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## The Compressibility of Media under Extreme Pressures

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2172	Lattice dynamics and thermal expansion of lutetium. <b>1979</b> , 36, 279-291	3

2171	An examination of the elasticity of hot-pressed MgO. <b>1979</b> , 5, 21-31	2
2170	A critical evaluation of equations of state by piezo-optic measurements. <b>1979</b> , 50, 1328-1333	7
2169	Lattice dynamics, thermal and elastic properties of hafnium. <b>1979</b> , 40, 769-778	
2168	Applicability of quadratic Murnaghan equation of state and Morse potential to diamond compressibility data. <b>1980</b> , 41, 679-680	2
2167	The thermodynamics of elastic deformation□ <b>1980</b> , 41, 837-850	174
2166	References. <b>1980</b> , 324-342	
2165	The second- and third-order elastic constants of amorphous arsenic. <b>1980</b> , 42, 127-148	47
2164	Study of the localized vibrations of boron in heavily doped Si. <b>1980</b> , 22, 4825-4833	83
2163	Equation of state from weak shocks in solids. <b>1980</b> , 22, 1495-1502	32
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2161	Dependence of the phonon spectrum of InP on hydrostatic pressure. <b>1980</b> , 21, 4869-4878	190
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2159	Piezo- and elasto-optic properties of liquids under high pressure. III. Results on twelve more liquids. <b>1980</b> , 73, 4577-4584	23
2158	Microscopic Theory of the Phase Transformation and Lattice Dynamics of Si. <b>1980</b> , 45, 1004-1007	465
2157	Piezo- and elasto-optic properties of deuterium oxide under high pressure. <b>1980</b> , 72, 1410-1411	1
2156	Ground-state properties of diamond. <b>1981</b> , 24, 6121-6124	129
2155	The pressure dependence of elastic constants and bond bending in HgTe. <b>1981</b> , 43, 1447-1471	48
2154	X-ray Measurements of the Bulk Modulus of the Myofilament Liquid Crystal in Striated Muscle. <b>1981</b> , 75, 211-216	4

2153	Pressure dependences of the elastic constants of PbTe, SnTe and Ge <sub>0.08</sub> Sn <sub>0.92</sub> Te. <b>1981</b> , 14, 1569-1584	81
2152	Evaluation of crystallization temperatures of mineral paragenesis in consolidated crust and uppermost mantle from explosion seismology data. <b>1981</b> , 119, 854-864	1
2151	Garnet inclusions in diamond and the state of the upper mantle. <b>1981</b> , 7, 216-222	7
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2143	The effects of pressure on the elastic constants of mercury selenide up to the phase transition. <b>1982</b> , 15, 657-671	39
2142	Elastic properties of GaS under high pressure by Brillouin scattering. <b>1982</b> , 25, 2767-2775	57
2141	Pressure-induced valence transition in TmSe: An x-ray-diffraction study. <b>1982</b> , 25, 3841-3845	25
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2136	The hydrostatic pressure derivatives of the elastic constants of the scheelites LiYF <sub>4</sub> and LiY <sub>0.5</sub> Tb <sub>0.5</sub> F <sub>4</sub> . <b>1982</b> , 15, 2081-2092	13

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2117	Total energy method for solids and solid surfaces. <b>1984</b> , 26, 105-120	20
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2041	On the use of shock-wave data in evaluations of thermodynamic properties. <b>1987</b> , 48, 819-825	8
2040	Elastic behaviour under pressure of the binary tellurite glasses TeO <sub>2</sub> -ZnCl <sub>2</sub> and TeO <sub>2</sub> -WO <sub>3</sub> . <b>1987</b> , 6, 443-446	46
2039	On the use of Grüneisen