemistry, 2012, 10, 1391-1422.	1.0	11
1383	Magnetism induced by nonmagnetic dopant in Li2O, Na2O, K2O and Rb2O: first-principles calculations. Journal of Materials Science, 2012, 47, 2316-2321.	1.7	2
1384	Elastic properties of random L12â€“Al3(Sc0.5TM0.5) alloys from first-principle SQSs calculations. Journal of Materials Science, 2012, 47, 3793-3800.	1.7	7
1385	Structural transformations in cubic Dy2O3 at high pressures. Solid State Communications, 2013, 169, 37-41.	0.9	29
1386	Geophysical and crystal chemical significance of (Mg, Fe)SiO₃perovskite. Geophysical Monograph Series, 0, , 1-12.	0.1	13
1387	Electronic Structure and Total Energy Calculations for Oxide Perovskites and Superconductors. Geophysical Monograph Series, 0, , 55-66.	0.1	11
1388	First-principles study of L12â€“Al3(Sc1â^'xTMx) alloys using special quasirandom structures. Computational Materials Science, 2013, 79, 136-142.	1.4	10
1389	Pressure effect on structural, elastic and electronic properties of (B3) BSb compound. Indian Journal of Physics, 2013, 87, 355-362.	0.9	11

#	Article	IF	Citations
1390	Theoretical investigation of the Alâ€“Crâ€“B orthorhombic ternary compounds. Computational and Theoretical Chemistry, 2013, 1020, 51-56.	1.1	18
1391	Equation of state of CaMnO3: a combined experimental and computational study. Applied Physics A: Materials Science and Processing, 2013, 112, 839-845.	1.1	12
1392	Advanced Nanoscale Characterization of Cement Based Materials Using X-Ray Synchrotron Radiation: A Review. International Journal of Concrete Structures and Materials, 2013, 7, 95-110.	1.4	51
1393	Pressure-induced volume collapse and structural phase transitions in SrRuO3. Journal of Solid State Chemistry, 2013, 205, 177-182.	1.4	11
1394	Phase transition and thermodynamic properties of CaF2 via first principles. Physica B: Condensed Matter, 2013, 426, 13-19.	1.3	15
1395	Structural and optoelectronic properties of NiTiX and CoVX (X = Sb and Sn) half-Heusler compounds: An ab initio study. Optik, 2013, 124, 570-574.	1.4	70
1396	Assessing modern GGA functionals for solids. Journal of Molecular Modeling, 2013, 19, 2791-2796.	0.8	14
1397	Phase transition and possible metallization in CeVO4 under pressure. Journal of Solid State Chemistry, 2013, 203, 273-280.	1.4	37
1398	Density functional study of elastic, mechanical and thermodynamic properties of MgCu with a CsCl-type structure. Journal of Magnesium and Alloys, 2013, 1, 128-133.	5.5	20
1399	Pressure-induced phase transitions in LnTe (Ln=La, Gd, Ho, Yb) and AmTe. Journal of Physics Condensed Matter, 2013, 25, 265401.	0.7	3
1400	Highâ€pressure Singleâ€crystal Xâ€ray Diffraction Study of the Photomagnetic Switching Complex â€” [Y(DMF)4(H2O)3(Î¼â€CN)Fe(CN)5]·H2O. Journal of the Chinese Chemical Society, 2013, 60, 929-934.	0.8	6
1401	Insights into the phase diagram of bismuth ferrite from quasiharmonic free-energy calculations. Physical Review B, 2013, 88, .	1.1	50
1402	X-ray diffraction study on pressure-induced phase transformations and the equation of state of ZnGa2Te4. Journal of Applied Physics, 2013, 114, .	1.1	37
1403	Elastic and thermodynamic properties of ZnSc2S4 and CdSc2S4 compounds under pressure and temperature effects. Computational Materials Science, 2013, 70, 107-113.	1.4	18
1404	Electronic, elastic and thermal properties of SrCu2As2 via first principles calculation. Journal of Alloys and Compounds, 2013, 570, 156-161.	2.8	9
1405	Ab Initio Study of Thermodynamic Properties of Lithium, Sodium, and Potassium Sulfates. Russian Physics Journal, 2013, 56, 638-646.	0.2	0
1406	Stability, elastic properties and fracture toughness of Al_{0.75}X_{0.75}B₁₄(X=Sc, Ti, V, Cr, Y, Zr, Nb, Mo) investigated usingab initiocalculations. Journal of Physics Condensed Matter, 2013, 25, 335501.	0.7	11
1407	First-principles theory and calculation of flexoelectricity. Physical Review B, 2013, 88, .	1.1	179

#	Article	IF	Citations
1408	Bonding and elastic properties of amorphous AlYB. Solid State Communications, 2013, 169, 6-9.	0.9	31
1409	First-principles calculations of structural, electronic and optical properties of BaGaXH (X=Si, Ge, Sn). Materials Science in Semiconductor Processing, 2013, 16, 1558-1565.	1.9	3
1410	High pressure Raman spectroscopy of layered matlockite, PbFCl. Journal of Physics Condensed Matter, 2013, 25, 155401.	0.7	16
1411	First-principles investigations on physical properties of NdN under high pressure. Journal of Physics and Chemistry of Solids, 2013, 74, 1504-1508.	1.9	5
1412	First-principles study of the structural, mechanical, magnetic, and electronic properties of Cr4AlN3 under pressure. Intermetallics, 2013, 43, 71-78.	1.8	9
1413	Thermodynamic assessment of the Gdâ€“Bi and the Hoâ€“Bi systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2013, 41, 1-5.	0.7	10
1414	Pressure-induced phase transition for ScVO4: A first-principles study. Physica B: Condensed Matter, 2013, 426, 20-23.	1.3	3
1415	Calculation of thermodynamic potentials with the inclusion of fractional occupation numbers and investigation of FCC-BCC structural phase transitions in alkaline-earth metals. Physics of the Solid State, 2013, 55, 1991-2000.	0.2	2
1416	Prediction Study of the Mechanical and Thermodynamic Properties of the $$hbox {RBRh}_{3}$$ RBRh 3 (R $$=$$ = Sm, Eu, Gd, and Tb) Compounds. International Journal of Thermophysics, 2013, 34, 2102-2118.	1.0	0
1417	The electronic and optical properties of the fluoroperovskite XLiF3 (X=Ca, Sr, and Ba) compounds. Computational Materials Science, 2013, 79, 201-205.	1.4	28
1418	High pressure equation of state and ideal compressive and tensile strength of MgO single crystal: Ab-initio calculations. Journal of Applied Physics, 2013, 113, 233504.	1.1	5
1419	Determination of the elastic properties of amorphous materials: Case study of alkaliâ€“silica reaction gel. Cement and Concrete Research, 2013, 54, 55-60.	4.6	24
1420	High-pressure structural transformations of Sn up to 138 GPa: Angle-dispersive synchrotron x-ray diffraction study. Physical Review B, 2013, 88, .	1.1	54
1421	Highâ€Pressure Behavior of Mullite: An Xâ€Ray Diffraction Investigation. Journal of the American Ceramic Society, 2013, 96, 1635-1642.	1.9	9
1422	Predictions of the structural, electronic and thermodynamic properties of the anti-fluorite-type Mg₂Sn under pressure from first principles. Physica Scripta, 2013, 88, 045302.	1.2	24
1423	Thermodynamic properties of magnesium alloys. , 2013, , 85-124.		0
1424	Phase diagram and equation of state of TiH2 at high pressures and high temperatures. Journal of Alloys and Compounds, 2013, 546, 270-274.	2.8	8
1425	Structural and mechanical stability of dilute yttrium doped chromium. Applied Physics Letters, 2013, 102, 021901.	1.5	4

#	Article	IF	Citations
1426	Crystal size effect on the compressibility of nano-crystalline uranium dioxide. Journal of Nuclear Materials, 2013, 435, 123-127.	1.3	23
1427	The Pâ€“Vâ€“T equation of state of CaPtO3 post-perovskite. Physics and Chemistry of Minerals, 2013, 40, 73-80.	0.3	3
1428	New type of possible high-pressure polymorphism in NiAs minerals in planetary cores. Physics and Chemistry of Minerals, 2013, 40, 183-193.	0.3	10
1429	The effect of the phase transition on the elasticity of cubic platinum carbide. Journal of Materials Science, 2013, 48, 1660-1668.	1.7	4
1430	Tight-binding studies of bulk properties and hydrogen vacancies in KBH4. Computational Materials Science, 2013, 79, 888-895.	1.4	3
1431	Ideal strength of Mg2X (XÂ=ÂSi, Ge, Sn and Pb) from first-principles. Journal of Magnesium and Alloys, 2013, 1, 163-168.	5.5	23
1432	Crystal structure of HgGa2Se4 under compression. Materials Research Bulletin, 2013, 48, 2128-2133.	2.7	18
1433	First principles study of the electronic and magnetic structures and bonding properties of UCoC2 ternary, characteristic of Câ€“C units. Solid State Sciences, 2013, 17, 128-133.	1.5	1
1434	A comparison of ice VII formed in the H2O, NaClâ€“H2O, and CH3OHâ€“H2O systems: Implications for H2O-rich planets. Physics of the Earth and Planetary Interiors, 2013, 215, 12-20.	0.7	11
1435	Changes in electronic, magnetic and bonding properties from Zr2FeH5 to Zr3FeH7 addressed from ab initio. Solid State Sciences, 2013, 25, 55-62.	1.5	2
1436	High-pressure polymorphs of TbVO4: A Raman and ab initio study. Journal of Alloys and Compounds, 2013, 577, 327-335.	2.8	45
1437	Bonds, bands and elasticity of smithsonite rock. Solid State Communications, 2013, 166, 76-82.	0.9	15
1438	Drastic changes of electronic, magnetic, mechanical and bonding properties in Zr2Co by hydrogenation. Intermetallics, 2013, 36, 25-30.	1.8	9
1439	High-pressure structural behaviour of Cu0.5Fe0.5Cr2S4: An experimental and theoretical study. Journal of Alloys and Compounds, 2013, 578, 202-207.	2.8	3
1440	Elasticity of single-crystal iron-bearing pyrope up to 20 GPa and 750 K. Earth and Planetary Science Letters, 2013, 361, 134-142.	1.8	45
1441	The phase transitions and electronic structures of crystalline BeF2 under high-pressure: First-principle calculations. Solid State Communications, 2013, 169, 14-19.	0.9	5
1442	Structural, electronic and dynamical stability of heavy metal iron pernitride: a spin polarized first-principles study. European Physical Journal B, 2013, 86, 1.	0.6	9
1443	First-principles calculations of the elastic, and electronic properties of YFe2, NiFe2 and YNiFe4 intermetallic compounds. Computational Materials Science, 2013, 73, 56-64.	1.4	10

#	Article	IF	Citations
1444	Garnet-to-Perovskite Transition in Gd₃Sc₂Ga₃O₁₂ at High Pressure and High Temperature. Inorganic Chemistry, 2013, 52, 431-434.	1.9	10
1445	Ab initio study on structural stability of uranium carbide. Journal of Nuclear Materials, 2013, 437, 81-86.	1.3	21
1446	Material and Elastic Properties of <scp><scp>Al</scp></scp>â€Tobermorite in Ancient Roman Seawater Concrete. Journal of the American Ceramic Society, 2013, 96, 2598-2606.	1.9	106
1447	Thermodynamic assessment of the Biâ€“Er and the Biâ€“Dy systems. Thermochimica Acta, 2013, 566, 44-49.	1.2	11
1448	Structural Transformations and Disordering in Zirconolite (CaZrTi₂O₇) at High Pressure. Inorganic Chemistry, 2013, 52, 1550-1558.	1.9	40
1449	A first principles lattice dynamics and Raman spectra of the ferroelastic rutile to CaCl₂ phase transition in SnO₂ at high pressure. Journal of Raman Spectroscopy, 2013, 44, 926-933.	1.2	40
1450	Pressure induced phase transitions in multiferroic BiFeO3. Solid State Communications, 2013, 154, 72-76.	0.9	15
1451	Pressure-induced structural phase transition and equation of state of LiTaO₃. Journal of Physics Condensed Matter, 2013, 25, 215401.	0.7	4
1452	Review on cerium intermetallic compounds: A bird's eye outlook through DFT. Progress in Solid State Chemistry, 2013, 41, 55-85.	3.9	28
1453	Newly synthesized nanolaminate Nb2GeC: Hardness, thermodynamic and optical properties by first-principles method. Computational Materials Science, 2013, 74, 119-123.	1.4	18
1454	Mechanical and optical properties of inverse-perovskites Sc3InX (X=B, C, N). Computational Materials Science, 2013, 73, 1-8.	1.4	13
1455	Phase stability, mechanical properties and electronic structure of hexagonal and trigonal Ti5Al2C3: An ab initio study. Intermetallics, 2013, 33, 105-112.	1.8	12
1456	First-principles study of structural, electronic and magnetic properties of AeX (Ae=Be, Mg, Sr, Ba; X=Si,) Tj ETQq0 0 0 rgBT /Overlock 10	1.0	9
1457	High pressure structural and vibrational properties of the spin-gap system Cu₂PO₄(OH). Journal of Physics Condensed Matter, 2013, 25, 045402.	0.7	7
1458	Nonlinear Eulerian thermoelasticity for anisotropic crystals. Journal of the Mechanics and Physics of Solids, 2013, 61, 1983-2014.	2.3	46
1459	The alunite supergroup under high pressure: the case of natrojarosite, NaFe₃(SO₄)₂(OH)₆. Mineralogical Magazine, 2013, 77, 3007-3017.	0.6	4
1460	Electronic properties and structural phase transition in A4 [M4O4] (A=Li, Na, K and Rb; M=Ag and Cu): A first principles study. Solid State Communications, 2013, 155, 62-68.	0.9	11
1461	ELECTRONIC STRUCTURE, MAGNETIC ORDERING AND PHASE STABILITY OF LiFeX (X =) Tj ETQq1 1 0.784314 rgBT /Ove 2013, 27, 1350236.	1.0	8

#	Article	IF	Citations
1462	Dynamics in molecular and molecular-ionic crystals: A combined experimental and molecular simulation study of reorientational motions in benzene, pyridinium iodide, and pyridinium nitrate. Journal of Chemical Physics, 2013, 138, 024508.	1.2	1
1463	Ab Initio Investigation of Nitride in Comparison with Carbide Phase of Superconducting InX (Xâ€‰=â€‰C, N). , 2013, 2013, 1-9.		14
1464	Elastic Properties, Mechanical Stability, and State Densities of Aluminnides. Acta Physica Polonica A, 2013, 123, 668-672.	0.2	5
1465	First-Principles Calculations of Electronic and Structural Properties of LaN under High Pressure. Applied Mechanics and Materials, 0, 331, 563-566.	0.2	4
1466	Electronic Structure and Ground State Properties of A₄[Ag₄O₄] (A=Na, K and Rb): A First-Principles Study. Advanced Materials Research, 0, 665, 43-48.	0.3	0
1467	A benchmark for some bulk properties of bcc iron. International Journal of Multiphysics, 2013, 7, 95-100.	0.3	6
1468	Structural, elastic, and thermodynamic properties under pressure of the FeC in the martensitic phase: an ab-initio study. High Pressure Research, 2013, 33, 572-583.	0.4	1
1469	Theoretical study of elastic properties and phase stability of M0.5Al0.5N1â^'xOx (Mâ€‰=â€‰Sc, Ti,) Tj ETQq1 1 0.784	1.1	14
1470	Pressure-induced structural evolution and amorphization in Eu3Ga5O12. Journal of Applied Physics, 2013, 114, 163521.	1.1	9
1471	Radial x-ray diffraction of tungsten tetraboride to 86â€‰GPa under nonhydrostatic compression. Journal of Applied Physics, 2013, 113, 033507.	1.1	23
1472	Stabilization of tetragonal phase in LaN under high pressure via Peierls distortion. High Pressure Research, 2013, 33, 563-571.	0.4	10
1473	Stability, metastability, and elastic properties of a dense silica polymorph, seifertite. Journal of Geophysical Research: Solid Earth, 2013, 118, 4745-4757.	1.4	52
1474	Compression of scheelite-type SrMoO4 under quasi-hydrostatic conditions: Redefining the high-pressure structural sequence. Journal of Applied Physics, 2013, 113, .	1.1	66
1475	High-pressure x-ray diffraction and Raman spectroscopy of phase transitions in Sm2O3. Journal of Applied Physics, 2013, 113, .	1.1	51
1476	Pressure-induced phase transitions of multiferroic BiFeO ₃. Chinese Physics C, 2013, 37, 128001.	1.5	5
1477	Nonmetal sublattice population induced defect structure in transition metal aluminum oxynitrides. Applied Physics Letters, 2013, 103, .	1.5	31
1478	BAND STRUCTURE, HARDNESS, THERMODYNAMIC AND OPTICAL PROPERTIES OF SUPERCONDUCTING Nb₂AsC, Nb₂InC AND Mo₂GaC. International Journal of Computational Materials Science and Engineering, 2013, 02, 1350007.	0.5	28
1479	Sound velocities for hexagonally closeâ€packed iron compressed hydrostatically to 136â€‰GPa from phonon density of states. Geophysical Research Letters, 2013, 40, 2983-2987.	1.5	16

#	Article	IF	Citations
1480	Phase stability and elastic properties of titanium aluminum oxynitride studied byab initiocalculations. Journal Physics D: Applied Physics, 2013, 46, 084002.	1.3	21
1482	Static Compression Measurements of Equations of State. AGU Reference Shelf, 0, , 98-142.	0.6	86
1483	Hugoniot Sound Velocities in Metals with Applications to the Earth's Inner Core. Geophysical Monograph Series, 0, , 353-361.	0.1	5
1484	A spectroscopic Study of the High-Pressure Behavior of the O₄H₄Substitution in Garnet. Geophysical Monograph Series, 0, , 297-304.	0.1	10
1485	Differential Finite-Strain Equations of State. Geophysical Monograph Series, 2013, , 147-156.	0.1	2
1486	Electron Momentum Density and Phase Transition in ZnS. Journal of Theoretical Chemistry, 2013, 2013, 1-7.	1.5	1
1487	Structural properties of (B3) TlP under pressure. International Journal of Physical Research, 2014, 2, .	0.5	3
1488	Structural and optical investigations of Fe_{1.03}Se_{0.5}Te_{0.5}under high pressure. Journal of Physics Condensed Matter, 2014, 26, 125701.	0.7	7
1489	PHASE TRANSITION AND THERMODYNAMIC PROPERTIES OF MAGNESIUM FLUORIDE BY FIRST PRINCIPLES. International Journal of Modern Physics B, 2014, 28, 1450026.	1.0	7
1490	Zirconium metal-based MAX phases Zr₂AC (A =) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 5 International Journal of Modern Physics B, 2014, 28, 1550022.	1.0	41
1491	High-pressure structural stability of the ductile intermetallic compound, ErCu. Bulletin of Materials Science, 2014, 37, 1343-1345.	0.8	2
1492	First-Principles Study of the Structural, Elastic, and Mechanical Properties of Ni₃Ga Compound under Pressure. Acta Physica Polonica A, 2014, 125, 54-59.	0.2	4
1493	First-principles elasticity of monocarboaluminate hydrates. American Mineralogist, 2014, 99, 1360-1368.	0.9	21
1494	Strength and structural phase transitions of gadolinium at high pressure from radial X-ray diffraction. Journal of Applied Physics, 2014, 116, .	1.1	5
1495	Exploring the behavior of molybdenum diboride (MoB2): A high pressure x-ray diffraction study. Journal of Applied Physics, 2014, 115, .	1.1	17
1496	High-pressure structural and elastic properties of Tl2O3. Journal of Applied Physics, 2014, 116, .	1.1	20
1497	Revisit of the relationship between the elastic properties and sound velocities at high pressures. Journal of Applied Physics, 2014, 116, 104904.	1.1	4
1498	Effect of oxygen incorporation on the structure and elasticity of Ti-Al-O-N coatings synthesized by cathodic arc and high power pulsed magnetron sputtering. Journal of Applied Physics, 2014, 116, .	1.1	51

#	Article	IF	Citations
1499	High-pressure behavior of amorphous selenium from ultrasonic measurements and Raman spectroscopy. Applied Physics Letters, 2014, 105, 011901.	1.5	10
1500	Structural and Vibrational Study of Pseudocubic CdIn₂Se₄ under Compression. Journal of Physical Chemistry C, 2014, 118, 26987-26999.	1.5	7
1501	Electronic and bonding analysis of hardness in pyrite-type transition-metal pernitrides. Physical Review B, 2014, 90, .	1.1	108
1502	Calcium Sulfoaluminate Sodalite (<scp><scp>Ca₄Al₆O₁₂SO₄</scp></scp>) Crystal Structure Evaluation and Bulk Modulus Determination. Journal of the American Ceramic Society, 2014, 97, 892-898.	1.9	36
1503	High-pressure elasticity of sodium majorite garnet, Na2MgSi5O12. American Mineralogist, 2014, 99, 2416-2423.	0.9	6
1504	On combining temperature and pressure effects on structural properties of crystals with standard ab initio techniques. Journal of Chemical Physics, 2014, 141, 124115.	1.2	68
1505	Ab initio prediction of the structural, electronic, elastic and thermodynamic properties of the tetragonal ternary intermetallics XCu2Si2 (X = Ca, Sr). European Physical Journal B, 2014, 87, 1.	0.6	10
1506	First principles study on structural and electronic properties and defect formation enthalpies of cubic Hf₃N₄ under high pressure. Canadian Journal of Physics, 2014, 92, 1581-1586.	0.4	1
1507	Structure and compressibility of the high-pressure molecular phase II of carbon dioxide. Physical Review B, 2014, 89, .	1.1	23
1508	Pressure Induced Structural and Electronic Properties of Thulium Nitride. Advanced Materials Research, 0, 1047, 147-150.	0.3	0
1509	Equation of state of bcc-Mo by static volume compression to 410â€‰GPa. Journal of Applied Physics, 2014, 116, .	1.1	16
1510	First Principle Calculations of Pressure Induced Structural and Electronic Properties in Americium Monochalcogenides. Advanced Materials Research, 0, 1047, 35-40.	0.3	1
1511	First-principles investigations on structural, elastic, thermodynamic and electronic properties of Ni3X (XÂ=ÂAl, Ga and Ge) under pressure. Intermetallics, 2014, 44, 110-115.	1.8	72
1512	First-principle calculations of the electronic, optical and elastic properties of ZnSiP2 semiconductor. Journal of Alloys and Compounds, 2014, 582, 101-107.	2.8	50
1513	First-principles study of mechanical and electronic properties of TiB compound under pressure. Intermetallics, 2014, 52, 64-71.	1.8	21
1514	In situ high-pressure synchrotron X-ray diffraction study of the structural stability in NdVO4 and LaVO4. Materials Research Bulletin, 2014, 50, 279-284.	2.7	60
1515	Structure and elasticity of phlogopite under compression: Geophysical implications. Physics of the Earth and Planetary Interiors, 2014, 233, 1-12.	0.7	36
1516	Structural and elastic properties of defect chalcopyrite HgGa2S4 under high pressure. Journal of Alloys and Compounds, 2014, 583, 70-78.	2.8	32

#	Article	IF	Citations
1517	Formation of a solid solution in the MgSiO3â€“MnSiO3 perovskite system. Physics and Chemistry of Minerals, 2014, 41, 431-437.	0.3	2
1518	Theoretical predictions of the structural and thermodynamic properties of MgZn2 Laves phase under high pressure. Applied Physics A: Materials Science and Processing, 2014, 115, 323-331.	1.1	17
1519	A new temperature-dependent equation of state of solids. Pramana - Journal of Physics, 2014, 82, 549-561.	0.9	3
1520	Ab-initio investigation of half-metallic ferromagnetism in half-Heusler compounds XYZ (X=Li, Na, K and) Tj ETQq1 1 0.784314 rgBT /Ov	1.0	59
1521	Electronic, elastic and optical properties of ZnGeP2 semiconductor under hydrostatic pressures. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2014, 182, 52-58.	1.7	50
1522	First-principles calculations on mechanical and elastic properties of 2H- and 3R-WS2 under pressure. Solid State Communications, 2014, 187, 43-47.	0.9	23
1523	Hydrogen-bonded structure and mechanical chiral response of a silver nanoparticle superlattice. Nature Materials, 2014, 13, 807-811.	13.3	128
1524	Electronic and elastic properties of Al4Ce binary compound under pressure via first-principles. Superlattices and Microstructures, 2014, 69, 76-86.	1.4	8
1525	Mechanical, electronic and thermodynamic properties of Mg2Ca Laves phase under high pressure: A first-principles calculation. Computational Materials Science, 2014, 88, 61-70.	1.4	38
1526	High pressure elastic properties of minerals from ab initio simulations: The case of pyrope, grossular and andradite silicate garnets. Journal of Chemical Physics, 2014, 140, 124703.	1.2	66
1527	Thermal equation of state and spin transition of magnesiosiderite at high pressure and temperature. American Mineralogist, 2014, 99, 84-93.	0.9	48
1528	Ab initio study of the structural, electronic and elastic properties of anti-fluorite Li2X (X=S and Te) compounds under pressure effect. Computational Materials Science, 2014, 86, 49-56.	1.4	12
1529	On equation of state, elastic, and lattice dynamic stability of bcc bismuth under high pressure: Ab-initio calculations. Journal of Applied Physics, 2014, 115, .	1.1	11
1530	Experimental evidence for pressure-driven isostructural and symmetry-breaking phase transitions on Bi14CrO24. Solid State Communications, 2014, 182, 50-54.	0.9	7
1531	Influence of (Al, Fe, Mg) Impurities on Triclinic Ca₃SiO₅: Interpretations from DFT Calculations. Crystal Growth and Design, 2014, 14, 2158-2171.	1.4	29
1532	Mechanical and electronic properties of Rh and Rh3Zr from first-principles calculation. Solid State Communications, 2014, 189, 43-46.	0.9	8
1533	Systematic analysis of the structural, elastic, and electronic properties of Tiâ€“Cuâ€“Me (Me=Al, Ga and) Tj ETQq0 0 0 rgBT /Overlock 10	1.9	2
1534	Equation of state of zircon- and scheelite-type dysprosium orthovanadates: a combined experimental and theoretical study. Journal of Physics Condensed Matter, 2014, 26, 025401.	0.7	12

#	Article	IF	Citations
1535	Pressure-induced volume anomaly and structural phase transition in nanocrystalline SnO₂. Physica Status Solidi (B): Basic Research, 2014, 251, 1380-1385.	0.7	7
1536	Towards designing La 1â^'x Sr x Co y Fe 1â^'y O 3â^'d with enhanced phase stability: Role of the defect structure. Solid State Ionics, 2014, 255, 108-112.	1.3	14
1537	Structural, elastic, electronic and optical properties of the newly synthesized monoclinic Zintl phase BaIn2P2. Solid State Sciences, 2014, 29, 12-23.	1.5	54
1538	Compression behavior of nanocrystalline TiN. Solid State Communications, 2014, 182, 26-29.	0.9	7
1539	Structural, elastic, thermal, electronic and optical properties of Ag2O under pressure. Computational Materials Science, 2014, 83, 474-480.	1.4	14
1540	Theoretical study of structural, elastic and thermodynamic properties of CZTX (X=S and Se) alloys. Journal of Alloys and Compounds, 2014, 589, 137-142.	2.8	19
1541	Compressibility and Structural Stability of Nanocrystalline TiO₂ Anatase Synthesized from Freeze-Dried Precursors. Inorganic Chemistry, 2014, 53, 11598-11603.	1.9	28
1542	SHOCK COMPRESSION OF METAL CRYSTALS: A COMPARISON OF EULERIAN AND LAGRANGIAN ELASTIC-PLASTIC THEORIES. International Journal of Applied Mechanics, 2014, 06, 1450048.	1.3	23
1543	Multiferroic CuCrO2 under high pressure: In situ X-ray diffraction and Raman spectroscopic studies. Journal of Applied Physics, 2014, 116, 133514.	1.1	31
1544	Equation of state of liquid mercury to 520 K and 7 GPa from acoustic velocity measurements. Journal of Chemical Physics, 2014, 140, 244201.	1.2	22
1545	Strength and equation of state of NaCl from radial x-ray diffraction. Journal of Applied Physics, 2014, 115, .	1.1	11
1546	Ab Initio Study of Pressure Induced Structural, Magnetic and Electronic Properties in Plutonium Pnictides. Advanced Materials Research, 2014, 1047, 11-17.	0.3	1
1547	Exploring the high pressure behavior of 2D and quasi-3D boron layers in MoB2. RSC Advances, 2014, 4, 52878-52882.	1.7	8
1548	From superhard to hard: A review of transition metal dioxides TiO2, ZrO2, and HfO2 hardness. Journal of Superhard Materials, 2014, 36, 231-245.	0.5	20
1549	Effects of atomic ordering on the elastic properties of TiN- and VN-based ternary alloys. Thin Solid Films, 2014, 571, 145-153.	0.8	34
1550	Elasticity of grossularâ€“andradite solid solution: an ab initio investigation. Physical Chemistry Chemical Physics, 2014, 16, 15331.	1.3	16
1551	First-principles study of structural, electronic and optical properties of the KCaX₃Â(X = F and Cl) compounds. International Journal of Modern Physics B, 2014, 28, 1450139.	1.0	19
1552	Anomalous pressure-induced phase transformation in nano-crystalline erbium sesquioxide (Er₂O₃): partial amorphization under compression. High Pressure Research, 2014, 34, 70-77.	0.4	10

#	Article	IF	Citations
1553	Equations of state of ice VI and ice VII at high pressure and high temperature. Journal of Chemical Physics, 2014, 141, 104505.	1.2	49
1554	High Pressure Crystal and Magnetic Phase Transitions in Multiferroic Bi_{0.9}La_{0.1}FeO₃. Chemistry of Materials, 2014, 26, 1180-1186.	3.2	19
1555	High-pressure structural transformations of PbCrO4 up to 51.2 GPa: An angle-dispersive synchrotron X-ray diffraction study. Materials Research Bulletin, 2014, 60, 206-211.	2.7	10
1556	Compression of lithium fluoride to 92ÂGPa. High Pressure Research, 2014, 34, 39-48.	0.4	26
1557	First-principles study of the electronic and structural properties of (CdTe)n/(ZnTe)n superlattices. Superlattices and Microstructures, 2014, 75, 818-830.	1.4	12
1558	X-ray diffraction studies of Sr3Cr2O8 and Ba3Cr2O8 at high pressures. Solid State Communications, 2014, 200, 5-8.	0.9	2
1559	Degradation Mechanism against Hydrogenation Cycles in Mg_{2â€“x}Pr_xNi₄ (x = 0.6 and 1.0). Journal of Physical Chemistry C, 2014, 118, 6697-6705.	1.5	23
1560	Phase diagram of the CuInSe2-CuGaSe2 pseudobinary system studied by combined ab initio density functional theory and thermodynamic calculation. Journal of Applied Physics, 2014, 116, .	1.1	16
1561	Magnetism and Sound Velocities of Iron Carbide (Fe3C) under Pressure. Chinese Journal of Chemical Physics, 2014, 27, 297-301.	0.6	2
1562	Equation of state of single-crystal cubic boron phosphide. Journal of Superhard Materials, 2014, 36, 61-64.	0.5	8
1563	Evolution of the optical properties of chromium spinels CdCr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>, HgCr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow	1.1	10
1564	Density and sound speed measurements on model basalt (Anâ€“Diâ€“Hd) liquids at one bar: New constraints on the partial molar volume and compressibility of the FeO component. Earth and Planetary Science Letters, 2014, 388, 283-292.	1.8	20
1565	Vibrational and elastic properties of 2D carbon allotropes: A first principles study. Solid State Communications, 2014, 189, 58-62.	0.9	10
1566	Reversible Structural Phase Transition in ZnV₂O₆ at High Pressures. Journal of Physical Chemistry C, 2014, 118, 10560-10566.	1.5	37
1567	Effect of Pressure on the Electronic and Magnetic Properties of a Few Mn-Based Half-Metallic Compounds. Arabian Journal for Science and Engineering, 2014, 39, 475-483.	1.1	2
1568	Single-crystal elasticity of the deep-mantle magnesite at high pressure and temperature. Earth and Planetary Science Letters, 2014, 392, 292-299.	1.8	39
1569	Ab initio study of the structural, electronic and optical properties of the fluoropervskite SrXF3 (X=Li,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	1.4	37
1570	Mechanical behaviors and phase transition of Ho2O3 nanocrystals under high pressure. Journal of Applied Physics, 2014, 116, .	1.1	18

#	Article	IF	Citations
1571	Compressibility Systematics of Calcite-Type Borates: An Experimental and Theoretical Structural Study on ABO₃ (A = Al, Sc, Fe, and In). Journal of Physical Chemistry C, 2014, 118, 4354-4361.	1.5	22
1572	Polymorphism in Paracetamol: Evidence of Additional Forms IV and V at High Pressure. Journal of Physical Chemistry A, 2014, 118, 6068-6077.	1.1	31
1573	Quasi-hydrostatic X-ray powder diffraction study of the low- and high-pressure phases of CaWO4 up to 28ÂGPa. Solid State Sciences, 2014, 36, 16-23.	1.5	18
1574	First-principles study of structural stabilities of AlH3 under high pressure. Journal of Physics and Chemistry of Solids, 2014, 75, 803-807.	1.9	6
1575	Pressure induced metallization of fordite SnNb2O6 from first principles. Computational Materials Science, 2014, 84, 355-359.	1.4	3
1576	Electronic structures of long periodic stacking order structures in Mg: A first-principles study. Journal of Alloys and Compounds, 2014, 586, 656-662.	2.8	42
1577	First-Principles Calculation of structural, electronic and magnetic properties of half-Heusler LiCaC and NaCaC compounds. Physica B: Condensed Matter, 2014, 448, 256-259.	1.3	24
1578	Structural, electronic and thermodynamic properties of BiF3-type Mg3Gd compound: A first-principle study. Physica B: Condensed Matter, 2014, 432, 33-39.	1.3	26
1579	Mechanical properties of doped g-C3N4 â€“ A first-principle study. Vacuum, 2014, 106, 79-85.	1.6	33
1580	Equation of state of Fe3S at room temperature up to 2 megabars. Physics of the Earth and Planetary Interiors, 2014, 228, 106-113.	0.7	14
1581	Structural, elastic, electronic, chemical bonding and optical properties of Cu-based oxides ACuO (A=Li, Na, K and Rb): An ab initio study. Computational Materials Science, 2014, 81, 561-574.	1.4	53
1582	In silico CrNF, a half-metallic ferromagnetic nitrideâ€“fluoride mimicking CrO2. Journal of Magnetism and Magnetic Materials, 2014, 368, 105-110.	1.0	7
1583	First-principles investigation of mechanical, electronic and optical properties of Al3Sc intermetallic compound under pressure. Computational Materials Science, 2014, 91, 165-172.	1.4	28
1584	Mechanical properties, hardness and electronic structures of new post-cotunnite phase (Fe2P-type) of TiO2. Physica B: Condensed Matter, 2014, 433, 48-54.	1.3	11
1585	Half-metallic ferromagnetism in Al1â^'xCrxP and superlattices (AlP)n/(CrP)m by density functional calculations. Superlattices and Microstructures, 2014, 65, 195-205.	1.4	20
1586	Single-crystal elastic constants of magnesium difluoride (MgF2) to 7.4GPa. Journal of Physics and Chemistry of Solids, 2014, 75, 136-141.	1.9	7
1587	Drastic changes of electronic structure, bonding properties and crystal symmetry in Zr2Cu by hydrogenation, from ab initio. Intermetallics, 2014, 45, 5-10.	1.8	3
1588	Unusually large shear wave anisotropy for chlorite in subduction zone settings. Geophysical Research Letters, 2014, 41, 1506-1513.	1.5	58

#	Article	IF	Citations
1589	Equations of state in the Feâ€FeSi system at high pressures and temperatures. Journal of Geophysical Research: Solid Earth, 2014, 119, 2810-2827.	1.4	71
1590	Computational Electronic Study of ScS. Procedia Computer Science, 2015, 57, 160-167.	1.2	6
1591	Enhanced thermoelectric performance of amorphous Nb based oxynitrides. Physica B: Condensed Matter, 2015, 479, 96-100.	1.3	10
1592	Pressure-induced novel compounds in the Hf-O system from first-principles calculations. Physical Review B, 2015, 92, .	1.1	44
1593	Structure and stability of as cast AlCrFeMnNiTi high entropy alloy. Materials Science and Technology, 2015, 31, 1153-1158.	0.8	5
1594	Finding the stable structures of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mtext>N</mml:mtext><mml:mrow><mml:mn1 anab initiohigh-throughput approach. Physical Review B, 2015, 91, .	1.1	54
1595	Development and application of a Ni-Ti interatomic potential with high predictive accuracy of the martensitic phase transition. Physical Review B, 2015, 92, .	1.1	187
1596	First-principles modeling of three-body interactions in highly compressed solid helium. Physical Review B, 2015, 92, .	1.1	11
1597	Equation of state of liquid Indium under high pressure. AIP Advances, 2015, 5, .	0.6	8
1598	Strength of polycrystalline niobium from high-pressure x-ray diffraction data: A comparison of results from line-width and line-shift analyses. Journal of Applied Physics, 2015, 118, .	1.1	5
1599	Theoretical investigations on the structural, elastic and electronic properties of binary Beryllides under pressure. Journal of Nuclear Materials, 2015, 464, 230-235.	1.3	11
1600	Elasticity of Ferropericlase across the Spin Crossover in the Earthâ€™s Lower Mantle. Scientific Reports, 2015, 5, 17188.	1.6	44
1601	The high pressure structure and equation of state of 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105) up to 20 GPa: X-ray diffraction measurements and first principles molecular dynamics simulations. Journal of Chemical Physics, 2015, 143, 144506.	1.2	36
1602	High-Pressure Orthorhombic Ferromagnesite as a Potential Deep-Mantle Carbon Carrier. Scientific Reports, 2015, 5, 7640.	1.6	51
1603	Pressure effects on structural and elastic properties of BeO from first-principles calculations. Physica Status Solidi (B): Basic Research, 2015, 252, 212-218.	0.7	5
1604	Limitations on silicon in the outer core: Ultrasonic measurements at high temperatures and high dK/dP values of Feâ€Niâ€Si liquids at high pressures. Journal of Geophysical Research: Solid Earth, 2015, 120, 6846-6855.	1.4	9
1605	Bottom-up formation of robust gold carbide. Scientific Reports, 2015, 5, 8891.	1.6	11
1606	Anomalous compression behavior of germanium during phase transformation. Applied Physics Letters, 2015, 106, .	1.5	16

#	Article	IF	Citations
1607	First-principles calculations of structural, electronic, elastic and thermal properties of phase M2SiC (M=Ti, V, Cr, Zr, Nb, Mo, Hf, Ta and W). Transactions of Nonferrous Metals Society of China, 2015, 25, 915-925.	1.7	25
1608	Formation of As-As Interlayer Bonding in the collapsed tetragonal phase of NaFe2As2 under pressure. Scientific Reports, 2015, 5, 9868.	1.6	16
1609	Electronic-band structures and optical properties of transition metal doped Zinc oxide. , 2015, , .		0
1610	Equation of State, Nonlinear Elastic Response, and Anharmonic Properties of Diamond-Cubic Silicon and Germanium: First-Principles Investigation. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 403-412.	0.7	4
1611	Phase transition and bulk properties of some polonide compounds: a comparative study. Phase Transitions, 2015, 88, 859-876.	0.6	5
1612	Structural, electronic and elastic properties of the B2-ScM (M =Au, Hg and Tl) intermetallic compounds: Ab initio calculations. International Journal of Computational Materials Science and Engineering, 2015, 04, 1550020.	0.5	1
1613	Accurate calculations of the high-pressure elastic constants based on the first-principles. Chinese Physics B, 2015, 24, 086201.	0.7	1
1614	Anab initiostudy of the structural, elastic, electronic and optical properties of the newly synthesized nitridoaluminate LiCaAlN₂. Philosophical Magazine, 2015, 95, 41-63.	0.7	4
1615	The elastic, electronic and thermodynamic properties of PdTe under high pressure from first-principles calculations. Physica C: Superconductivity and Its Applications, 2015, 509, 34-41.	0.6	13
1616	DFT calculations of structural, electronic, optical and elastic properties of scintillator materials BaCl₂and BaBr₂. Journal Physics D: Applied Physics, 2015, 48, 105301.	1.3	8
1617	First-principles calculations of two cubic fluoropervskite compounds: RbFeF3 and RbNiF3. Journal of Magnetism and Magnetic Materials, 2015, 382, 211-218.	1.0	53
1618	A first-principles study of structure, elasticity and thermal decomposition of Ti1â^'xTMxN alloys (TM=Y,) Tj ETQq1 1 0.784314 rgBT /O	2.2	36
1619	Pressure-Induced Reversible Phase Transformation in Nanostructured Bi₂Te₃ with Reduced Transition Pressure. Journal of Physical Chemistry C, 2015, 119, 3843-3848.	1.5	30
1620	External pressure and composition effects on the atomic and electronic structure of SnWO4. Solar Energy Materials and Solar Cells, 2015, 143, 627-634.	3.0	19
1621	Katoite under pressure: an ab initio investigation of its structural, elastic and vibrational properties sheds light on the phase transition. Physical Chemistry Chemical Physics, 2015, 17, 2660-2669.	1.3	16
1622	Investigations on Radiation Tolerance of M_{n+1}AX_n Phases: Study of Ti₃SiC₂, Ti₃AlC₂, Cr₂AlC, Cr₂GeC, Ti₂AlC, and Ti₂AlN. Journal of the American Ceramic Society, 2015, 98, 1323-1331.	1.9	83
1623	Electronic properties and Schottky barriers at ZnOâ€"metal interfaces from first principles. Journal of Physics Condensed Matter, 2015, 27, 015006.	0.7	16
1624	Band gap behavior of scandium aluminum phosphide and scandium gallium phosphide ternary alloys and superlattices. Materials Science in Semiconductor Processing, 2015, 31, 493-500.	1.9	14

#	Article	IF	Citations
1625	Stiffness and toughness prediction of Coâ€“Feâ€“Taâ€“B metallic glasses, alloyed with Y, Zr, Nb, Mo, Hf, W, C, N and O byab initiomolecular dynamics. Journal of Physics Condensed Matter, 2015, 27, 105502.	0.7	5
1626	Mechanical properties of jennite: A theoretical and experimental study. Cement and Concrete Research, 2015, 71, 106-114.	4.6	33
1627	First-principles investigation of thermodynamic, elastic and electronic properties of Al3V and Al3Nb intermetallics under pressures. Journal of Applied Physics, 2015, 117, .	1.1	44
1628	Electronic Structure and Thermodynamic Properties of RNi₅Sn (R = La, Ce, Pr, Nd) Compounds. Acta Physica Polonica A, 2015, 127, 257-259.	0.2	1
1629	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	1.2	28
1630	CuMo_{0.9}W_{0.1}O₄ phase transition with thermochromic, piezochromic, and thermosalient effects. Journal of Materials Chemistry C, 2015, 3, 2918-2924.	2.7	26
1631	A Protocol to Fabricate Nanostructured New Phase: B31-Type MnS Synthesized under High Pressure. Journal of the American Chemical Society, 2015, 137, 10297-10303.	6.6	67
1632	Compressibility and structural stability of spinel-type MnIn2O4. Journal of Solid State Chemistry, 2015, 230, 301-308.	1.4	13
1633	Quenching rattling modes in skutterudites with pressure. Physical Review B, 2015, 91, .	1.1	15
1634	Elasticity of single-crystal olivine at high pressures and temperatures. Earth and Planetary Science Letters, 2015, 426, 204-215.	1.8	61
1635	First principle calculations of elastic and thermodynamic properties of Ir3Nb and Ir3V with L12 structure under high pressure. Intermetallics, 2015, 66, 103-110.	1.8	11
1636	First principles calculations of structural, elastic, electronic properties of Ir3Zr with L12 structure under high pressure. Materials Chemistry and Physics, 2015, 162, 807-812.	2.0	12
1637	Structural, elastic, electronic and optical properties of the quaternary nitridogallate LiCaGaN2: First-principles study. Materials Science in Semiconductor Processing, 2015, 40, 64-76.	1.9	19
1638	Structural, Mechanical, and Electronic Properties of Monoclinic N2H5N3 Under Pressure. Brazilian Journal of Physics, 2015, 45, 399-403.	0.7	3
1639	Theory and Practice: Techniques for Measuring High-Pâ€“T Elasticity. , 2015, , 293-312.		7
1640	Crystal Structure of Sinhalite MgAlBO4 under High Pressure. Journal of Physical Chemistry C, 2015, 119, 6777-6784.	1.5	5
1641	Holistic quantum design of thermoelectric niobium oxynitride. Solid State Communications, 2015, 212, 5-9.	0.9	14
1642	First-principles study of the nickelâ€“silicon binary compounds under pressure. Journal of Alloys and Compounds, 2015, 640, 233-239.	2.8	23

#	Article	IF	Citations
1643	The equations of state of forsterite, wadsleyite, ringwoodite, akimotoite, MgSiO3-perovskite, and postperovskite and phase diagram for the Mg2SiO4 system at pressures of up to 130 GPa. Russian Geology and Geophysics, 2015, 56, 172-189.	0.3	28
1644	Pressureâ€“Temperature Dependence of Thermodynamic Properties of $$hbox {ScAlO}_{3}$$ ScAlO 3 Perovskite from First Principles. International Journal of Thermophysics, 2015, 36, 2273-2282.	1.0	2
1645	Coherent view of crystal chemistry and ab initio analyses of Pb(II) and Bi(III) lone pair in square planar coordination. Progress in Solid State Chemistry, 2015, 43, 82-97.	3.9	21
1646	A comparative study of high pressure behaviors of pyrochlore-type and thortveitite-type In₂Ge₂O₇. RSC Advances, 2015, 5, 44121-44127.	1.7	9
1647	Theoretical study of the structural, elastic, electronic and optical properties of XCaF3 (XÂ=ÂK and Rb). Solid State Sciences, 2015, 43, 9-14.	1.5	22
1648	Exploring the high-pressure behavior of the three known polymorphs of BiPO4: Discovery of a new polymorph. Journal of Applied Physics, 2015, 117, .	1.1	55
1649	Electronic structure and thermodynamic properties of Cu₃V₂O₈compound. Phase Transitions, 2015, 88, 970-978.	0.6	7
1650	Doping effect on electronic band structure and magnetic properties of MFeAs(M = Li, Na). International Journal of Computational Materials Science and Engineering, 2015, 04, 1550005.	0.5	1
1651	First-principles investigation on mechanical, electronic, and thermodynamic properties of Mg2Sr under high pressure. Journal of Applied Physics, 2015, 117, .	1.1	19
1652	LaMgX and CeMgX (XÂ=ÂGa, In, Tl, Pd, Ag, Pt, Au) with ZrNiAl type structure â€“ A systematic view on electronic structure and chemical bonding. Solid State Sciences, 2015, 43, 28-34.	1.5	3
1653	A comparative study of Burakovsky's and Jacobs's volume dependence GrÃ¼neisen parameter for fcc aluminum. Physica B: Condensed Matter, 2015, 468-469, 7-10.	1.3	8
1654	Anisotropy in elastic properties of TiSi₂(C49,C40 andC54), TiSi and Ti₅Si₃: anab-initiodensity functional study. Materials Research Express, 2015, 2, 096302.	0.8	10
1655	Electronic, optical and thermal properties of TiCr2 and TiMn2 by ab initio simulations. International Journal of Modern Physics B, 2015, 29, 1550223.	1.0	5
1656	The structural, elastic, electronic properties and Debye temperature of D022-Ni3V under pressure from first-principles. Journal of Alloys and Compounds, 2015, 647, 1104-1110.	2.8	98
1657	Pressure, stress, and strain distribution in the double-stage diamond anvil cell. Journal of Applied Physics, 2015, 118, .	1.1	22
1658	Strength and texture of Pt compressed to 63â€‰GPa. Journal of Applied Physics, 2015, 117, .	1.1	12
1659	Elastic anisotropy, vibrational, and thermodynamic properties of U2Ti intermetallic compound with AlB2-type structure under high pressure up to 100â€‰GPa. Journal of Applied Physics, 2015, 117, .	1.1	5
1660	Hugoniot equation of state and dynamic strength of boron carbide. Journal of Applied Physics, 2015, 117, 165904.	1.1	44

#	Article	IF	Citations
1661	First-principles modeling of quantum nuclear effects and atomic interactions in solid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mmultiscripts><mml:mi mathvariant="normal">He</mml:mi><mml:mprescripts /><mml:none /><mml:mrow><mml:mn>4</mml:mn></mml:mrow></mml:mmultiscripts></mml:math>at high pressure. Physical Review B, 2015, 91, .	1.1	18
1662	Equations of state of anhydrous AlF3 and AlI3: Modeling of extreme condition halide chemistry. Journal of Chemical Physics, 2015, 142, 214506.	1.2	6
1663	Structural phase transition of ternary dielectric SmGdO3: Evidence from angle dispersive x-ray diffraction and Raman spectroscopic studies. Journal of Applied Physics, 2015, 117, 094101.	1.1	9
1664	First-Principles Study of Electronic, Elastic, and Optical Properties of Yb:CaF₂ Crystals. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2015, 70, 889-896.	0.7	3
1665	Equation of state and elasticity of the 3.65 Ã... phase: Implications for the X-discontinuity. American Mineralogist, 2015, 100, 2199-2208.	0.9	17
1666	Ab initio Predictions of Structural and Thermodynamic Properties of Zr2AlC Under High Pressure and High Temperature. Chinese Journal of Chemical Physics, 2015, 28, 263-268.	0.6	9
1667	Lattice distortion induced anomalous ferromagnetism and electronic structure in FCC Fe and Fe-TM (TMÂ=ÂCr, Ni, Ta and Zr) alloys. Materials Chemistry and Physics, 2015, 162, 748-756.	2.0	17
1668	The structural, elastic, electronic properties and Debye temperature of Ni3Mo under pressure from first-principles. Journal of Alloys and Compounds, 2015, 621, 383-388.	2.8	82
1669	Thermodynamic, elastic and electronic properties of AlSc2Si2. Materials Letters, 2015, 138, 148-150.	1.3	16
1670	First principles account for large changes in electronic structure and bonding from LaCu to LaCuMg and LaCuMg4. Computational Materials Science, 2015, 97, 231-236.	1.4	0
1671	Elasticity of superhydrous phase, B, Mg10Si3O14(OH)4. Physics of the Earth and Planetary Interiors, 2015, 238, 42-50.	0.7	15
1672	Crystal and chemical anisotropy effects in AE2ZnN2, (AEÂ=ÂCa, Sr, Ba) from ab initio. Solid State Sciences, 2015, 39, 10-14.	1.5	3
1673	Radial X-ray diffraction study of the static strength and equation of state of MoB2 to 85 GPa. Journal of Alloys and Compounds, 2015, 623, 442-446.	2.8	7
1674	Picosecond acoustics method for measuring the thermodynamical properties of solids and liquids at high pressure and high temperature. Ultrasonics, 2015, 56, 129-140.	2.1	24
1675	Mechanical, electronic, optical, thermodynamic properties and superconductivity of ScGa. Physica B: Condensed Matter, 2015, 457, 320-325.	1.3	24
1676	Elasticity of single-crystal quartz to 10ÂGPa. Physics and Chemistry of Minerals, 2015, 42, 203-212.	0.3	57
1677	LDA+U/GGA+U calculations of structural and electronic properties of CdTe: Dependence on the effective U parameter. Computational Materials Science, 2015, 98, 18-23.	1.4	25
1678	Pâ€“Vâ€“T equation of state of spessartineâ€“almandine solid solution measured using a diamond anvil cell and in situ synchrotron X-ray diffraction. Physics and Chemistry of Minerals, 2015, 42, 63-72.	0.3	9

#	Article	IF	Citations
1679	Electronic structure, elastic anisotropy, thermal conductivity and optical properties of calcium apatite Ca5(PO4)3X (X = F, Cl or Br). Journal of Alloys and Compounds, 2015, 619, 66-77.	2.8	84
1680	Unusual Compression Behavior of Nanocrystalline CeO2. Scientific Reports, 2014, 4, 4441.	1.6	21
1681	Structural, elastic, thermal and electronic properties of M2X (MÂ=ÂSr, Ba and XÂ=ÂSi, Ge, Sn) compounds in anti-fluorite structure: first principle calculations. Indian Journal of Physics, 2015, 89, 369-375.	0.9	10
1682	The K₂CO₃ fusion curve revisited: New experiments at pressures up to 12 GPa. Journal of Mineralogical and Petrological Sciences, 2016, 111, 241-251.	0.4	8
1683	Electronic and elastic properties of BaLiF₃with pressure effects: First-principles study. Physica Status Solidi (B): Basic Research, 2016, 253, 1788-1794.	0.7	8
1684	Phase Stability of Lanthanum Orthovanadate at High Pressure. Journal of Physical Chemistry C, 2016, 120, 13749-13762.	1.5	42
1685	Properties of samarium nitride: First principle calculations. AIP Conference Proceedings, 2016, , .	0.3	3
1686	Micro-stress dominant displacive reconstructive transition in lithium aluminate. Applied Physics Letters, 2016, 109, .	1.5	8
1687	Structural and Electronic Properties of Thulium Compounds. Journal of Metastable and Nanocrystalline Materials, 2016, 28, 59-64.	0.1	0
1688	Elasticity of methane hydrate phases at high pressure. Journal of Chemical Physics, 2016, 144, 154501.	1.2	4
1689	High-pressure X-ray diffraction, Raman and computational studies of MgCl2 up to 1 Mbar: Extensive pressure stability of the Î²-MgCl2 layered structure. Scientific Reports, 2016, 6, 30631.	1.6	15
1690	The structural, elastic and optical properties of ScM (M = Rh, Cu, Ag, Hg) intermetallic compounds under pressure by ab initio simulations. International Journal of Computational Materials Science and Engineering, 2016, 05, 1650024.	0.5	7
1691	Behaviors of Zn ₂ GeO ₄ under high pressure and high temperature. Chinese Physics B, 2016, 25, 076101.	0.7	8
1692	Anomalous expansion of Nb nanowires in a NiTi matrix under high pressure. Applied Physics Letters, 2016, 109, 161903.	1.5	1
1693	Guiding ab initio calculations by alchemical derivatives. Journal of Chemical Physics, 2016, 144, 104103.	1.2	25
1694	High-pressure structure and elastic properties of tantalum single crystal: First principles investigation. Chinese Physics B, 2016, 25, 126103.	0.7	9
1695	Band structure, Fermi surface, elastic, thermodynamic, and optical properties of AlZr₃, AlCu₃, and AlCu₂Zr: First-principles study. Chinese Physics B, 2016, 25, 083101.	0.7	11
1696	Thermomechanical response of thermoelectrics. Applied Physics Letters, 2016, 109, 223903.	1.5	23

#	Article	IF	Citations
1697	Structural and electronic properties of thallium compounds. AIP Conference Proceedings, 2016, , .	0.3	0
1698	Exploring the coordination change of vanadium and structure transformation of metavanadate MgV2O6 under high pressure. Scientific Reports, 2016, 6, 38566.	1.6	25
1699	Band structure and phonon properties of lithium fluoride at high pressure. AIP Conference Proceedings, 2016, , .	0.3	1
1700	Electronic hybridisation implications for the damage-tolerance of thin film metallic glasses. Scientific Reports, 2016, 6, 36556.	1.6	26
1701	The equation of state of 5-nitro-2,4-dihydro-1,2,4,-triazol-3-one determined via in-situ optical microscopy and interferometry measurements. Journal of Applied Physics, 2016, 119, 135904.	1.1	10
1702	High-throughput exploration of thermoelectric and mechanical properties of amorphous NbO2 with transition metal additions. Journal of Applied Physics, 2016, 120, .	1.1	11
1703	Equation of state of synthetic qandilite Mg2TiO4 at ambient temperature. Physics and Chemistry of Minerals, 2016, 43, 301-306.	0.3	6
1704	Self-consistent modeling of thermal and elastic properties of unconventional superconductor PuCoGa5. Physica B: Condensed Matter, 2016, 491, 17-21.	1.3	4
1705	Phase transformation and fluorescent enhancement of ErF3 at high pressure. Solid State Communications, 2016, 242, 30-35.	0.9	6
1706	Elasticity and phase transformation at high pressure in coesite from experiments and first-principles calculations. American Mineralogist, 2016, 101, 1190-1196.	0.9	5
1707	Tuning of the electronic and optical properties of single-layer boron nitride by strain and stress. Diamond and Related Materials, 2016, 66, 163-170.	1.8	24
1708	Choice of hybrid functional and basis set optimization to calculate the structural, electronic, mechanical, and vibrational properties of BaSnO3. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	10
1709	Tuning of the electronic and optical properties of single-layer indium nitride by strain and stress. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 372-377.	1.3	28
1710	Structural, elastic and thermodynamic properties of tetragonal and orthorhombic polymorphs of Sr₂GeN₂: an ab initio investigation. High Pressure Research, 2016, 36, 198-219.	0.4	15
1711	Applications of the modified Rydbergâ€“Vinet equation-of-state to the lower mantle and core. Modern Physics Letters B, 2016, 30, 1650015.	1.0	0
1712	Electronic structure and optical properties of (BeTe)_n/(ZnSe)_m superlattices. Materials Science-Poland, 2016, 34, 115-125.	0.4	9
1713	Crystal structure of the superconducting phase of sulfur hydride. Nature Physics, 2016, 12, 835-838.	6.5	392
1714	Electronic and structural properties of rare earth pnictides. Materials Science-Poland, 2016, 34, 45-52.	0.4	2

#	Article	IF	Citations
1715	Structural, elastic, electronic and thermodynamic investigations of neptunium chalcogenides: First-principles calculations. Chinese Journal of Physics, 2016, 54, 33-41.	2.0	30
1716	Electronic and magnetic structures and bonding properties of Ce 2 CrN 3 and U 2 CrN 3 from first principles. Computational Condensed Matter, 2016, 9, 13-18.	0.9	3
1717	The structural, elastic, electronic and optical properties of MgCu under pressure: A first-principles study. International Journal of Modern Physics B, 2016, 30, 1650199.	1.0	73
1718	How far away are accurate equations of state determinations? Some issues on pressure scales and non-hydrostaticity in diamond anvil cells. Matter and Radiation at Extremes, 2016, 1, 224-236.	1.5	6
1719	Thallium under extreme compression. Journal of Physics Condensed Matter, 2016, 28, 445401.	0.7	30
1720	Electronic and optical properties of beryllium carbide monolayer: First principles calculations. Optik, 2016, 127, 12063-12068.	1.4	3
1721	Drastic changes of electronic structure and crystal chemistry upon oxidation of SnII2TiO4E2 into SnIV2TiO6: An ab initio study. Solid State Sciences, 2016, 59, 25-31.	1.5	2
1722	Pressure-induced transition to Ni2In-type phase in lithium sulfide (Li2S). Solid State Sciences, 2016, 61, 220-224.	1.5	4
1723	Structural and anisotropic elastic properties of hexagonal MP (M = Ti, Zr, Hf) monophosphides determined by first-principles calculations. Philosophical Magazine, 2016, 96, 3654-3670.	0.7	24
1724	Superhard Rhenium/Tungsten Diboride Solid Solutions. Journal of the American Chemical Society, 2016, 138, 14398-14408.	6.6	48
1725	Compression of a multiphase mantle assemblage: Effects of undesirable stress and stress annealing on the iron spin state crossover in ferropericlase. Journal of Geophysical Research: Solid Earth, 2016, 121, 3377-3392.	1.4	17
1726	Equation of state and thermodynamic GrÃ¼neisen parameter of monoclinic 1,1-diamino-2,2-dinitroethylene. Journal of Physics Condensed Matter, 2016, 28, 395402.	0.7	3
1728	A comparative first-principles study on electronic structures and mechanical properties of ternary intermetallic compounds Al8Cr4Y and Al8Cu4Y: Pressure and tension effects. Journal of Physics and Chemistry of Solids, 2016, 98, 298-308.	1.9	15
1729	Elasticity of singleâ€crystal superhydrous phase B at simultaneous high pressureâ€temperature conditions. Geophysical Research Letters, 2016, 43, 8458-8465.	1.5	18
1730	Electronic and optical properties of beryllium sulfide monolayer: Under stress and strain conditions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2016, 380, 3546-3552.	0.9	11
1731	Synthesis of Ultra-incompressible sp³-Hybridized Carbon Nitride with 1:1 Stoichiometry. Chemistry of Materials, 2016, 28, 6925-6933.	3.2	41
1732	High-temperature superconductivity at high pressures for H3Si P1â^', H3P S1â^', and H3Cl S1â^'. Journal of Physics and Chemistry of Solids, 2016, 99, 105-110.	1.9	25
1733	Lattice dynamics, thermodynamics and elastic properties of C22-Zr6FeSn2 from first-principles calculations. Journal of Nuclear Materials, 2016, 479, 461-469.	1.3	12

#	Article	IF	Citations
1734	Elasticity of singleâ€crystal NAL phase at high pressure: A potential source of the seismic anisotropy in the lower mantle. Journal of Geophysical Research: Solid Earth, 2016, 121, 5696-5707.	1.4	7
1735	Pressure effect on the structural, electronic, and elastic properties and Debye temperature of Rh3Nb: first-principles calculations. RSC Advances, 2016, 6, 78028-78035.	1.7	6
1736	Elasticity of ferropericlase and seismic heterogeneity in the Earth's lower mantle. Journal of Geophysical Research: Solid Earth, 2016, 121, 8488-8500.	1.4	17
1737	Pressure induced elastic softening in framework aluminosilicate- albite (NaAlSi3O8). Scientific Reports, 2016, 6, 34815.	1.6	19
1738	A ZrNiAl related high-pressure modification of CeRuSn. Dalton Transactions, 2016, 45, 14216-14229.	1.6	6
1739	High-pressure structural study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MnF</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review B, 2016, 93, .	1.1	26
1740	Unusual onset of p-element magnetization in a two dimensional structure. Solid State Sciences, 2016, 60, 55-58.	1.5	3
1741	Theoretical study of phase stability and elastic properties ofT0.75Y0.75B14(Tâ€‰â€‰=â€‰â€‰Sc, Ti, V, Y, Zr, Nb, Si). Journal of Physics Condensed Matter, 2016, 28, 105501.	0.7	3
1742	Phase stability, elastic anisotropy and electronic structure of cubic MAl₂(M = Mg, Ca, Sr) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.8	23
1743	Electronic structural and bulk properties of ScSe: ab initio study. Physics of the Solid State, 2016, 58, 2081-2087.	0.2	5
1744	Monazite-type <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>SrCr</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> under compression. Physical Review B, 2016, 94, .	1.1	30
1745	Structural phase transition and electronic properties in samarium chalcogenides. AIP Conference Proceedings, 2016, , .	0.3	2
1746	Elastic and electronic properties calculations of the filled skutterudite CeOs₄P₁₂. Journal of Physics: Conference Series, 2016, 758, 012010.	0.3	3
1747	A Theoretical Investigation on Structural and Electronic Properties of MgTl. Journal of Metastable and Nanocrystalline Materials, 2016, 28, 27-31.	0.1	0
1748	High-pressure behavior of the polymorphs of FeOOH. American Mineralogist, 2016, 101, 1483-1488.	0.9	8
1749	High-pressure polymorphism of the electrochemically active organic molecule tetrahydroxy-p-benzoquinone. Journal of Molecular Structure, 2016, 1119, 71-77.	1.8	1
1750	Ab initio proposition of novel BCN3 hard material based on the intergrowth of wurtzite and pyrite-like motifs. Computational Condensed Matter, 2016, 7, 14-19.	0.9	2
1751	First-principles investigation of mechanical and electronic properties of LaAg5 Laves phase under pressure. Journal of Rare Earths, 2016, 34, 105-112.	2.5	0

#	Article	IF	Citations
1752	Resolving the structure of TiBe₁₂. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 277-280.	0.5	11
1753	Potassium chloride-bearing ice VII and ice planet dynamics. Geochimica Et Cosmochimica Acta, 2016, 174, 156-166.	1.6	4
1754	Elastic and thermodynamic properties of Fe3Ga from first-principles calculations. Solid State Communications, 2016, 230, 43-48.	0.9	9
1755	Recent progress and new directions in density functional theory based design of hard coatings. Surface and Coatings Technology, 2016, 286, 178-190.	2.2	56
1756	Electronic structure, thermodynamic properties and hydrogenation of LaPtIn and CePtIn compounds by ab-initio methods. Journal of Solid State Chemistry, 2016, 234, 48-54.	1.4	2
1757	Crystal structure, equation of state, and elasticity of hydrous aluminosilicate phase, topaz-OH (Al2SiO4(OH)2) at high pressures. Physics of the Earth and Planetary Interiors, 2016, 251, 24-35.	0.7	18
1758	Predicting finite-temperature properties of crystalline carbon dioxide from first principles with quantitative accuracy. Chemical Science, 2016, 7, 246-255.	3.7	64
1759	Pressure effect on the structural, electronic, optical and elastic properties of Zn0.75Be0.25O from first-principles calculations. Optik, 2016, 127, 1754-1761.	1.4	9
1760	The effect of subducting slabs in global shear wave tomography. Geophysical Journal International, 2016, 205, 1074-1085.	1.0	44
1761	Mechanical properties of metal dihydrides. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 035005.	0.8	17
1762	A density functional study on properties of a Cu3Zn material and CO adsorption onto its surfaces. Applied Surface Science, 2016, 363, 128-139.	3.1	12
1763	Structural, elastic and thermodynamic properties of Mo3Si and Mo3Ge. European Physical Journal B, 2016, 89, 1.	0.6	18
1764	Lithium halide monolayers: Structural, electronic and optical properties by first principles study. Physica E: Low-Dimensional Systems and Nanostructures, 2016, 83, 426-433.	1.3	11
1765	Thermodynamic properties of calcium ferrite-type MgAl2O4: A first principles study. Science China Earth Sciences, 2016, 59, 831-839.	2.3	4
1766	Elastic, Electronic, Optical and Thermal Properties of Na2Po: An Ab Initio Study. Journal of Electronic Materials, 2016, 45, 435-443.	1.0	1
1767	Pressure-induced structural transition of Y 2 Zr 2 O 7. Journal of Alloys and Compounds, 2016, 660, 446-449.	2.8	19
1768	Pressure-induced amorphization of YVO₄:Eu³⁺nanoboxes. Nanotechnology, 2016, 27, 025701.	1.3	19
1769	Phase stability, mechanical and thermodynamic properties of orthorhombic and trigonal MgSiN₂: an ab initio study. Phase Transitions, 2016, 89, 480-513.	0.6	69

#	Article	IF	Citations
1770	n s 2 n p 4 (n Â=Â4, 5) lone pair triplets whirling in M*F 2 E 3 (M*Â=ÂKr, Xe): Stereochemistry and ab initio analyses. Solid State Sciences, 2017, 64, 114-124.	1.5	5
1771	Pressure-induced fcc to hcp phase transition in Ni-based high entropy solid solution alloys. Applied Physics Letters, 2017, 110, .	1.5	62
1772	First-principles investigations of structural, mechanical, electronic and optical properties of U3Si2-type AlSc2Si2 under high pressure. Transactions of Nonferrous Metals Society of China, 2017, 27, 148-156.	1.7	8
1773	Electronic and optical properties of Î± -InX (X = S, Se and Te) monolayer: Under strain conditions. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 1313-1320.	0.9	39
1774	Elastic properties of amorphousT0.75Y0.75B14(Tâ€‰â€‰=â€‰â€‰Sc, Ti, V, Y, Zr, Nb) and the effect of O incorporation on bonding, density and elasticity (Tâ€²â€‰â€‰=â€‰â€‰Ti, Zr). Journal of Physics Condensed Matter, 2017, 29, 085404.	2.7	2
1775	Thermal expansion of SiC at high pressureâ€temperature and implications for thermal convection in the deep interiors of carbide exoplanets. Journal of Geophysical Research E: Planets, 2017, 122, 124-133.	1.5	29
1776	FeCr2O4spinel to near megabar pressures: Orbital moment collapse and site-inversion facilitated spin crossover. Physical Review B, 2017, 95, .	1.1	10
1777	Elastic anharmonicity of bcc Fe and Fe-based random alloys from first-principles calculations. Physical Review B, 2017, 95, .	1.1	4
1778	Pressure effect on the mechanical, electronic and thermodynamic properties of Ba2Bi3: First-principle calculations. Journal of Physics and Chemistry of Solids, 2017, 104, 293-303.	1.9	5
1779	Determination of the phase boundary of GaP using in situ high pressure and high-temperature X-ray diffraction. High Pressure Research, 2017, 37, 28-35.	0.4	12
1780	Ab initio study of the structural, electronic, elastic and thermal conductivity properties of SrClF with pressure effects. Philosophical Magazine, 2017, 97, 743-758.	0.7	8
1781	Elastic, electronic and optical properties of cubic Mg2C under hydrostatic pressure: Modified Beckeâ€“Johnson calculations. Optik, 2017, 136, 411-420.	1.4	9
1782	Unprecedented Al supersaturation in single-phase rock salt structure VAlN films by Al+ subplantation. Journal of Applied Physics, 2017, 121, .	1.1	40
1783	Abnormal Elasticity of Single-Crystal Magnesiosiderite across the Spin Transition in Earthâ€™s Lower Mantle. Physical Review Letters, 2017, 118, 036402.	2.9	34
1784	Pressure-induced phase transitions in HoDyYGdTb high-entropy alloy. Materials Letters, 2017, 196, 137-140.	1.3	39
1785	Ab initio study of the mechanical and electronic properties of scheelite-type XWO₄(X = Ca, Sr, Ba) compounds. International Journal of Modern Physics B, 2017, 31, 1750086.	1.0	22
1786	First-principles study of the structural, electronic, elastic, and thermodynamic properties of Rh3Sc compound under high pressure. Journal of Alloys and Compounds, 2017, 704, 484-490.	2.8	16
1787	Elastic properties and thermal conductivities of fluor-, chlor- and brom-barium apatites predicted by first-principles simulations. Philosophical Magazine, 2017, 97, 1708-1728.	0.7	1

#	Article	IF	Citations
1788	Structural Phase Transition of ThC Under High Pressure. Scientific Reports, 2017, 7, 96.	1.6	18
1789	Theoretical study of elastic and electronic properties of Al5Mo and Al5W intermetallics under pressure. Materials Chemistry and Physics, 2017, 197, 145-153.	2.0	13
1790	Electronic, elastic, lattice dynamic and thermal conductivity properties of Na₃OBr via first principles. Physica Status Solidi (B): Basic Research, 2017, 254, 1700089.	0.7	15
1791	Polyamorphism in Yb-based metallic glass induced by pressure. Scientific Reports, 2017, 7, 46762.	1.6	13
1792	A study of tantalum pentoxide Ta2O5 structures up to 28â€‰GPa. Journal of Applied Physics, 2017, 121, 175901.	1.1	3
1793	Hardness and compression behavior of niobium carbide. High Pressure Research, 2017, 37, 244-255.	0.4	8
1794	Electronic and optical properties of pentagonal-B₂C monolayer: A first-principles calculation. International Journal of Modern Physics B, 2017, 31, 1750044.	1.0	32
1795	Structural, mechanical, dynamical and electronic properties and high-pressure behavior of Mo2GeC: A first-principles study. Computational Materials Science, 2017, 137, 306-313.	1.4	7
1796	Strength and equation of state of molybdenum triboride under 80 GPa pressure, using radial X-ray diffraction. High Pressure Research, 2017, 37, 334-344.	0.4	2
1797	Structural stability of ultra-high temperature refractory material MoSi ₂ and Mo ₅ Si ₃ under high pressure. Chinese Physics B, 2017, 26, 053101.	0.7	11
1798	Phase stability and incompressibility of tungsten boride (WB) researched by in-situ high pressure x-ray diffraction. Physica B: Condensed Matter, 2017, 521, 6-12.	1.3	19
1799	Arsenic carbide monolayer: First principles prediction. Applied Surface Science, 2017, 423, 566-570.	3.1	45
1800	The nitridoborate nitrides Mg₃[BN₂]N and Ca₃[BN₂]N â€“ electronic structure and chemical bonding. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 433-439.	0.3	4
1801	The mechanism of anomalous hardening in transition-metal monoborides. Nanoscale, 2017, 9, 9112-9118.	2.8	21
1802	Correlative plasma-surface model for metastable Cr-Al-N: Frenkel pair formation and influence of the stress state on the elastic properties. Journal of Applied Physics, 2017, 121, .	1.1	27
1803	Elasticity of phase-Pi (Al3Si2O7(OH)3) â€“ A hydrous aluminosilicate phase. Physics of the Earth and Planetary Interiors, 2017, 269, 91-97.	0.7	8
1804	Ultra-stiff metallic glasses through bond energy density design. Journal of Physics Condensed Matter, 2017, 29, 265502.	0.7	11
1805	Investigation of thermodynamic stability, mechanical and electronic properties of superhard tetragonal B 4 CO 4 compound: Ab initio calculations. Computational Condensed Matter, 2017, 12, 1-8.	0.9	7

#	Article	IF	Citations
1806	Structural, elastic, electronic and optical properties of the novel quaternary diamond-like semiconductors Cu2MgSiS4 and Cu2MgGeS4. Solid State Sciences, 2017, 70, 21-35.	1.5	24
1807	Mechanical, elastic and thermodynamic properties of crystalline lithium silicides. Computational Materials Science, 2017, 134, 48-57.	1.4	4
1808	Physical properties and Debye temperature of Al7Cu2Fe alloy under various pressures analyzed by first-principles. Solid State Communications, 2017, 257, 6-10.	0.9	16
1809	Intrinsic Properties and Structure of AB2 Laves Phase ZrW2. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2017, 48, 3082-3089.	1.1	2
1810	Physical properties of fluorine based perovskites for vacuum-ultraviolet-transparent lens materials. Chinese Journal of Physics, 2017, 55, 893-903.	2.0	13
1811	Pressure effects on the thermodynamic and mechanical properties of zinc-blende ZnTe compound. European Physical Journal B, 2017, 90, 1.	0.6	4
1812	Electronic and optical properties of paratellurite TeO2 under pressure: A first-principles calculation. Optik, 2017, 139, 9-15.	1.4	24
1813	Experimental and theoretical high pressure study of calcium hydroxyaluminate phases. Cement and Concrete Research, 2017, 97, 1-10.	4.6	8
1814	Pressure-induced disordering and phase transformations in Eu₂Zr₂O₇ pyrochlore. High Pressure Research, 2017, 37, 256-266.	0.4	9
1815	Strong p -magnetism in carbon suboxide C 2 O devised from first principles. Chemical Physics Letters, 2017, 674, 115-119.	1.2	4
1816	New pressure-induced polymorphic transitions of anhydrous magnesium sulfate. Dalton Transactions, 2017, 46, 5058-5068.	1.6	23
1817	Ab Initio Study of Electronic Structure, Elastic and Transport Properties of Fluoroperovskite LiBeF3. Journal of Electronic Materials, 2017, 46, 2205-2210.	1.0	19
1818	Magnesium carbide monolayer: A novel quasi-planar semiconductor. Superlattices and Microstructures, 2017, 102, 134-140.	1.4	18
1819	Metal mono-chalcogenides ZnX and CdX (X = S, Se and Te) monolayers: Chemical bond and optical interband transitions by first principles calculations. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 663-670.	0.9	43
1820	Interatomic potential that describes martensitic phase transformations in pure lithium. Computational Materials Science, 2017, 129, 202-210.	1.4	10
1821	Electronic and optical investigations of Be 2 C monolayer: Under stress and strain conditions. Materials Research Bulletin, 2017, 88, 49-55.	2.7	40
1822	Zinc-Blende MnTe Under Pressure: Structural, Mechanical, and Optical Properties from Ab Initio Calculation. Journal of Superconductivity and Novel Magnetism, 2017, 30, 1533-1538.	0.8	3
1823	Elastic, thermodynamic and optical behavior of V2AC (A= Al, Ga) MAX phases. Results in Physics, 2017, 7, 3634-3639.	2.0	31

#	Article	IF	Citations
1824	First-principles investigation of the structural, mechanical and thermodynamic properties of Al 2 Cu phase under various pressure and temperature conditions. Solid State Communications, 2017, 268, 44-50.	0.9	31
1825	A correlative experimental and ab initio approach to improve the fracture behavior of Mo thin films by alloying with Cu. Applied Physics Letters, 2017, 111, 134101.	1.5	5
1826	First-principles investigations of the electronic and magnetic structures and the bonding properties of uranium nitride fluoride (UNF). Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2017, 72, 725-730.	0.3	1
1827	Hydrostatic pressure effects on the structural, elastic and thermodynamic properties of the complex transition metal hydrides A₂OsH₆ (Aâ€‰=â€‰Mg, Ca, Sr and Ba). High Pressure Research, 2017, 37, 558-578.	0.4	13
1828	Experimental and theoretical exploration of mechanical stability of Pt/NbO2interfaces for thermoelectric applications. Journal Physics D: Applied Physics, 2017, 50, 455502.	1.3	4
1829	Pressure-induced abnormal insulating state in triangular layered cobaltite Li_xCoO₂ (x = 0.9). Journal of Materials Chemistry A, 2017, 5, 19390-19397.	5.2	9
1830	Thermodynamic properties of liquid sodium under high pressure. AIP Advances, 2017, 7, .	0.6	7
1831	An experimental and first-principles investigation of noncentrosymmetric cubic Re3W. Journal of Alloys and Compounds, 2017, 728, 984-991.	2.8	3
1832	First-principles study of structural, elastic, electronic, thermodynamic and optical properties of Sc 3 Sn X (X Â=ÂB, C). Computational Condensed Matter, 2017, 13, 41-48.	0.9	5
1833	Structural, mechanical, electronic and thermal properties of the newly predicted NB2 from ab initio calculations. Chinese Journal of Physics, 2017, 55, 2540-2547.	2.0	5
1834	Stoichiometric Î´-NbN: The Most Incompressible Cubic Transition Metal Mononitride. Physica Status Solidi (B): Basic Research, 2017, 254, 1700063.	0.7	3
1835	(CaO) IrO2 (n = 1, 2, 4) family: Chemical scissors effects of CaO on structural characteristics correlated to physical properties. Ab initio study. Journal of Solid State Chemistry, 2017, 255, 82-88.	1.4	10
1836	The pressureâ€“temperature phase diagram of pure Co based on first-principles calculations. Physical Chemistry Chemical Physics, 2017, 19, 22061-22068.	1.3	2
1837	Direct Measurement of the Magnetocaloric Effect in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>La</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>Fe</mml:mi><mml:mo>,</mml:mo><mml:mi>Si</mml:mi><mml:mo>,</mml:mo><mml:mi>Co</mml:mi> In Pulsed Magnetic Fields. Physical Review Applied, 2017, 8, .	1.5	28
1838	First-principles prediction of a novel cadmium disulfide monolayer (penta-CdS2): Indirect to direct band gap transition by strain engineering. Chemical Physics Letters, 2017, 685, 310-315.	1.2	45
1839	Deformation behavior of Re alloyed Mo thin films on flexible substrates: In situ fragmentation analysis supported by first-principles calculations. Scientific Reports, 2017, 7, 7374.	1.6	17
1840	Effect of pressure on structural, elastic and mechanical properties of transition metal hydrides Mg7TMH16 (TMÂ=ÂSc, Ti, V, Y, Zr and Nb): First-principles investigation. Journal of Physics and Chemistry of Solids, 2017, 111, 229-237.	1.9	7
1841	Phase transition and equation of state of dense hydrous silica up to 63ÂGPa. Journal of Geophysical Research: Solid Earth, 2017, 122, 6972-6983.	1.4	22

#	Article	IF	Citations
1842	Thermodynamic characterization of lithium monosilicide (LiSi) by means of calorimetry and DFT-calculations. International Journal of Materials Research, 2017, 108, 942-958.	0.1	8
1843	<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:mn>2</mml:mn></mml:msub><mml:mr Glass Density to Lower-Mantle Pressures. Physical Review Letters, 2017, 119, 215701.	2.9	38
1844	Crystallite size-dependent metastable phase formation of TiAlN coatings. Scientific Reports, 2017, 7, 16096.	1.6	34
1845	First principles investigation of structural, mechanical, dynamical and thermodynamic properties of AgMg under pressure. Materials Research Express, 2017, 4, 126507.	0.8	0
1846	Thermal expansion of Pd-based metallic glasses by ab initio methods and high energy X-ray diffraction. Scientific Reports, 2017, 7, 15744.	1.6	14
1847	First-Principles Study on Polymorphs of AgVO₃: Assessing to Structural Stabilities and Pressure-Induced Transitions. Journal of Physical Chemistry C, 2017, 121, 27624-27642.	1.5	22
1848	First-principles calculations of structural and thermodynamic properties of Î² -PbO. Chinese Physics B, 2017, 26, 116501.	0.7	5
1849	Pressure Impact on the Stability and Distortion of the Crystal Structure of CeScO₃. Inorganic Chemistry, 2017, 56, 8363-8371.	1.9	18
1850	Site-specific spin crossover in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">F</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> post-spinel under high pressure up to nearly a megabar. Physical Review B, 2017, 96, .	1.1	8
1851	Extended metastable Al solubility in cubic VAlN by metal-ion bombardment during pulsed magnetron sputtering: film stress vs subplantation. Journal of Applied Physics, 2017, 122, .	1.1	19
1852	Critical behavior of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">M</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â€“</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mi mathvariant="normal">F</mml:mi><mml:msub><mml:mi mathvariant="normal">e</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">O	1.1	8
1853	The EOS of Iɛ-NTO through high-pressure microscopy-interferometry measurements. AIP Conference Proceedings, 2017, , .	0.3	0
1854	A first-principles study of elastic, magnetic, and structural properties of PrX2 (X=Fe, Mn, Co) compounds. Journal of Magnetism and Magnetic Materials, 2017, 423, 447-452.	1.0	9
1855	Combinatorial synthesis of high entropy alloys: Introduction of a novel, single phase, body-centered-cubic FeMnCoCrAl solid solution. Journal of Alloys and Compounds, 2017, 691, 683-689.	2.8	60
1856	Phase formation of Nb2AlC investigated by combinatorial thin film synthesis and ab initio calculations. Journal of the European Ceramic Society, 2017, 37, 35-41.	2.8	7
1857	Principles of Energetic Structure and Excitation-Energy Transfer Based on High-Pressure Measurements. , 2017, , 67-151.		6
1858	Shear induced weakening of the hydrogen bonding lattice of the energetic material 5,5â€²-Hydrazinebistetrazole at high-pressure. Journal of Molecular Structure, 2017, 1129, 313-318.	1.8	6
1859	Thermoelastic properties of grossularâ€“andradite solid solution at high pressures and temperatures. Physics and Chemistry of Minerals, 2017, 44, 137-147.	0.3	8

#	Article	IF	Citations
1860	Elasticity under pressure and thermal property of Mg2La from first-principles calculations. Journal of Central South University, 2017, 24, 1713-1719.	1.2	1
1861	Elastic, thermodynamic, electronic, and optical properties of recently discovered superconducting transition metal boride NbRuB: An ab-initio investigation. Chinese Physics B, 2017, 26, 106201.	0.7	31
1862	Noncovalent Interactions in Molecular Crystals. , 2017, , 303-331.		7
1863	Possible bcc â† sc phase transitions in Caâ€“Sr solid solutions under pressure. Physics of Metals and Metallography, 2017, 118, 723-730.	0.3	1
1864	Insight into solid-solution strengthened bulk and stacking faults properties in Ti alloys: a comprehensive first-principles study. Journal of Materials Science, 2018, 53, 7493-7505.	1.7	17
1865	Understanding How Bonding Controls Strength Anisotropy in Hard Materials by Comparing the High-Pressure Behavior of Orthorhombic and Tetragonal Tungsten Monoboride. Journal of Physical Chemistry C, 2018, 122, 5647-5656.	1.5	10
1866	First principle studies of structural, magnetic and elastic properties of orthorhombic rare-earth diaurides intermetallics RAu2 (R=La, Ce, Pr and Eu). Materials Chemistry and Physics, 2018, 212, 44-50.	2.0	11
1867	Anomalous compression behaviour in Nd2O3 studied by x-ray diffraction and Raman spectroscopy. AIP Advances, 2018, 8, .	0.6	19
1868	Experimental and Theoretical Study of Bi₂O₂Se Under Compression. Journal of Physical Chemistry C, 2018, 122, 8853-8867.	1.5	46
1869	Strength and texture of sodium chloride to 56â€‰GPa. Journal of Applied Physics, 2018, 123, 135901.	1.1	10
1870	Interplay between structural and magnetic-electronic responses of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>FeA</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> to a megabar: Site inversion and spin crossover. Physical Review B, 2018, 97, .	1.1	5
1871	Pressure and Temperature Dependent Structural Studies on Hollandite Type Ferrotitanate and Crystal Structure of a High Pressure Phase. Inorganic Chemistry, 2018, 57, 2157-2168.	1.9	4
1872	Strong electronic metal-support interaction of Pt/CeO2 enables efficient and selective hydrogenation of quinolines at room temperature. Journal of Catalysis, 2018, 359, 101-111.	3.1	146
1873	Investigation of different physical aspects such as structural, mechanical, optical properties and Debye temperature of Fe₂ScM (M=P and As) semiconductors: A DFT-based first principles study. International Journal of Modern Physics B, 2018, 32, 1850121.	1.0	33
1874	Origin of negative thermal expansion in Zn₂GeO₄ revealed by high pressure study. Journal Physics D: Applied Physics, 2018, 51, 095303.	1.3	11
1875	Evidence of low-symmetry phases in pressure-dependent Raman spectroscopic study of BaTiO3. Journal of Materials Science, 2018, 53, 7224-7232.	1.7	8
1876	A comprehensive study of the high-pressureâ€“temperature phase diagram of silicon. Journal of Materials Science, 2018, 53, 7475-7485.	1.7	14
1877	Highâ€Pressure Geophysical Properties of Fcc Phase FeH_X. Geochemistry, Geophysics, Geosystems, 2018, 19, 305-314.	1.0	37

#	Article	IF	Citations
1878	Vanadium Diboride (VB₂) Synthesized at High Pressure: Elastic, Mechanical, Electronic, and Magnetic Properties and Thermal Stability. Inorganic Chemistry, 2018, 57, 1096-1105.	1.9	64
1879	Pressure induced solid-solid reconstructive phase transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LiGa</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> dominated by elastic strain. Physical Review B, 2018, 97, .	1.1	10
1880	Pressure-dependent mechanical and thermodynamic properties of newly discovered cubic Na 2 He. Chinese Journal of Physics, 2018, 56, 231-237.	2.0	16
1881	From quantum to continuum mechanics: studying the fracture toughness of transition metal nitrides and oxynitrides. Materials Research Letters, 2018, 6, 142-151.	4.1	30
1882	High-Pressure Formation of Cobalt Polyhydrides: A First-Principle Study. Inorganic Chemistry, 2018, 57, 181-186.	1.9	22
1883	Computational thermomechanics of crystalline rock, Part I: A combined multi-phase-field/crystal plasticity approach for single crystal simulations. Computer Methods in Applied Mechanics and Engineering, 2018, 338, 657-691.	3.4	49
1884	Theoretical Prediction of an Antimony-Silicon Monolayer $$(hbox {penta-Sb}_{2}hbox) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 507 Td ({S 2290-2297.	1.0	31
1885	First-principles study of mechanical and magnetic properties of transition metal (M) nitrides in the cubic M4N structure. Journal of Physics and Chemistry of Solids, 2018, 120, 197-206.	1.9	41
1886	Spreadsheets to calculatePâ€“Vâ€“Trelations, thermodynamic and thermoelastic properties of silicates in the MgSiO₃â€“MgO system. High Pressure Research, 2018, 38, 193-211.	0.4	10
1887	The Nature of Bonding in Bulk Tellurium Composed of One-Dimensional Helical Chains. Inorganic Chemistry, 2018, 57, 5083-5088.	1.9	49
1888	Recent progress on the characterization of the high-pressure behaviour of AVO4 orthovanadates. Progress in Materials Science, 2018, 97, 123-169.	16.0	105
1889	Theoretical exploring the mechanical and electrical properties of tI12-B6C4O2. Computational Materials Science, 2018, 150, 259-264.	1.4	4
1890	First principles study of structural, electronic and optical properties of perovskites CaZrO 3 and CaHfO 3 in cubic phase. Solid State Communications, 2018, 275, 29-34.	0.9	41
1891	Structural phase transition, strength, and texture in vanadium at high pressure under nonhydrostatic compression. Chinese Physics B, 2018, 27, 036101.	0.7	5
1892	High pressure in solid state chemistry: Combined experimental and modeling approaches for assessing and predicting properties. Solid State Sciences, 2018, 80, 178-195.	1.5	1
1893	The structural, mechanical and thermodynamic properties of Ti-B compounds under the influence of temperature and pressure: First-principles study. Materials Chemistry and Physics, 2018, 209, 200-207.	2.0	26
1894	Atomistic insights into the effect of polymerization on the thermophysical properties of 2-D C60 molecular solids. Carbon, 2018, 133, 267-274.	5.4	7
1895	Effect of Explosion on Materials. Engineering Materials, 2018, , 1-152.	0.3	0

#	Article	IF	Citations
1896	Selective Semihydrogenation of Phenylacetylene to Styrene Catalyzed by Alloyed Palladium/Gold Catalysts Anchored on Cerium Oxide. ChemNanoMat, 2018, 4, 472-476.	1.5	11
1897	First-principles investigations on elastic, thermodynamic and lattice thermal conductivity of topological insulator LaAs. Philosophical Magazine, 2018, 98, 1900-1918.	0.7	11
1898	Single-crystal elasticity of MgAl2O4-spinel up to 10.9 GPa and 1000 K: Implication for the velocity structure of the top upper mantle. Earth and Planetary Science Letters, 2018, 481, 41-47.	1.8	13
1899	Stability and high-temperature superconductivity in hydrogenated chlorine. Quantum Studies: Mathematics and Foundations, 2018, 5, 23-33.	0.4	6
1900	First-principles study of the third-order elastic constants and related anharmonic properties in refractory high-entropy alloys. Acta Materialia, 2018, 142, 29-36.	3.8	25
1901	Atomic and electronic basis for solutes strengthened (010) anti-phase boundary of L12 Co3(Al, TM): A comprehensive first-principles study. Acta Materialia, 2018, 145, 30-40.	3.8	40
1902	Ab initio dynamical stability of tungsten at high pressures and high temperatures. Computational Materials Science, 2018, 144, 32-35.	1.4	10
1903	Structural Phase Transition, Electronic, and Mechanical Properties of Beryllium Oxide: Temperature and Pressureâ€induced Effects. Physica Status Solidi (B): Basic Research, 2018, 255, 1700524.	0.7	2
1904	Radial X-ray diffraction study of the static strength and texture of tungsten to 96ÂGPa. Solid State Communications, 2018, 269, 83-89.	0.9	6
1905	Tuning the electronic and optical properties of XP(Xâ€¯=â€¯Al,Ga) monolayer semiconductors using biaxial strain effect: Modified Becke-Johnson calculations. Chemical Physics Letters, 2018, 691, 181-189.	1.2	18
1906	Pressureâ€“induced structural changes of basaltic glass. Journal of Mineralogical and Petrological Sciences, 2018, 113, 286-292.	0.4	5
1907	Evaluating physical properties of the orthorhombic crystal phase of ammonium perchlorate using a Class II force field. Journal of Chemical Physics, 2018, 149, 244502.	1.2	7
1908	Structure, Elastic Properties, Thermodynamic and Electronic Properties of Al-Y Alloy Under Pressure from First-principles Calculations. Rare Metal Materials and Engineering, 2018, 47, 1325-1332.	0.8	7
1909	First-principles Study on Effect of Pressure and Temperature on Mechanical, Thermodynamic Properties, and Electronic Structure of Ni3Al Alloy. Rare Metal Materials and Engineering, 2018, 47, 3651-3658.	0.8	1
1910	Equation of State of a Natural Chromian Spinel at Ambient Temperature. Minerals (Basel, Switzerland), 2018, 8, 591.	0.8	6
1911	Atomistic Simulations of Pure Tin Based on a New Modified Embedded-Atom Method Interatomic Potential. Metals, 2018, 8, 900.	1.0	22
1912	Six Polymorphs of Sodium Chloride upon Depth-Sensing Macroindentation with Unusual Long-Range Cracks Requiring 30 N Load. Journal of Material Science & Engineering, 2018, 07, .	0.2	12
1913	Thermoelastic Properties of Aluminous Phases in MORB from Firstâ€principles Calculation: Implications for Earth's Lower Mantle. Journal of Geophysical Research: Solid Earth, 2018, 123, 10,583.	1.4	4

#	Article	IF	Citations
1914	Peculiar magnetic properties of NC6 and NC12 layered compounds from first principles. Journal of Theoretical and Applied Physics, 2018, 12, 209-217.	1.4	0
1915	Fragmentation and stress diversification in diamond powder under high pressure. Journal of Applied Physics, 2018, 124, .	1.1	24
1916	Anharmonicity-induced first-order isostructural phase transition of zirconium under pressure. Physical Review B, 2018, 98, .	1.1	15
1917	Investigation on the structural, elastic, electronic, and magnetic properties of half-metallic $$hbox {Co}_{2}hbox {MnSi}$$ Co 2 MnSi and CoMnIrSi via first-principles calculations. Journal of Computational Electronics, 2018, 17, 1470-1477.	1.3	18
1918	First principles investigation of pressure dependent stability, phonon, Debye temperature, physical, mechanical and thermodynamic properties of Rh3Al intermetallic compound. Molecular Simulation, 2018, 44, 1554-1563.	0.9	2
1919	B1 to B2 structural phase transition in LiF under pressure. AIP Conference Proceedings, 2018, , .	0.3	2
1920	Unusual optical isotropy in anisotropic alkali metal perchlorates MClO₄(Mâ€‰â€‰=â€‰â€‰Li, Na,) Tj ETQq0 0 0	0.7	3
1921	Band gap behavior of thallium phosphide and gallium phosphide binary compounds and Ga_x Tl_{1-x} P ternary alloys. Journal of Physics: Conference Series, 2018, 1081, 012011.	0.3	0
1922	Pressure-induced ordering phase transition in high-entropy alloy. Intermetallics, 2018, 103, 63-66.	1.8	10
1923	Metalliclike thermoelectric Ti-V oxide nanocomposites. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2018, 36, .	0.9	1
1924	Investigation on structural, electronic, optical and elastic properties of thallium phosphide and gallium phosphide binary compounds and their ternary alloys and superlattices. Computational Condensed Matter, 2018, 17, e00344.	0.9	7
1925	Search for new d0 half-metallic materials: theoretical investigation on KCaC1â^'xSi (x = 0; 0.25; 0.5; 0.75) Tj ETQq1 1 0.784314 rgBT /	2.0	7
1926	Elastic stability of CO2 phase I under high temperature and pressure. Physical Review B, 2018, 98, .	1.1	2
1927	Metastability in high-entropy alloys: A review. Journal of Materials Research, 2018, 33, 2924-2937.	1.2	85
1928	Compression behavior and phase transition of Î² -Si ₃ N ₄ under high pressure. Chinese Physics B, 2018, 27, 056101.	0.7	3
1929	Structural, mechanical and electronic properties of (TaNbHfTiZr)C high entropy carbide under pressure: Ab initio investigation. Physica B: Condensed Matter, 2018, 550, 163-170.	1.3	75
1930	Electrical resistivity modulation of thermoelectric iron based nanocomposites. Vacuum, 2018, 157, 384-390.	1.6	3
1931	Pressure-induced structural and electronic transitions in kesterite-type Cu2ZnSnS4. Journal of Applied Physics, 2018, 124, 085905.	1.1	7

#	Article	IF	Citations
1932	Strongly correlated intermetallic rare-earth monoaurides (Ln-Au): Ab-initio study. Journal of Rare Earths, 2018, 36, 1106-1111.	2.5	9
1933	First principles study on structural, electronic and optical properties of Ga 1â^'x B x P ternary alloys () Tj ETQq1 1 0.784314 rgBT /Over 1942-1949.	0.9	10
1934	Structural, elastic, and optoelectronic properties of ternary alloyBxAl1â^'xAs. Physica B: Condensed Matter, 2018, 544, 52-60.	1.3	2
1935	Density functional study of the phase stability and Raman spectra of Yb₂O₃, Yb₂SiO₅ and Yb₂Si₂O₇ under pressure. Physical Chemistry Chemical Physics, 2018, 20, 16518-16527.	1.3	30
1936	Universal link of magnetic exchange and structural behavior under pressure in chromium spinels. Physical Review B, 2018, 97, .	1.1	24
1937	Insight into the structural, elastic, electronic and thermal properties of YMgX₄ (X = Co,) Tj ETQq1 1 0.784314 rgBT /Over	0.8	9
1938	Pressure Impact on the Crystal Structure, Optical, and Transport Properties in Layered Oxychalcogenides BiCuChO (Ch = S, Se). Journal of Physical Chemistry C, 2018, 122, 15929-15936.	1.5	15
1939	Comparative study of 9R and 12R hexagonal diamond by first-principles calculations. International Journal of Modern Physics B, 2018, 32, 1850211.	1.0	2
1940	Double-A layered ceramics. , 2018, , 331-354.		2
1941	Third-order elastic constants and anharmonic properties of three fcc high-entropy alloys from first-principles. Journal of Alloys and Compounds, 2018, 764, 906-912.	2.8	11
1942	Tuning magnetic coercivity with external pressure in iron-rhenium based ferrimagnetic double perovskites. Physical Review B, 2018, 98, .	1.1	12
1943	Copper Delafossites under High Pressureâ€"A Brief Review of XRD and Raman Spectroscopic Studies. Crystals, 2018, 8, 255.	1.0	23
1944	Pressure-induced disruption of the local environment of Fe-Fe dimers in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>FeGa</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> by metallization. Physical Review B, 2018, 98, .	1.1	3
1945	Superconducting and magnetic phase diagram of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>RbEuFe</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>CsEuFe</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> at high pressure. Physical Review B, 2018, 98, .	1.1	31
1946	Effect of High Pressure on the Crystal Structure and Vibrational Properties of Olivine-Type LiNiPO₄. Inorganic Chemistry, 2018, 57, 10265-10276.	1.9	16
1947	First Principles Study of Topochemical Effects and Electronic Structure Relationships between ANCl and A2N2Se (A = Zr, Ce) Assimilated to Pseudo-Binaries: {AN}Cl and {A2N2}Se. Computation, 2018, 6, 30.	1.0	1
1948	Structural Phase Transition and Compressibility of CaF2 Nanocrystals under High Pressure. Crystals, 2018, 8, 199.	1.0	10
1949	Effects of pressure on the structure and lattice dynamics of ammonium perchlorate: A combined experimental and theoretical study. Journal of Chemical Physics, 2018, 149, 034501.	1.2	6

#	Article	IF	Citations
1950	A unified model for the uniaxial and hydrostatic pressure dependence of T in YBa2Cu3O (xâ€¯â‰ˆâ€¯6.95â€“7.0). Computational Materials Science, 2018, 153, 268-274.	1.4	1
1951	Equation of state, phase stability, and phase transformations of uranium-6 wt.â€‰% niobium under high pressure and temperature. Journal of Applied Physics, 2018, 123, .	1.1	9
1952	Melts Under Extreme Conditions From Shock Experiments. , 2018, , 387-418.		5
1953	Density functional theory study of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mo stretchy="false">{</mml:mo><mml:mn>1</mml:mn><mml:mspace width="0.12em" /><mml:mn>0</mml:mn><mml:mspace width="0.12em" /><mml:mover accent="true"><mml:mrow><mml:mn>1</mml:mn></mml:mrow><mml:mrow><mml:mo>Â¯</mml:mo></mml:mrow></mml:mover><mml:mo stretchy="false">}</mml:mo></mml:mrow></mml:math> twin boundaries of Zn under high pressure. C	1.4	5
1954	Chemical composition and stress dependence of the elastic properties of Î·-(Fe,Mn)3AlC thin films. Scripta Materialia, 2018, 153, 49-53.	2.6	7
1955	Structural, Mechanical and Thermodynamic Properties of Cu2CoXS4 (X = Si, Ge, Sn) Studied by Density Functional Theory. Semiconductors, 2018, 52, 414-419.	0.2	2
1956	High-pressure investigations on the semi-Heusler compound CuMnSb. Physical Review B, 2018, 98, .	1.1	4
1957	A new antimony carbide monolayer: An indirect semiconductor with a tunable band gap. Chemical Physics Letters, 2018, 708, 188-193.	1.2	14
1958	Ab-initio investigation of structural, electronic, magnetic, and thermodynamic properties of XPt3 (X=V, Cr, Mn, and Fe) intermetallic compounds. Computational Condensed Matter, 2018, 16, e00328.	0.9	3
1959	In situ high-pressure measurement of crystal solubility by using neutron diffraction. Review of Scientific Instruments, 2018, 89, 053906.	0.6	6
1960	High pressure high temperature devitrification of Fe78B13Si9 metallic glass with simultaneous x-ray structural characterization. Journal of Applied Physics, 2018, 123, 215901.	1.1	0
1961	Structural, elastic and optoelectronic properties of Sr-based perovskite-type oxides SrXO3 (Mâ€“â€“Th, Zr) via first-principles calculations. Chinese Journal of Physics, 2018, 56, 1515-1524.	2.0	10
1962	First principles study of structural, electronic, elastic and thermodynamic properties of cubic HfO2 under pressure. Physica B: Condensed Matter, 2018, 545, 55-61.	1.3	15
1963	Pressure-induced structural and electronic transitions, metallization, and enhanced visible-light responsiveness in layered rhenium disulphide. Physical Review B, 2018, 97, .	1.1	35
1964	Ab Initio Investigation of Structural, Electronic, and Magnetic Properties of Cr-Doped ZnS and ZnSe in Wurtzite Structure. Journal of Superconductivity and Novel Magnetism, 2019, 32, 413-423.	0.8	4
1965	Magnetization on nitrogen in extended honeycomb carbon layers from first principles: Case studies of CxN (xâ€“=â€“2, 6, 12). Journal of Magnetism and Magnetic Materials, 2019, 469, 46-51.	1.0	3
1966	Buckling strain effects on electronic and optical aspects of penta-graphene nanostructure. Superlattices and Microstructures, 2019, 133, 106217.	1.4	14
1967	Intermetallic M Pt₃ (M = Ti, Zr, Hf): Elastic, electronic, optical and thermal properties. International Journal of Modern Physics B, 2019, 33, 1950189.	1.0	10

#	Article	IF	Citations
1968	When a defect is a pathway to improve stability: a case study of the L12 Co3TM superlattice intrinsic stacking fault. Journal of Materials Science, 2019, 54, 13609-13618.	1.7	16
1969	Synthesis and High-Pressure Mechanical Properties of Superhard Rhenium/Tungsten Diboride Nanocrystals. ACS Nano, 2019, 13, 10036-10048.	7.3	12
1970	Structural Characterization of Aurophilic Gold(I) Iodide under High Pressure. Inorganic Chemistry, 2019, 58, 10665-10670.	1.9	15
1971	High-pressure isothermal equation of state of composite materials: A case study of LX-17 polymer bonded explosive. Applied Physics Letters, 2019, 115, 051902.	1.5	4
1972	Runaway climate cooling of ocean planets in the habitable zone: a consequence of seafloor weathering enhanced by melting of high-pressure ice. Monthly Notices of the Royal Astronomical Society, 2019, 488, 1580-1596.	1.6	13
1973	Improving the Calculations of Electronic and Magnetic Properties of Sr2CrMoO6 Double-Perovskite with LDA+U and mBJ Potential. Journal of Electronic Materials, 2019, 48, 6406-6413.	1.0	8
1974	Elastic, electronic, chemical bonding and thermodynamic properties of the ternary nitride Ca4TiN4: Ab initio predictions. Journal of Molecular Graphics and Modelling, 2019, 92, 74-85.	1.3	5
1975	Nitrided FeNi: Chemical versus magnetovolume effects from ab initio. Journal of Magnetism and Magnetic Materials, 2019, 491, 165555.	1.0	1
1976	Anomalous elastic behavior of phase egg, AlSiO3(OH), at high pressures. American Mineralogist, 2019, 104, 130-139.	0.9	7
1977	Elasticity of single-crystal low water content hydrous pyrope at high-pressure and high-temperature conditions. American Mineralogist, 2019, 104, 1022-1031.	0.9	9
1978	Equation of state and strain-induced stabilization of Î´-phase stabilized plutonium alloys. Journal of Nuclear Materials, 2019, 524, 54-59.	1.3	2
1979	Stability and Compressibility of Cation-Doped High-Entropy Oxide MgCoNiCuZnO₅. Journal of Physical Chemistry C, 2019, 123, 17735-17744.	1.5	50
1980	Phase stability and electronic structure of iridium metal at the megabar range. Scientific Reports, 2019, 9, 8940.	1.6	17
1981	How to Quench Ferromagnetic Ordering in a CN-Bridged Ni(II)-Nb(IV) Molecular Magnet? A Combined High-Pressure Single-Crystal X-Ray Diffraction and Magnetic Study. Magnetochemistry, 2019, 5, 33.	1.0	9
1982	Biaxial strain and external electric field effects on the electronic structure of hydrogenated GaN monolayer. Superlattices and Microstructures, 2019, 136, 106270.	1.4	13
1983	First-principles design of strong solids: Approaches and applications. Physics Reports, 2019, 826, 1-49.	10.3	31
1984	Computational investigation of the structural, electronic, optical and thermoelectric properties of T2-Al2MgC2 compound. Journal of Solid State Chemistry, 2019, 280, 120999.	1.4	6
1985	Finite Strain Analysis of Shear and Compressional Wave Velocities. Journal of Geophysical Research: Solid Earth, 2019, 124, 11651-11677.	1.4	3

#	Article	IF	Citations
1986	Structural stability of uranium carbide (UC) under high pressure: ab-initio study. Computational Condensed Matter, 2019, 21, e00431.	0.9	8
1987	Melting curve and phase diagram of vanadium under high-pressure and high-temperature conditions. Physical Review B, 2019, 100, .	1.1	42
1988	Intrinsic Thermal Shock Behavior of Common Rutile Oxides. Physics, 2019, 1, 290-300.	0.5	6
1989	High pressure studies on Î±-cristobalite form of Al_{0.5}Ga_{0.5}PO₄: hydrostatic versus non-hydrostatic conditions. High Pressure Research, 2019, 39, 81-91.	0.4	2
1990	Structural, electronic and elastic properties of ZnGeN2 and WZ-GaN under different hydrostatic pressures: A first-principle study. International Journal of Modern Physics B, 2019, 33, 1950297.	1.0	3
1991	First principles investigation on elastic, optoelectronic and thermoelectric properties of KYX (XÂ= Ge,) Tj ETQq1 1 0.784314 rgBT /Ove	1.3	18
1992	First-principles investigation into the effect of pressure on structural, electronic, elastic, elastic anisotropy, thermoelectric and thermodynamic properties of CaMgSi. Results in Physics, 2019, 14, 102483.	2.0	7
1993	Thermodynamic description of the Coâ€“Niâ€“Ta system. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 66, 101649.	0.7	13
1994	Effects of Zn and Cr additions on precipitation and creep behavior of a dilute Alâ€“Zrâ€“Erâ€“Si alloy. Acta Materialia, 2019, 181, 249-261.	3.8	35
1995	Stress-Dependent Elasticity of TiAlN Coatings. Coatings, 2019, 9, 24.	1.2	20
1996	Effects of pressure on the structure and lattice dynamics of Î±-glycine: a combined experimental and theoretical study. CrystEngComm, 2019, 21, 4457-4464.	1.3	16
1997	High-Pressure Third-Order Elastic Constants of MgO Single Crystal: First-Principles Investigation. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2019, 74, 447-456.	0.7	3
1998	Theoretical study of electronic structure, thermoelectric and thermodynamic properties of 2H-AgAlO2. Physica B: Condensed Matter, 2019, 558, 109-115.	1.3	6
1999	Understanding the mechanism of hardness enhancement in tantalum-substituted tungsten monoboride solid solutions. Journal of Applied Physics, 2019, 125, .	1.1	9
2000	First principles investigation into the phase stability and enhanced hardness of TiN-ScN and TiN-YN alloys. Thin Solid Films, 2019, 688, 137284.	0.8	16
2001	Elasticity of single-crystal periclase at high pressure and temperature: The effect of iron on the elasticity and seismic parameters of ferropericlase in the lower mantle. American Mineralogist, 2019, 104, 262-275.	0.9	27
2002	FP-LMTO study of structural, electronic and optical properties of wurtzite (CdS)n/(CdSe)n superlattices. Chinese Journal of Physics, 2019, 60, 462-472.	2.0	1
2003	Equation of state of LiNi0.8Co0.1Mn0.1O2 at high pressure. Solid State Communications, 2019, 299, 113656.	0.9	9

#	Article	IF	Citations
2004	Upper mantle temperature structure of the North China Craton. Physics of the Earth and Planetary Interiors, 2019, 293, 106269.	0.7	8
2005	Superconductivity in the van der Waals layered compound PS2. Physical Review B, 2019, 99, .	1.1	11
2006	Pressure effect on the structural, elastic and thermodynamic properties of the BeP2N4 compound: First-principles investigation. Computational Condensed Matter, 2019, 21, e00408.	0.9	1
2007	Prediction of novel SiX2(Xâ€¯=â€¯S, Se) monolayer semiconductors by density functional theory. Physica E: Low-Dimensional Systems and Nanostructures, 2019, 114, 113581.	1.3	25
2008	Equation of state and phase evolution of U-7.7Nb with implications for the understanding of dynamic behavior of U-Nb alloys. Applied Physics Letters, 2019, 114, .	1.5	6
2009	Revealing the ductility of nanoceramic MgAl₂O₄. Journal of Materials Research, 2019, 34, 1489-1498.	1.2	6
2010	Calculation of the anisotropic coefficients of thermal expansion: A first-principles approach. Computational Materials Science, 2019, 167, 257-263.	1.4	16
2011	Pressure-induced reentrant transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Nb</mml:mi><mml:msub><mml:mi mathvariant="normal">S</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> phases: Combined Raman scattering and x-ray diffraction study. Physical Review B, 2019, 99, .	1.1	5
2012	Local Lattice Distortion Mediated Formation of Stacking Faults in Mg Alloys. SSRN Electronic Journal, 0, , .	0.4	0
2013	Gold(<scp>i</scp>) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. Chemical Science, 2019, 10, 6467-6475.	3.7	12
2014	First principles investigation of magnetic new carbon-rich layered compounds UC (n= 2, 6, 12). Computational Condensed Matter, 2019, 21, e00397.	0.9	0
2015	Cohesive zone method based multi particle finite element simulation of compaction densification process of Al and NaCl laminar composite powders. Journal of Physics and Chemistry of Solids, 2019, 134, 35-42.	1.9	8
2016	Structural, electronic, optical and thermodynamic properties of AeBi2O6 (AeÂ= Sr and Ba): Insights from first principles study. Journal of Molecular Graphics and Modelling, 2019, 90, 153-160.	1.3	8
2017	Pressure-induced phase transition in 1,3,5-triamino-2,4,6-trinitrobenzene (TATB). Applied Physics Letters, 2019, 114, .	1.5	34
2018	Investigation on new equiatomic quaternary Heusler compound CoCrIrSi via FP-LAPW calculations. Chemical Physics, 2019, 523, 130-137.	0.9	25
2019	A new stable BeP2C monolayer with visible light sensitivity: A first principles study. Chemical Physics Letters, 2019, 728, 14-18.	1.2	2
2020	Equation of state of LiCoO ₂ under 30 GPa pressure. Chinese Physics B, 2019, 28, 016402.	0.7	6
2021	Firstâ€Principles Study of FeO 2 H x Solid and Melt System at High Pressures: Implications for Ultralowâ€Velocity Zones. Journal of Geophysical Research: Solid Earth, 2019, 124, 4566-4575.	1.4	6

#	Article	IF	Citations
2022	Density functional investigation of structural, electronic, optical and thermodynamic properties of Zn1â^'xBexO semiconductor. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	1.1	10
2023	Correlating Structure and Magnetic Behavior at High Pressure. , 2019, , 546-546.		0
2024	Thermal Boundary Characteristics of Homo-/Heterogeneous Interfaces. Nanomaterials, 2019, 9, 663.	1.9	5
2025	2D Li2S monolayer: A global minimum lithium sulfide sandwich. Chemical Physics Letters, 2019, 722, 58-63.	1.2	12
2026	Local lattice distortion mediated formation of stacking faults in Mg alloys. Acta Materialia, 2019, 170, 231-239.	3.8	45
2027	Computational investigation of CrFeZ [Z = Si, Sn and Ge] half-Heusler compounds ferromagnets. Physica B: Condensed Matter, 2019, 563, 50-55.	1.3	12
2028	Stability of Zirconium Carbide under High Pressure and High Temperature. Journal of Physical Chemistry C, 2019, 123, 10051-10056.	1.5	13
2029	Pressure-Induced Hexagonal to Monoclinic Phase Transition of Partially Hydrated CePO₄. Inorganic Chemistry, 2019, 58, 4480-4490.	1.9	11
2030	Liquid Iron Equation of State to the Terapascal Regime From Ab Initio Simulations. Journal of Geophysical Research: Solid Earth, 2019, 124, 3350-3364.	1.4	23
2031	Mechanical properties of boron arsenide single crystal. Applied Physics Letters, 2019, 114, .	1.5	31
2032	High-Pressure Phase Transitions of Cubic Y ₂ O ₃ under High Pressures by In-situ Synchrotron X-Ray Diffraction. Chinese Physics Letters, 2019, 36, 046103.	1.3	10
2033	High pressure behavior of mercury difluoride (HgF2). Chemical Physics Letters, 2019, 724, 35-41.	1.2	7
2034	Radial Xâ€Ray Diffraction Study of Superhard Early Transition Metal Dodecaborides under High Pressure. Advanced Functional Materials, 2019, 29, 1900293.	7.8	12
2035	First principle investigation of the structural, electronic and elastic properties of the Laves phase compounds SrX2 (Xâ€¯=â€¯Pd and Pt). Chinese Journal of Physics, 2019, 59, 210-219.	2.0	6
2036	Phase transitions and chemical reactions of octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine under high pressure and high temperature. RSC Advances, 2019, 9, 5825-5833.	1.7	21
2037	Crossover in the pressure evolution of elementary distortions in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>R</mml:mi><mml:mi>Fe</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>perovskites and its impact on their phase transition. Physical Review B, 2019, 99, .	1.1	21
2038	Effect of anharmonicity on the hcp to bcc transition in beryllium at high-pressure and high-temperature conditions. Physical Review B, 2019, 99, .	1.1	14
2039	A Series of MAX Phases with MAâ€Triangularâ€Prism Bilayers and Elastic Properties. Angewandte Chemie - International Edition, 2019, 58, 4576-4580.	7.2	20

#	Article	IF	Citations
2040	Structural, optoelectronic and thermoelectric properties of antiperovskite compounds Ae3PbS (Ae =) Tj ETQq0 0 0 rgBT /Overlock 10 Tf Physics, 2019, 383, 1648-1654.	0.9	22
2041	A Series of MAX Phases with MAâ€Triangularâ€Prism Bilayers and Elastic Properties. Angewandte Chemie, 2019, 131, 4624-4628.	1.6	2
2042	Advanced Spectral Analysis Program. Review of Scientific Instruments, 2019, 90, 023903.	0.6	0
2043	First-principles calculations of mechanical and thermodynamic properties of tetragonal Be₁₂Ti. RSC Advances, 2019, 9, 5302-5312.	1.7	17
2044	Structure and superconductivity of protactinium hydrides under high pressure. Journal of Physics Condensed Matter, 2019, 31, 315403.	0.7	6
2045	Investigation on structural, electronic, magnetic and thermodynamic properties of antiperovskites Mn₃XC (X=Al, Zn and Ga). International Journal of Modern Physics B, 2019, 33, 1950337.	1.0	4
2046	Numerical and theoretical determination of various materials Hugoniot relations based on the equation of state in high-temperature shock loading. High Pressure Research, 2019, 39, 666-690.	0.4	3
2047	Abnormal physical behaviors of hafnium diboride under high pressure. Applied Physics Letters, 2019, 115, .	1.5	15
2048	First-principles study of structural, mechanical, and electronic properties of typical iron-containing phases in Al-Cu alloys under different pressures. Physica B: Condensed Matter, 2019, 555, 112-117.	1.3	4
2049	Robust half metallicity state with the hydrostatic and tetragonal distortion for a new quaternary Heusler ZrTiRhGa: FP-LAPW calculations. Physica B: Condensed Matter, 2019, 557, 56-62.	1.3	13
2050	Comparative study of structural, electronic, optical and thermoelectric properties of GaS bulk and monolayer. Philosophical Magazine, 2019, 99, 736-751.	0.7	14
2051	High pressure structural investigations on hexagonal YInO₃. High Pressure Research, 2019, 39, 17-35.	0.4	6
2052	Electronic structure and thermoelectric properties of Ta-based half-Heusler compounds with 18 valence electrons. Computational Materials Science, 2019, 159, 470-477.	1.4	41
2053	Pressure effects on the optical and electronic aspects of T-Carbon: A first principles calculation. Optik, 2019, 180, 125-133.	1.4	22
2054	Nitrogen Content in the Earth's Outer Core. Geophysical Research Letters, 2019, 46, 89-98.	1.5	10
2055	SiP2S monolayer: A two dimensional semiconductor with a moderate band gap. Chemical Physics Letters, 2019, 715, 100-104.	1.2	5
2056	Firstâ”principles study: Structural, mechanical, electronic and thermodynamic properties of simpleâ”cubicâ”perovskite (Ba0.62K0.38)(Bi0.92Mg0.08)O3. Solid State Communications, 2019, 288, 22-27.	0.9	22
2057	A DFT based prediction of a new 2D zirconium disulfide Pmmm-ZrS2 monolayer: A quasi direct band gap semiconductor. Results in Physics, 2019, 12, 903-907.	2.0	10

#	Article	IF	Citations
2058	Recordâ€High Superconductivity in Niobiumâ€“Titanium Alloy. Advanced Materials, 2019, 31, e1807240.	11.1	27
2059	Theoretical investigations on physical properties of SrFCuCh (Ch=S and Se). Journal of Solid State Chemistry, 2019, 271, 191-198.	1.4	2
2060	The effect of high pressure on the structure and stability of sodium formate: Probed by in situ synchrotron X-ray diffraction technique. Solid State Communications, 2019, 289, 67-70.	0.9	2
2061	Size-Dependent Adsorption of Styrene on Pd Clusters: A Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 2182-2188.	1.5	12
2062	Tuneable thermal expansion of poly (3,4-ethylenedioxythiophene) polystyrene sulfonate. Journal of Physics Condensed Matter, 2019, 31, 125101.	0.7	7
2063	Systematic study of structural, electronic, optical and thermodynamic properties of SrFCuTe compound. Journal of Solid State Chemistry, 2019, 270, 85-91.	1.4	10
2064	High pressure synchrotron x-ray diffraction study of the Mn0.94Ti0.06CoGe alloy. Physica B: Condensed Matter, 2019, 554, 5-8.	1.3	1
2065	Kâ€Birnessite Electrode Obtained by Ion Exchange for Potassiumâ€Ion Batteries: Insight into the Concerted Ionic Diffusion and K Storage Mechanism. Advanced Energy Materials, 2019, 9, 1802739.	10.2	80
2066	Synthesis, crystal structure, microstructure and mechanical properties of (Ti1-Zr)3SiC2 MAX phase solid solutions. Ceramics International, 2019, 45, 1400-1408.	2.3	21
2067	Phase transition, mechanical stability and optical response of MnSe: Pressure effect. Physica B: Condensed Matter, 2019, 553, 6-10.	1.3	4
2068	Thermal expansion, compressibility and bulk modulus of ilmenite-type CoTiO3: X-ray diffraction at high pressures and temperatures. Solid State Sciences, 2019, 88, 1-5.	1.5	5
2069	First principles investigations of Fe, Co, Ni in model honeycomb carbon networks. Solid State Sciences, 2019, 87, 155-162.	1.5	2
2070	Structural, electronic, and mechanical properties of anatase titanium dioxide. Multidiscipline Modeling in Materials and Structures, 2019, 15, 306-316.	0.6	8
2071	Structural, elastic, electronic, thermodynamic, and optical properties of layered BaPd2As2 pnictide superconductor: A first principles investigation. Journal of Alloys and Compounds, 2019, 780, 452-460.	2.8	61
2072	Theoretical study of structural, electronic and optical properties of ScxTl1-xP ternary alloys and (ScP)n/(TlP)n superlattices by FP-LMTO method. Optik, 2019, 178, 243-250.	1.4	2
2073	Theoretical study on the stability, electronic, mechanical, vibrational and thermodynamic properties of rare-earth intermetallic compound Rh₃Ce. Molecular Simulation, 2019, 45, 40-49.	0.9	1
2074	Electronic, Structural, and Magnetic Properties of Hole-Doped Iron-Based Superconductors Using First Principle Study. Journal of Superconductivity and Novel Magnetism, 2020, 33, 921-930.	0.8	2
2075	Experimental and theoretical study on elastic properties of crystalline alkali silicate hydrate. Materials and Design, 2020, 185, 108240.	3.3	1

#	Article	IF	Citations
2076	Electronic and thermoelectric properties of RbYSn half-Heusler compound with 8 valence electrons: Spin-orbit coupling effect. Chemical Physics, 2020, 528, 110510.	0.9	20
2077	Electronic structure based design of thin film metallic glasses with superior fracture toughness. Materials and Design, 2020, 186, 108327.	3.3	13
2078	Carbon at the nanoscale: Ultrastiffness and unambiguous definition of incompressibility. Carbon, 2020, 160, 228-235.	5.4	10
2079	DFT investigations into the physical properties of a MAB phase Cr4AlB4. Journal of Alloys and Compounds, 2020, 821, 153547.	2.8	15
2080	Experimental and Theoretical Study of SbPO4 under Compression. Inorganic Chemistry, 2020, 59, 287-307.	1.9	14
2081	High-pressure X-ray diffraction and MÃ¶ssbauer spectroscopy study of Fe1.087Te. Physica B: Condensed Matter, 2020, 578, 411875.	1.3	0
2082	High-pressure structural investigations on InPO4. Journal of Solid State Chemistry, 2020, 282, 121065.	1.4	4
2083	Electronic structure and dynamics analysis of the Cu-Ag binary alloy by a tight-binding parametrization. Computational Materials Science, 2020, 173, 109454.	1.4	2
2084	Examining the uniform strain effect on elastic, electronic and optical properties of CsPbCl3 through FP-LAPW calculations. Chemical Physics, 2020, 531, 110654.	0.9	8
2085	Tungsten solubility in L12-ordered Al3Er and Al3Zr nanoprecipitates formed by aging in an aluminum matrix. Journal of Alloys and Compounds, 2020, 820, 153383.	2.8	16
2086	On the structural, electronic, optical and thermoelectric properties of CdIn2Se4 ordered-vacancy compound. Journal of Solid State Chemistry, 2020, 282, 121078.	1.4	2
2087	Second nearest-neighbor modified embedded atom method interatomic potentials for the Na unary and Na-Sn binary systems. Computational Materials Science, 2020, 185, 109953.	1.4	8
2088	High pressure chemical reactivity and structural study of the Naâ€“P and Liâ€“P systems. Journal of Materials Chemistry A, 2020, 8, 21797-21803.	5.2	5
2089	Diiron in extended carbon networks: Magnetic properties of model Fe2C6 and Fe2C12 from first principles. Journal of Magnetism and Magnetic Materials, 2020, 514, 167213.	1.0	2
2090	Comprehensive first-principles calculations on physical properties of ScV2Ga4 and ZrV2Ga4 in comparison with superconducting HfV2Ga4. Materials Today Communications, 2020, 24, 100935.	0.9	23
2091	Examining the half-metallicity and thermoelectric properties of new equiatomic quaternary Heusler compound CoVRhGe under pressure. Physica B: Condensed Matter, 2020, 583, 412058.	1.3	23
2092	High-Pressure Equation of State of 1,3,5-triamino-2,4,6-trinitrobenzene: Insights into the Monoclinic Phase Transition, Hydrogen Bonding, and Anharmonicity. Journal of Physical Chemistry A, 2020, 124, 10580-10591.	1.1	16
2093	Magnetic Phase Transition, Elastic and Thermodynamic Properties of L12-(Ni,Cu)3(Al,Fe,Cr) in 3d High-Entropy Alloys. Crystals, 2020, 10, 1102.	1.0	1

#	Article	IF	Citations
2094	Effects of W and Si microadditions on microstructure and the strength of dilute precipitation-strengthened Alâ€“Zrâ€“Er alloys. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 798, 140159.	2.6	17
2095	Investigation on properties of FeNi intermetallics under pressure by First-principles. Journal of Physics: Conference Series, 2020, 1507, 082026.	0.3	3
2096	Insights into the predicted Hf2SN in comparison with the synthesized MAX phase Hf2SC: A comprehensive study. Computational Condensed Matter, 2020, 24, e00485.	0.9	17
2097	Electronic and structural properties of the honeycomb iridates A2IrO3 (A=Na , Li) at elevated pressures. Physical Review B, 2020, 102, .	1.1	8
2098	A high-pressure study of HfC and nano-crystalline TiC by X-ray diffraction and density functional theory calculations. Modern Physics Letters B, 2020, 34, 2050393.	1.0	7
2099	Key Experiments and Thermodynamic Description of the Co-Nb-Ni System. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2020, 51, 5892-5911.	1.1	11
2100	Thermal Pressure in the Laserâ€Heated Diamond Anvil Cell: A Quantitative Study and Implications for the Density Versus Mineralogy Correlation of the Mantle. Journal of Geophysical Research: Solid Earth, 2020, 125, e2020JB020006.	1.4	6
2101	Insight View of Topological Nontrivial Nature in the Novel Alkali Metalâ€“Based Quaternary Heusler Compounds via Ab Initio Calculations. Journal of Superconductivity and Novel Magnetism, 2020, 33, 3875-3881.	0.8	4
2102	Multi-fidelity machine-learning with uncertainty quantification and Bayesian optimization for materials design: Application to ternary random alloys. Journal of Chemical Physics, 2020, 153, 074705.	1.2	45
2103	Thermoelastic properties of tungsten at simultaneous high pressure and temperature. Journal of Applied Physics, 2020, 128, .	1.1	7
2104	Distance-Selected Topochemical Dehydro-Dielsâ€“Alder Reaction of 1,4-Diphenylbutadiyne toward Crystalline Graphitic Nanoribbons. Journal of the American Chemical Society, 2020, 142, 17662-17669.	6.6	23
2105	Elastic Coefficients of Î²-HMX as Functions of Pressure and Temperature from Molecular Dynamics. Crystals, 2020, 10, 1123.	1.0	23
2106	Physical properties of a novel boron-based ternary compound Ti2InB2. Materials Today Communications, 2020, 25, 101600.	0.9	14
2107	Detonation-induced transformation of graphite to hexagonal diamond. Physical Review B, 2020, 102, .	1.1	13
2108	Effect of the Free Volume on the Electronic Structure of Cu70Zr30 Metallic Glasses. Materials, 2020, 13, 4911.	1.3	2
2109	Equation of state of LiNi0Â·5Mn1Â·5O4 at high pressure. Solid State Communications, 2020, 321, 114045.	0.9	2
2110	Effect of chemical composition, defect structure, and stress state on the elastic properties of (V_{1â^'x}Al_x)_{1â^'yâ€Š}N_{yâ€Š}. Journal of Physics Condensed Matter, 2020, 32, 025901.	2.7	7
2111	Change mechanism of the pressure-induced quantum phase transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>EuC</mml:mi><mml:msub><mml:mi		

#	Article	IF	Citations
2112	Structural and vibrational behavior of cubic Cu1.80(3)Se cuprous selenide, berzelianite, under compression. Journal of Alloys and Compounds, 2020, 830, 154646.	2.8	1
2113	Se2TiO6E2 Ternary Oxide Characteristic of Isolated TiO6 Octahedra with the Shear Effect of SeIVE Electron Lone Pair (E): Combined Crystal Chemistry and ab Initio Study. Journal of Physical Chemistry C, 2020, 124, 12281-12285.	1.5	0
2114	On thermal conductivity of amorphous niobium monoxide. Journal Physics D: Applied Physics, 2020, 53, 285303.	1.3	10
2115	P-substitution effects on the electronic structure and thermal properties of the half-metallic half-Heusler NaCrBi compound. Chemical Physics, 2020, 537, 110848.	0.9	8
2116	Strain tunable electrical and optical properties of two dimensional tetragonal MgX (X=S, Se) monolayer semiconductors. Superlattices and Microstructures, 2020, 144, 106570.	1.4	7
2117	Mechanism for structure conversion of FeSi under pressures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126598.	0.9	3
2118	Thermal expansion and vibrational properties of Î±-Se and Î±-TeSe2 based on first-principles calculations. Solid State Communications, 2020, 314-315, 113912.	0.9	1
2119	Mn2CoX (X = P and As) full-Heusler compounds for spintronic applications: Half-metallicity and elastic properties. Physics Letters, Section A: General, Atomic and Solid State Physics, 2020, 384, 126589.	0.9	28
2120	Application of the training of density functional theory potentials within machine learning to adsorptions and reactionÂpaths on Platinum surfaces. Materials Chemistry and Physics, 2020, 253, 123407.	2.0	5
2121	Thermoelasticity of tremolite amphibole: Geophysical implications. American Mineralogist, 2020, 105, 904-916.	0.9	11
2122	First-principles predictions of electronic, elastic, and optical properties of ScBC and YBC ternary cermet phases. Vacuum, 2020, 179, 109488.	1.6	29
2123	First principle calculation of the effect of Cr, Ti content on the properties of VMoNbTaWMx (M = Cr,) Tj ETQq1 1 0.784314 rgBT /Over	1.6	22
2124	Elastic and thermodynamic properties of high entropy carbide (HfTaZrTi)C and (HfTaZrNb)C from ab initio investigation. Ceramics International, 2020, 46, 15104-15112.	2.3	58
2125	Evolution of Ni/Li antisites under the phase transition of a layered LiNi_{1/3}Co_{1/3}Mn_{1/3}O₂ cathode. Journal of Materials Chemistry A, 2020, 8, 6337-6348.	5.2	36
2126	Electronic structures and optical properties of two-dimensional (W2âˆ•3X1âˆ•3)2CO2 (X=SC,Y) iMXene by first-principles calculations. Materials Chemistry and Physics, 2020, 248, 122896.	2.0	3
2127	Elasticity of single-crystal Fe-enriched diopside at high-pressure conditions: Implications for the origin of upper mantle low-velocity zones. American Mineralogist, 2020, 105, 363-374.	0.9	5
2128	The Raman and IR vibration modes of metal pentazolate hydrates [Na(H2O)(N5)]Â·2H2O and [Mg(H2O)6(N5)2]Â·4H2O. Journal of Molecular Modeling, 2020, 26, 84.	0.8	3
2129	Computational prediction of the spin-polarized semiconductor equiatomic quaternary Heusler compound MnVZrP as a spin-filter. RSC Advances, 2020, 10, 25609-25617.	1.7	4

#	Article	IF	Citations
2130	Evidence of shock-compressed stishovite above 300â€‰GPa. Scientific Reports, 2020, 10, 10197.	1.6	8
2131	Thermal boundary conductance between high thermal conductivity boron arsenide and silicon. Journal of Applied Physics, 2020, 127, 055105.	1.1	6
2132	DFT prediction of structural, electronic and magnetic properties of Sr_{0.75}TM_{0.25}S (TM is 3d transition metals). Philosophical Magazine Letters, 2020, 100, 95-104.	0.5	4
2133	First principles insight into the structural, electronic, optical and thermodynamic properties of CsPb2Br5 compound. Chemical Physics, 2020, 533, 110704.	0.9	7
2134	An assessment of the structural, electronic, optical and thermoelectric properties of the BaAg2GeS4 compound. Journal of Solid State Chemistry, 2020, 285, 121260.	1.4	8
2135	Pressureâ€induced anomalous behavior of thaumasite crystal. Journal of the American Ceramic Society, 2020, 103, 3763-3775.	1.9	3
2136	Pressureâ€Induced Structural Evolution and Bandgap Optimization of Leadâ€Free Halide Double Perovskite (NH₄)₂SeBr₆. Advanced Science, 2020, 7, 1902900.	5.6	44
2137	A high-pressure study of Cr3C2 by XRD and DFT. Chinese Physics B, 2020, 29, 086401.	0.7	3
2138	Structure and Behavior of the Ni End-Member Schreibersite Ni3P under Compression to 50 GPa. Minerals (Basel, Switzerland), 2020, 10, 306.	0.8	2
2139	Structural, mechanical, electronic, and thermodynamic properties of pure tungsten metal under different pressures: A firstâ€principles study. International Journal of Quantum Chemistry, 2020, 120, e26231.	1.0	14
2140	Structural, mechanical, electronic and thermodynamic properties of cubic TiC compounds under different pressures: A first-principles study. Solid State Communications, 2020, 311, 113856.	0.9	16
2141	First-Order Isostructural Phase Transition Induced by High Pressure in Fe(IO₃)₃. Journal of Physical Chemistry C, 2020, 124, 8669-8679.	1.5	24
2142	The Sensitivity of Joint Inversions of Seismic and Geodynamic Data to Mantle Viscosity. Geochemistry, Geophysics, Geosystems, 2020, 21, e2019GC008648.	1.0	11
2143	A comparative study of high-pressure behaviors of the two polymorphs of Ho₂Ge₂O₇. RSC Advances, 2020, 10, 10540-10545.	1.7	4
2144	Zirconium trigallide polymorphs with tetragonal and cubic structures: optical and thermodynamic properties. Indian Journal of Physics, 2021, 95, 587-594.	0.9	5
2145	Prediction of a new 2D B2CO monolayer from density functional theory. Computational Materials Science, 2021, 186, 109975.	1.4	4
2146	First principles analysis of the half-metallic ferromagnetism, elastic and thermodynamic properties of equiatomic quaternary Heusler compound CoCrRhSi. Materials Chemistry and Physics, 2021, 257, 123695.	2.0	8
2147	Effect of target peak power density on the phase formation, microstructure evolution, and mechanical properties of Cr2AlC MAX-phase coatings. Journal of the European Ceramic Society, 2021, 41, 1841-1847.	2.8	13

#	Article	IF	Citations
2148	Tight-binding study of beryllium. Computational Materials Science, 2021, 188, 110142.	1.4	1
2149	Constraining the density evolution during destruction of the lithospheric mantle in the eastern North China Craton. Gondwana Research, 2021, 91, 18-30.	3.0	5
2150	First principles study on phonon dispersion, mechanical and thermodynamic properties of ThP. Materials Today Communications, 2021, 26, 101951.	0.9	3
2151	Lattice distortion in highâ€entropy carbide ceramics from firstâ€principles calculations. Journal of the American Ceramic Society, 2021, 104, 1874-1886.	1.9	50
2152	rh.-B12 as host of interstitial atoms: Review of a large family with illustrative study of B12{CN2} from first-principles. Progress in Solid State Chemistry, 2021, 61, 100296.	3.9	5
2153	Structural, mechanical and phonons properties of binary intermetallic compound BaSn3 under pressure. Solid State Communications, 2021, 323, 114110.	0.9	7
2154	High-pressure structural study of Î± -Mn: Experiments and calculations. Physical Review B, 2021, 103, .	1.1	1
2155	Pressure effects on electronic, elastic, and vibration properties of metallic antiperovskite PbNCa3 by ab initio calculations. Journal of Molecular Modeling, 2021, 27, 7.	0.8	3
2156	Structural, Electronic, Mechanical, and Optical Properties of LaIn3 under Pressure: A First Principle Investigation. Journal of Superhard Materials, 2021, 43, 31-44.	0.5	0
2157	First principle studies of ammonium chloride under high pressure. RSC Advances, 2021, 11, 5149-5155.	1.7	0
2158	The solubility behavior of NaCl in water at high pressure studied by neutron diffraction and Raman scattering. High Pressure Research, 2021, 41, 39-51.	0.4	1
2159	Phase transition and chemical reactivity of 1H-tetrazole under high pressure up to 100 GPa. Physical Chemistry Chemical Physics, 2021, 23, 19503-19510.	1.3	3
2160	Pressure-induced bandgap engineering of lead-free halide double perovskite (NH4)2SnBr6. Physical Chemistry Chemical Physics, 2021, 23, 19308-19312.	1.3	5
2161	DFT calculations on ZnO1â^'x compounds for optoelectronic applications. Journal of Computational Electronics, 2021, 20, 467-479.	1.3	8
2162	Equations of state for CaSiO3 phases based on the Helmholtz free energy. Journal of Physics: Conference Series, 2021, 1787, 012005.	0.3	1
2163	Pressure dependence of structural, elastic, electronic, thermodynamic, and optical properties of van der Waals-type NaSn2P2 pnictide superconductor: Insights from DFT study. Results in Physics, 2021, 21, 103848.	2.0	48
2164	Comparative computational study of antiferromagnetic and mixed-valent diamagnetic phase of AgF2: Crystal, electronic and phonon structure and p-T phase diagram. Computational Materials Science, 2021, 188, 110250.	1.4	7
2165	Electronic structure, elastic, optical and thermodynamic properties of cubic perovskite NaBaF3 with pressure effects: First-principles calculations. Results in Physics, 2021, 22, 103860.	2.0	28

#	Article	IF	Citations
2166	Equations of State of Ca-Silicates and Phase Diagram of the CaSiO3 System under Upper Mantle Conditions. Minerals (Basel, Switzerland), 2021, 11, 322.	0.8	8
2167	The effect of interstitial-site nitrogen on structural, elastic, and magnetic properties of face-center cubic Co. Journal of Applied Physics, 2021, 129, .	1.1	4
2168	An ab-initio study on structural, elastic, electronic, bonding, thermal, and optical properties of topological Weyl semimetal TaX (Xâ€‰=â€‰P, As). Scientific Reports, 2021, 11, 5592.	1.6	84
2169	Pressure effect of the mechanical, electronics and thermodynamic properties of Mgâ€“B compounds A first-principles investigations. Scientific Reports, 2021, 11, 6096.	1.6	5
2170	Structural, mechanical, electronic properties, and Debye temperature of quaternary carbide Ti₃NiAl₂C ceramics under high pressure: A first-principles study*. Chinese Physics B, 2021, 30, 036202.	0.7	1
2171	Ultra-incompressible High-Entropy Diborides. Journal of Physical Chemistry Letters, 2021, 12, 3106-3113.	2.1	17
2172	Post-lithium-ion batteries: characterization of phosphorous and tin for potassium-ion anodes. Journal of Materials Science, 2021, 56, 10926-10937.	1.7	3
2173	Strain effect on the electronic and optical properties of 2D Tetrahexcarbon: a DFT-based study. Indian Journal of Physics, 2021, 95, 2365-2373.	0.9	39
2174	An ab initio study of structural, elastic and electronic properties of hexagonal MAuGe (M = Lu, Sc) compounds. Condensed Matter Physics, 2021, 24, 13706.	0.3	3
2176	Equation of State for Natural Almandine, Spessartine, Pyrope Garnet: Implications for Quartz-In-Garnet Elastic Geobarometry. Minerals (Basel, Switzerland), 2021, 11, 458.	0.8	2
2177	Structural, elastic, thermodynamic, electronic, and optical properties of $$hbox {CaMg}_{2}hbox {AN}_{3}$$($$hbox {A}=hbox {Al}$$ and Ga): ab initio investigation. European Physical Journal B, 2021, 94, 1.	0.6	3
2178	The structural, electronic, and optical properties of hydrofluorinated germanene (GeH1-xFx): a first-principles study. Journal of Molecular Modeling, 2021, 27, 123.	0.8	0
2179	A comparison study of the structural electronic, elastic and lattice dynamic properties of ZrInAu and ZrSnPt. Zeitschrift Fur Naturforschung - Section A Journal of Physical Sciences, 2021, 76, 559-567.	0.7	3
2180	Normal and anomalous self-healing mechanism of crystalline calcium silicate hydrates. Cement and Concrete Research, 2021, 142, 106356.	4.6	15
2181	Ab-initio investigations on dynamical and lattice thermal behaviours of ThC. Bulletin of Materials Science, 2021, 44, 1.	0.8	3
2182	Ab initio investigations on lattice dynamics and thermal characteristics of ThO2 using Debyeâ€“Einstein model. Bulletin of Materials Science, 2021, 44, 1.	0.8	0
2183	Stability, Elastic and Electronic Properties of Ta2N by First-Principles Calculations. Crystals, 2021, 11, 445.	1.0	3
2184	DFT calculations of optoelectronic properties of cubic $$left({{ext{In}}_{1 - x} {ext{Al}}_{x} }) Tj ETQq1 1 0.784314 rgBT /Overlock	1.3	5

#	Article	IF	Citations
2185	Featureâ€rich structural, electronic, magnetic and optical properties of the fluorineâ€and nitrogenâ€incorporated CaF 2 compound. International Journal of Quantum Chemistry, 2021, 121, e26672.	1.0	0
2186	A computational prediction of a novel quasi hexagonal Al2SSi semiconductor monolayer. Chemical Physics, 2021, 545, 111148.	0.9	0
2187	First-Principle Studies of the Vibrational Properties of Carbonates under Pressure. Sensors, 2021, 21, 3644.	2.1	16
2188	Microscopic phase diagram of Eu(Fe1â^'xNix)As2 (x = 0,0.04) under pressure. Physical Review B, 2021, 103, .	1.1	5
2189	First-principles calculations of metal surfaces. I. Slab-consistent bulk reference for convergent surface properties. Physical Review B, 2021, 103, .	1.1	3
2190	High Pressureâ€Temperature Singleâ€Crystal Elasticity of Grossular: Implications for the Lowâ€Velocity Layer in the Bottom Transition Zone. Geophysical Research Letters, 2021, 48, e2021GL093540.	1.5	5
2191	Structural, electronic, magnetic and optical properties of CaO induced by oxygen incorporation effects: A first-principles study. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 397, 127241.	0.9	12
2192	First-principles calculations of metal surfaces. II. Properties of low-index platinum surfaces toward understanding electron emission. Physical Review B, 2021, 103, .	1.1	4
2193	Phase, microstructure and related mechanical properties of a series of (NbTaZr)C-Based high entropy ceramics. Ceramics International, 2021, 47, 14341-14347.	2.3	38
2194	Crystal Structure of Symmetric Ice X in H₂Oâ€“H₂ and H₂Oâ€“He under Pressure. Journal of Physical Chemistry Letters, 2021, 12, 4707-4712.	2.1	4
2195	Novel binder-free carbon anode for high capacity Li-ion batteries. Nano Energy, 2021, 83, 105816.	8.2	11
2196	Pressure effects on vibrational properties and structure of nanocrystalline Cu2ZnSnS4. Journal of Alloys and Compounds, 2021, 867, 159041.	2.8	3
2197	Elucidating the Phase Transformation and Metallization Behavior of Zinc Phosphide under High Pressure. Inorganic Chemistry, 2021, 60, 10315-10322.	1.9	3
2198	Atomic-scale Evidence for Open-system Thermodynamics in the Early Solar Nebula. Planetary Science Journal, 2021, 2, 115.	1.5	5
2199	Transition path to a dense efficient-packed post-delafossite phase. Crystal structure and evolution of the chemical bonding. Journal of Alloys and Compounds, 2021, 867, 159012.	2.8	1
2200	Site Occupation and Structural Phase Transformation of the (010) Antiphase Boundary in Boron-Modified L12 Ni3Al. Jom, 2021, 73, 2285-2292.	0.9	2
2201	Entropy, dynamics, and freezing of CaSiO3 liquid. Geochimica Et Cosmochimica Acta, 2021, 302, 1-17.	1.6	6
2202	Possible Deep Structure and Composition of Venus With Respect to the Current Knowledge From Geodetic Data. Journal of Geophysical Research E: Planets, 2021, 126, e2019JE006243.	1.5	6

#	Article	IF	Citations
2203	High-pressure behavior of disodered kesterite-type Cu2ZnSnS4. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	1.1	3
2204	Scalable High-Pressure Synthesis of sp²â€“sp³ Carbon Nanoribbon via [4 + 2] Polymerization of 1,3,5-Triethynylbenzene. Journal of Physical Chemistry Letters, 2021, 12, 7140-7145.	2.1	5
2205	Nonlinear effects of hydration on high-pressure sound velocities of rhyolitic glasses. American Mineralogist, 2021, 106, 1143-1152.	0.9	6
2206	The pressure effect on stability, electronic and optical properties of fluorine passivated graphene (CF)n: A first-principle study. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 269, 115163.	1.7	6
2207	Understanding the surface adsorption and oxidation of cubic Cr0.5Al0.5N by first-principles calculations. Computational Materials Science, 2021, 196, 110518.	1.4	6
2208	Understanding the interfacial properties in BN-SiO2 diphase ceramic/TiNiNb filler alloy systems: First-principles and mechanical studies. Applied Surface Science, 2021, 556, 149563.	3.1	5
2209	Equation of state and electrical transport properties of mixture of Li1.2Mn0.54Co0.13Ni0.13O₂ and LiNi0.87Co0.09Mn0.03Al0.01O₂ at high pressure. International Journal of Modern Physics B, 2021, 35, .	1.0	0
2210	First-principles investigation of rhodium hydrides under high pressure. Physical Review B, 2021, 104, .	1.1	4
2211	High-pressure compression behavior of isoelectronic pairs of alkali metal halides and noble gas solids. Physical Review B, 2021, 104, .	1.1	0
2212	Unravelling the ion-energy-dependent structure evolution and its implications for the elastic properties of (V,Al)N thin films. Acta Materialia, 2021, 214, 117003.	3.8	20
2213	Tin-pest problem as a test of density functionals using high-throughput calculations. Physical Review Materials, 2021, 5, .	0.9	7
2214	The coupling of lattice-strain and phonon induced order-disorder phase transition in layered LiGaO2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 407, 127464.	0.9	1
2215	Crystal chemistry and ab initio prediction of ultrahard rhombohedral B2N2 and BC2N. Solid State Sciences, 2021, 118, 106667.	1.5	13
2216	Phase transformations of zircon-type DyVO4 at high pressures up to 36.4ÂGPa: X-ray diffraction measurements. Journal of Alloys and Compounds, 2021, 875, 159926.	2.8	5
2217	A comprehensive study of the thermophysical and optoelectronic properties of Nb2P5 via ab-initio technique. Results in Physics, 2021, 28, 104623.	2.0	20
2218	Thermoelasticity of Water in Silicate Melts: Implications for Melt Buoyancy in Earth's Mantle. Journal of Geophysical Research: Solid Earth, 2021, 126, e2021JB022359.	1.4	2
2219	The interplay between twinning and cation inversion in MgAl2O4-spinel: Implications for a nebular thermochronometer. American Mineralogist, 2022, 107, 1470-1476.	0.9	1
2220	Experimental thermal equation of state of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>B</mml:mi><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:m Physical Review B, 2021, 104, .	1.1	7

#	Article	IF	Citations
2221	MechElastic: A Python library for analysis of mechanical and elastic properties of bulk and 2D materials. Computer Physics Communications, 2021, 267, 108068.	3.0	54
2222	First-principles study of structural, electronic, elastic, vibrational and thermodynamics properties of LaX3 (X=Sn, Tl, Pb and Bi) compounds under pressure. Solid State Communications, 2021, 336, 114431.	0.9	2
2223	Ultra-hard rhombohedral carbon by crystal chemistry and ab initio investigations. Journal of Solid State Chemistry, 2021, 302, 122354.	1.4	7
2224	Structural transition and ductility enhancement of a tungsten heavy alloy under high pressure. International Journal of Refractory Metals and Hard Materials, 2021, 100, 105632.	1.7	8
2225	CsIBr2 at high pressures: An insitu Raman and ADXRD investigation. Journal of Solid State Chemistry, 2021, 303, 122530.	1.4	2
2226	Pressure-induced band anticrossing in two adamantine ordered-vacancy compounds: CdGa2S4 and HgGa2S4. Journal of Alloys and Compounds, 2021, 886, 161226.	2.8	6
2227	Elucidating the structural properties and reversible regional texture effect of GdB6 under high pressure. Journal of Alloys and Compounds, 2021, 886, 161239.	2.8	1
2228	Small-scale analysis of brittle-to-ductile transition behavior in pure tungsten. Journal of Materials Science and Technology, 2022, 105, 242-258.	5.6	15
2229	Optoelectronic, thermodynamic and vibrational properties of intermetallic MgAl2Ge2: a first-principles study. SN Applied Sciences, 2021, 3, 1.	1.5	2
2230	Two-dimensional buckled tetragonal cadmium chalcogenides including CdS, CdSe, and CdTe monolayers as photo-catalysts for water splitting. Physical Chemistry Chemical Physics, 2021, 23, 12226-12232.	1.3	35
2233	Equation of State and Possible Critical Phase Transitions in MgSiO3 Perovskite at Lower-Mantle Conditions. , 1988, , 91-112.		13
2234	Reduction of Mantle and Core Properties to a Standard State by Adiabatic Decompression. , 1986, , 275-309.		33
2235	AB$$_{2}$$O$$_{4}$$ Compounds at High Pressures. Springer Series in Materials Science, 2014, , 53-73.	0.4	11
2236	$$mathrm{AB}_{2} ext {Se}_{4}$$ Ordered-Vacancy Compounds at High Pressures. Springer Series in Materials Science, 2014, , 163-184.	0.4	5
2237	Metal-Hydrogen System Under Extended p, T Conditions. Springer Series in Materials Science, 1993, , 71-119.	0.4	4
2238	Density Patterns of the Upper Mantle Under Asia and the Arctic: Comparison of Thermodynamic Modelling and Geophysical Data. Pure and Applied Geophysics, 2020, 177, 4289-4307.	0.8	2
2239	Newly synthesized A-site ordered cubic-perovskite superconductor (Ba0.54K0.46)4Bi4O12: A DFT investigation. Physica C: Superconductivity and Its Applications, 2020, 574, 1353669.	0.6	23
2240	Differentiating the Electrical and Optoelectrical Properties of Oxysulfides La₂Ta₂MS₂O₈ (M = Zr, Ti) via Application of Pressure. Journal of Physical Chemistry C, 2020, 124, 14477-14484.	1.5	5

#	Article	IF	Citations
2241	Pressure-induced polymorphism in hypervalent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Cs</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2017, 96, .	1.1	8
2242	Thermomechanical response of NiTi shape-memory nanoprecipitates in TiV alloys. Physical Review Materials, 2017, 1, .	0.9	23
2243	High-pressure behavior of CaMoO4. Physical Review Materials, 2017, 1, .	0.9	15
2244	High-enthalpy crystalline phases of cadmium telluride. Physical Review Research, 2020, 2, .	1.3	4
2245	Equation of state of phase E. Mineralogical Magazine, 2000, 64, 561-567.	0.6	18
2246	Equation of State of Zircon-Type TbVO4. Acta Physica Polonica A, 2010, 117, 319-322.	0.2	4
2247	A First Principle Study of Antifluorite Be₂X (X = C, Si) Polymorph. Acta Physica Polonica A, 2011, 119, 442-446.	0.2	4
2248	First-Principles Study of Structural, Elastic and Mechanical Properties of Zinc-Blende Boron Nitride (B3-BN). Acta Physica Polonica A, 2012, 122, 109-115.	0.2	16
2249	Hot Compression Test of Heat Resistant Steel. Acta Physica Polonica A, 2017, 131, 1340-1344.	0.2	1
2250	Investigation of the crystal structure of a low water content hydrous olivine to 29.9 GPa: A high-pressure single-crystal X-ray diffraction study. American Mineralogist, 2020, 105, 1857-1865.	0.9	7
2251	Phase transitions in Îµ-FeOOH at high pressure and ambient temperature. American Mineralogist, 2020, 105, 1769-1777.	0.9	20
2252	Thermodynamics of deep geophysical media. Russian Journal of Earth Sciences, 1999, 1, 11-49.	0.2	4
2254	Equations of State for High Pressure Phases.. Review of High Pressure Science and Technology/Koatsuryoku No Kagaku To Gijutsu, 2001, 11, 55-58.	0.1	4
2255	Electronic Band Structure and Heat Capacity Calculation of Some TlX (X = Sb, Bi) Compounds. Advances in Materials Physics and Chemistry, 2016, 06, 47-53.	0.3	1
2257	High-Pressure and High-Temperature Synthesis and In Situ High-Pressure Synchrotron X-ray Diffraction Study of HfSi₂. Inorganic Chemistry, 2021, 60, 15215-15222.	1.9	3
2258	Atomistic simulations of Agâ€“Cuâ€“Sn alloys based on a new modified embedded-atom method interatomic potential. Journal of Materials Research, 2022, 37, 145-161.	1.2	4
2259	Ethane and methane at high pressures: structure and stability. Journal of Chemical Physics, 2021, 155, 184503.	1.2	2
2260	Electronic Structure Methods Based on Density Functional Theory. , 2009, , 478-488.		0

#	Article	IF	Citations
2262	One New Isotherm Equation Expressed in Exp Form. Applied Physics, 2012, 02, 89-91.	0.0	0
2263	Theoretical calculations of high-pressure melting curves of five metals. Wuli Xuebao/Acta Physica Sinica, 2012, 61, 016401.	0.2	0
2264	Theoretical Assessment of the Mechanical, Electronic, and Vibrational Properties of the Paramagnetic Insulating Cerium Dioxide and Investigation of Intrinsic Defects. Advances in Chemical and Materials Engineering Book Series, 2014, , 431-446.	0.2	0
2266	Accuracy in Measurements and the Temperature and Volume Dependence of Thermoelastic Parameters. , 1993, , 327-339.		3
2268	Electronic Structure and Total Energy of Crystalline Approximants to Quasicrystalline Al-Cu-Fe Alloys. , 1994, , 323-331.		0
2270	Electronic Structure and Stability of Al-Ge Alloys Under Pressure. NATO ASI Series Series B: Physics, 1996, , 367-373.	0.2	0
2272	Modelling of Phase Transitions in Calciumâ€“Strontium Superstructures at Low Pressures.. Modelling and Simulation in Engineering, 2017, 39, 113-125.	0.0	0
2273	Elastic Anisotropic and Thermodynamic Properties of Two BC7 Phases. Acta Physica Polonica A, 2017, 132, 1340-1346.	0.2	1
2274	Eulerian Formulation. Shock Wave and High Pressure Phenomena, 2019, , 73-98.	0.1	0
2275	Comparison of Characteristics of Structural Phase Transitions under Pressure in Barium and Radium. Metallofizika I Noveishie Tekhnologii, 2019, 41, 851-861.	0.2	0
2276	Monoclinic semimetal IrSi synthesized under high pressure above 25 GPa: Crystal structure, electronic, and magnetic properties. Physical Review Materials, 2020, 4, .	0.9	1
2278	Unconventional iron-magnesium compounds at terapascal pressures. Physical Review B, 2021, 104, .	1.1	3
2279	Analysis of equations of state as applied to thermoelastic properties of C60 crystalline solid. Indian Journal of Physics, 2021, 95, 83-88.	0.9	0
2280	Evolutions of structural and optical properties of lead-free double perovskite Cs₂TeCl₆ under high pressure. Wuli Xuebao/Acta Physica Sinica, 2020, 69, 218801.	0.2	1
2281	Electronic and magnetic properties of new binary uranium-boron compounds with 2D and 3D boron networks: A revisit of the U:B system. Solid State Sciences, 2020, 101, 106150.	1.5	2
2282	High Pressure Study of HfNi Crystallographic and Electronic Structure. , 2005, , 786-791.		0
2283	Structural characteristics and elasticities of coesite and coesite-II at high pressure. New Journal of Physics, 2020, 22, 093044.	1.2	1
2284	INFLUENCE OF PRESSURE ON STRUCTURAL, ELECTRONIC, AND OPTICAL PROPERTIES OF CHOLINE IODIDE. Journal of Structural Chemistry, 2020, 61, 1503-1511.	0.3	0

#	Article	IF	Citations
2285	Ð†Ð¾Ð½Ð½Ð¸Ð¹ Ñ…Ð°Ñ€Ð°ÐºÑ‚ÐµÑ€, Ñ„Ð°Ð·Ð¾Ð²Ñ– Ð¿ÐµÑ€ÐµÑ…Ð¾Ð´Ð¸ Ð¿Ñ€Ð¸ Ð¾Ð´Ð½Ð¾Ð²Ñ–ÑÐ½Ð¾Ð¼Ñƒ Ñ‚Ð¸ÑÐºÑƒ Ñ– Ð¼Ð°Ð³Ð½Ñ–Ñ‚Ð½Ñ– Ð²Ð»Ð°ÑÑ‚Ð¸Ð²Ð¾ÑÑ‚Ñ– Ð¿ÐµÑ€Ð¾Ð²ÑÐºÑ–Ñ‚Ñ–Ð² KBeO3 Ñ– KMgO3. Ð¤Ñ–Ð·Ð¸ÐºÐ° Ð¢Ð²ÐµÑ€Ð´Ð¾Ð³Ð¾ Ð¢Ñ–Ð»Ð°, 2020, 62, 1.		
2286	High-pressure induced magnetic phase transition in half-metallic KBeO3 perovskite. Condensed Matter Physics, 2020, 23, 33601.	0.3	3
2287	Pressure induced phase transition of La-substituted BiFeO3. Solid State Communications, 2022, 341, 114595.	0.9	4
2288	Tunable indirect to direct band gap transition of Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1193" altimg="si40.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math>TaX (X=Al and Ga) Heusler alloy under hydrostatic pressure effect. Computational Materials Science, 2022, 203, 111049.	1.4	8
2289	MODEL OF POLYMORPHIC TRANSFORMATION IN A SHOCK WAVE. 3. BORON NITRIDE. Journal of Applied Mechanics and Technical Physics, 2021, 62, 542-551.	0.1	0
2290	Metallization and Superconductivity in the van der Waals Compound CuP₂Se through Pressure-Tuning of the Interlayer Coupling. Journal of the American Chemical Society, 2021, 143, 20343-20355.	6.6	10
2291	Structural and electronic properties of ternary alloys of alkaline-earth oxides and chalcogenides. Phase Transitions, 0, , 1-21.	0.6	0
2292	Crystal structures and mechanical properties of tungsten monocarbide predicted by first-principles investigations. Journal of Applied Physics, 2021, 130, 195902.	1.1	0
2293	Structural, elastic, electronic and optical properties of the half-Heusler ScPtSb and YPtSb compounds under pressure. Condensed Matter Physics, 2021, 24, 43702.	0.3	9
2294	A Comprehensive First Principles Calculations On (Ba _{0.82}K) Tj ETQq1 1 0.784314 rgBT /Overlock 10 ₃ Single-Cubic-Perovskite Superconductor. SSRN Electronic Journal, 0, , .	0.4	1
2295	Ferromagnetic half-metallicity of the cubic NaMgO₃ perovskite: from bulk to (001) surfaces. Physical Chemistry Chemical Physics, 2022, 24, 2209-2218.	1.3	3
2296	Equation of state of a new calcium magnesium silicate compound with the composition Ca3MgSi2O8 at pressures up to 23 GPa and ambient T. Physics and Chemistry of Minerals, 2022, 49, 1.	0.3	0
2297	First-principles study of the structural, electronic, optical, and thermoelectric properties of the RhVZ (Z= Si, Ge, Sn). Superlattices and Microstructures, 2022, 164, 107162.	1.4	3
2298	High pressure-induced phase transition in nanocrystalline iron confined by single-walled carbon nanohorns. Journal of Applied Physics, 2022, 131, .	1.1	5
2299	Theoretical calculations of the effect of nitrogen substitution on the structural, vibrational, and electronic properties of wolframite-type ScTaO₄at ambient conditions. Dalton Transactions, 2022, 51, 3642-3651.	1.6	3
2300	High-Pressure Properties of Wolframite-Type ScNbO₄. Journal of Physical Chemistry C, 2022, 126, 4664-4676.	1.5	14
2301	Deviation between quartzâ€inâ€garnet elastic geobarometry and equilibriumâ€based pressureâ€“temperature modelling in Barrovian metamorphic rocks. Journal of Metamorphic Geology, 2022, 40, 1067-1086.	1.6	2
2302	Structural, Electronic, and Magnetic Properties of Sr(_{1-x})Mn(_{x})F(_{2}) Alloys Studied by First-principles Calculations. Communications in Physics, 2022, 32, 157.	0.0	0

#	Article	IF	Citations
2303	First-principle studies of the pressure effect on metal carbonates elastic properties. Solid State Communications, 2022, 346, 114706.	0.9	4
2304	First-principles study of structural, mechanical, lattice dynamics, superconducting and optoelectronic properties of the Pd3Pb2Se2 shandite under hydrostatic pressure. Physica B: Condensed Matter, 2022, , 413920.	1.3	3
2305	Ab-initio method to investigate perovskites BiXO3(X = Be, Ca, Mg, Na, K, Li) for spintronics applications. Solid State Sciences, 2022, 126, 106839.	1.5	9
2306	Second nearest-neighbor modified embedded atom method interatomic potentials for Na-Mâ"Sn (MÂ=ÂCu,) Tj ETQq1 1 0.784314 rgBT	1.4	3
2307	Atomistic simulations of the deformation behavior of an Nb nanowire embedded in a NiTi shape memory alloy. Acta Materialia, 2022, 228, 117764.	3.8	5
2308	Structural, electronic, elastic, mechanical, magnetic and thermophysical insights of XCNi3 (X = Sc, Ti,) Tj ETQq1 1 0.784314 rgBT /Ove 144, 106617.	1.9	0
2309	Anomalous elasticity of talc at high pressures: Implications for subduction systems. Geoscience Frontiers, 2022, 13, 101381.	4.3	4
2310	Structural Stability of Pyrochlore Manganate In2Mn2O7 Under High Pressure. Frontiers in Physics, 2021, 9, .	1.0	0
2311	Structural, elastic, electronic and optical investigations of fluoride-perovskite NaBeF₃: first-principles calculations. Philosophical Magazine, 2022, 102, 634-649.	0.7	5
2312	Waterâ€"Solid Interface Engineering Stabilizes Kâ€Birnessite Cathode. Advanced Functional Materials, 2022, 32, 2108267.	7.8	2
2313	Enhancement of high entropy oxide (La0.2Nd0.2Sm0.2Gd0.2Y0.2)2Zr2O7 mechanical and photocatalytic properties via Eu doping. Journal of Materials Science, 2022, 57, 7863.	1.7	3
2314	Carbon and Silicon co-doping effect on microstructural and optoelectronic properties of ZnO: An ab initio study. Optik, 2022, , 169138.	1.4	0
2315	Drastic enhancement of magnetic critical temperature and amorphization in topological magnet EuSn2P2 under pressure. Npj Quantum Materials, 2022, 7, .	1.8	9
2316	Single-Crystal Elasticity of (Al,Fe)-bearing Bridgmanite up to 82 GPa. American Mineralogist, 2022, , .	0.9	0
2317	FIRST-PRINCIPLE STUDY OF THE BUCKLING COMPRESSIVE STRAIN INDUCED ON OPTOELECTRONIC ASPECTS OF TWO-DIMENSIONAL B₂C NANOSTRUCTURE. Surface Review and Letters, 2022, 29, .	0.5	3
2318	Magnetic, Electronic, Thermodynamic, and Thermoelectric Properties of Fe16N2 Alloys: Ab Initio Study. Journal of Superconductivity and Novel Magnetism, 0, , 1.	0.8	0
2319	Hard nanocrystalline gold materials prepared via high-pressure phase transformation. Nano Research, 0, , .	5.8	3
2321	First-principle studies of electronic, elastic and vibrational properties of barytocalcite and paralstonite. Materials Today Communications, 2022, 31, 103644.	0.9	0

#	Article	IF	Citations
2322	A high-pressure study of EuN using XRD and DFT. Solid State Communications, 2022, 351, 114811.	0.9	0
2323	Structural degradation behavior of Mg2-Pr Ni4 upon hydrogenation. Journal of Alloys and Compounds, 2022, 912, 165272.	2.8	4
2324	The structural, mechanical, and electronic properties of LiAlB ₄ under pressure from first principles. Physica Status Solidi C: Current Topics in Solid State Physics, 2017, 14, 1700080.	0.8	0
2325	Surface Structures and Their Relative Stabilities of Orthorhombic YAlO3: A First-Principles Study. Acta Metallurgica Sinica (English Letters), 0, , .	1.5	0
2326	Single-crystal elasticity of Zn2TiO4-spinel up to 18 GPa. Journal Physics D: Applied Physics, 0, , .	1.3	0
2327	Coordination Li diffusion chemistry in NASICON Li1.5Al0.5Ge1.5(PO4)3 solid electrolyte. Solid State Ionics, 2022, 381, 115947.	1.3	3
2328	Pressure-Quenched Superconductivity in Weyl Semimetal NbP Induced by Electronic Phase Transitions under Pressure. Journal of Physical Chemistry Letters, 2022, 13, 5514-5521.	2.1	6
2329	Equation of State and Electrical Transport Properties of Li2mno3 at High Pressure. SSRN Electronic Journal, 0, , .	0.4	0
2330	Novel Valence Transition in Elemental Metal Europium around 80ÂGPa. Physical Review Letters, 2022, 129, .	2.9	5
2331	Thermal and mechanical properties of the clathrate-II <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Na</mml:mi><mml:mn>24</mml:mn></mml:msub><mml:mi>Mn</mml:mi></mml:mrow></mml:math> Physical Review B, 2022, 105, .	1.1	2
2332	Development of slurry targets for high repetition-rate x-ray free electron laser experiments. Journal of Applied Physics, 2022, 131, .	1.1	3
2333	Equation of state of elbaite at high pressure up to 21.1 GPa and room temperature. Physics and Chemistry of Minerals, 2022, 49, .	0.3	1
2334	On the structure of SbTeI. Journal of Applied Physics, 2022, 132, 015106.	1.1	1
2335	Theoretical investigation of some fundamental physical properties of the ternary nitrides Ca4SiN4 and Ca4GeN4 under pressure and temperature effect. Computational Condensed Matter, 2022, 32, e00711.	0.9	5
2336	Highâ€Pressure and Highâ€Temperature Singleâ€Crystal Elasticity of Crâ€Pyrope: Implications for the Density and Seismic Velocity of Subcontinental Lithospheric Mantle. Geochemistry, Geophysics, Geosystems, 2022, 23, .	1.0	0
2337	Femtosecond diffraction studies of the sodium chloride phase diagram under laser shock compression. Journal of Applied Physics, 2022, 132, .	1.1	3
2338	Global water distribution in the mantle transition zone from a seismic isotropic velocity model and mineral physics modeling. Frontiers in Earth Science, 0, 10, .	0.8	0
2339	Spin resolved-Electronic, Magnetic and Thermodynamic properties of perovskites XTiO₃ (X= Rb, Cs) using GGA, TB-mBJ and GGA+U Potentials -A DFT approach. Canadian Journal of Physics, 0, , .	0.4	0

#	Article	IF	Citations
2340	Investigation of the Physical Properties of XCRh3 (Xâ€‰=â€‰Ti, V, Cr, Mn, Fe, Ni, Cu, Zn, Zr, Nb, Mo, Tc, Ru, Pd,) Ti ETQq0 0 0 rgBT /Ov	1.0	1
2341	Lattice distortion and the influence on mechanical and thermodynamic properties of high entropy (HfZrTaNbTi)X (X=C, N, NC) by Ab initio investigation. Ceramics International, 2022, 48, 35353-35364.	2.3	12
2342	Buckling variation effects on optical and electronic properties of GeP2S nanostructure: a first-principles calculation. Optical and Quantum Electronics, 2022, 54, .	1.5	1
2343	Abnormal Elastic Changes for Cubic-Tetragonal Transition of Single-crystal SrTiO₃. Chinese Physics Letters, 0, , .	1.3	2
2344	Thermal and rheological structure of lithosphere beneath Northeast China. Tectonophysics, 2022, 840, 229560.	0.9	2
2345	First principles study of adsorption and simulation of desorption properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si8.svg" display="inline" id="d1e1251"><mml:mrow><mml:msub><mml:mrow><mml:mi mathvariant="normal">Pd</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi mathvariant="normal">x</mml:mi></mml:mrow></mml:msub><mml:msub><mml:mrow><mml:mi mathvariant="normal">Ag</mml:mi></mml:mrow><mml:mrow><mml:mi	0.9	4
2346	First-principles calculations to investigate physical properties of single-cubic (Ba0.82K0.18)(Bi0.53Pb0.47)O3 novel perovskite superconductor. Materials Today Communications, 2022, 33, 104302.	0.9	22
2347	First-principles calculations to investigate mechanical, thermodynamic and electronic properties of Al2CuMg intermetallic compound under pressure effect. Computational Condensed Matter, 2022, 33, e00738.	0.9	3
2348	A new family of NaTMGe (TM = 3d transition metals) half-Heusler compounds: the role of TM modification. RSC Advances, 2022, 12, 26418-26427.	1.7	2
2349	Thermal expansion and compressibility of alamosite (PbSiO3) determined by in-situ synchrotron X-ray diffraction. Ceramics International, 2022, 48, 34350-34354.	2.3	2
2350	Experimental and theoretical study of anomalous temperature dependence of phonons in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Y</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi>Ti</mml:mi><mml:mn>2</mml:mn></m mathvariant="normal">O</mml:mi><mml:mn>7</mml:mn></mml:msub></mml:mrow></mml:math> pyrochlore. Physical Review B, 2022, 106, .	1.1	3
2351	Chemical Bonding Effects and Physical Properties of Noncentrosymmetric Hexagonal Fluorocarbonates ABCO3F (A: K, Rb, Cs; B: Mg, Ca, Sr, Zn, Cd). Molecules, 2022, 27, 6840.	1.7	3
2352	Temperature distribution in a laser-heated diamond anvil cell as described by finite element analysis. AIP Advances, 2022, 12, 105218.	0.6	1
2353	Vibration Spectra of Double Kâ€“Ca, Kâ€“Mg, and Naâ€“Mg Carbonates under Pressure. Geochemistry International, 2022, 60, 1103-1113.	0.2	1
2354	Theoretical Study of the Effect of Pressure on the Structure and Electronic Properties of Metal Carbonates. Bulletin of the Russian Academy of Sciences: Physics, 2022, 86, 1230-1241.	0.1	0
2355	Insulator-metal-superconductor transition in the medium-entropy van der Waals compound <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>M</mml:mi><mml:mi		

#	Article	IF	Citations
2358	Discovery of high-pressure post-perovskite phase in HoCrO3. Journal of Physics and Chemistry of Solids, 2023, 172, 111078.	1.9	4
2359	Determination of Pâ€“V equation of state of a natural clinoptilolite using high-pressure powder synchrotron X-ray diffraction. Physics and Chemistry of Minerals, 2022, 49, .	0.3	1
2360	Phase stability of stress-sensitive Ag2CO3 silver carbonate at high pressures and temperatures. Solid State Sciences, 2023, 135, 107068.	1.5	3
2361	Insights into crystal structure, elasticity, lattice dynamics, and thermodynamics of ternary magnesium alloy MgZn2Ce. Vacuum, 2023, 209, 111755.	1.6	1
2362	Ab Initio Studies of the Influence of Pressure on the Structure and Electronic and Elastic Properties of Carbonates of Alkaline and Alkaline-Earth Metals. Physics of the Solid State, 2022, 64, 405-415.	0.2	1
2363	Pressure-dependent electronic properties in the rocksalt structure of lithium fluoride: A DFT Study. Journal of Physics: Conference Series, 2022, 2376, 012010.	0.3	0
2364	Superconductivity arising from pressure-induced emergence of a Fermi surface in the kagome-lattice chalcogenide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Rb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:m Physical Review B, 2022, 106, .	1.1	3
2365	Singleâ€Crystal Elasticity of Phase E at High Pressure and Temperature: Implications for the Lowâ€Velocity Layer Atop the 410â€km Depth. Journal of Geophysical Research: Solid Earth, 2022, 127, .	1.4	1
2366	Influence of 3d-Fe substitution on structural, mechanical, electronic, and magnetic properties in rock-salt SrS: Insights from the first-principles study. Solid State Communications, 2023, 361, 115060.	0.9	1
2367	Thermodynamic Properties of MgAl2O4 Spinel at High Temperatures and High Pressures. Crystals, 2023, 13, 240.	1.0	0
2368	Solids that are also liquids: elastic tensors of superionic materials. Npj Computational Materials, 2023, 9, .	3.5	2
2369	An ab initio study of novel quaternary Heusler alloys for spin polarized and waste heat recycling systems. Journal of Magnetism and Magnetic Materials, 2023, 571, 170541.	1.0	5
2370	Ion kinetic energy- and ion flux-dependent mechanical properties and thermal stability of (Ti,Al)N thin films. Acta Materialia, 2023, 250, 118864.	3.8	9
2371	First-principles analysis of the physical properties of XAcTe2 (XÂ=ÂLi, Na) Heusler alloys for optoelectronic and thermoelectric devices. Computational Materials Science, 2023, 224, 112156.	1.4	6
2372	Visible light response in 2D QBi (Q=Si, Ge and Sn) monolayer semiconductors: A DFT based study. Materials Today Communications, 2023, 35, 105886.	0.9	0
2373	Electronic, mechanical, optical and thermodynamic properties of the quaternary semiconductors Sr3GeMgN4 and Ba3GeMgN4. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2023, 290, 116292.	1.7	0
2374	High-Pressure Structural and Thermodynamic Properties of Cerium Orthosilicates (CeSiO₄). Journal of Physical Chemistry C, 2023, 127, 4225-4238.	1.5	4
2375	DFT investigations of optoelectronic and thermoelectric properties of stannite phase of Cu₂SrXSe₄ (X = Ge, Si, Sn) compounds using TB-mBJ mechanism. Modern Physics Letters B, 2023, 37, .	1.0	0

#	Article	IF	Citations
2377	Theoretical study of void collapse and hot spot formation mechanism for energetic material. Philosophical Magazine, 2023, 103, 915-932.	0.7	0
2378	Equation of State, Compressibility, and Vibrational Properties of Brucite over Wide Pressure and Temperature Ranges: Atomistic Computer Simulations with the Modified ClayFF Classical Force Field. Minerals (Basel, Switzerland), 2023, 13, 408.	0.8	4
2379	Ordered Van der Waals Hetero-nanoribbon from Pressure-Induced Topochemical Polymerization of Azobenzene. Journal of the American Chemical Society, 2023, 145, 6845-6852.	6.6	1
2380	Exploring the hardness and high-pressure behavior of osmium and ruthenium-doped rhenium diboride solid solutions. APL Materials, 2023, 11, 031108.	2.2	1
2381	Intraband and interband transitions in X$$_2$$MnSi(X=Fe,Co,Ni), Fe$$_2$$YSi(Y=V,Cr,Mn) and Fe$$_2$$MnZ(Z=Si,Ge,Sn) full-Heusler alloys: first principles calculations. European Physical Journal Plus, 2023, 138, .	1.2	0
2382	High-Pressure Coupling Reactions to Produce a Spherical Bulk Re_xN/Fe₃N Composite. Inorganic Chemistry, 2023, 62, 6263-6273.	1.9	1
2383	Pressure-induced Mott insulator-metal transition and structural phase transitions in the triangular antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Ni</mml:mi><mml:msub><mml:mi>Ga</mml:mi><mml:mi><mml:m mathvariant="normal">S</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math>. Physical Review B, 2023, 107, .	0.0	0
2384	Improved Mechanical Characterization of LiCoO2 Cathode Material by Ab-Initio Calculations Using Density Functional Theory. Bulletin of the Chemical Society of Japan, 2023, 96, 475-483.	2.0	0
2385	DFT based comparative analysis of the physical properties of some binary transition metal carbides XC (X = Nb, Ta, Ti). Journal of Materials Research and Technology, 2023, 24, 4808-4832.	2.6	8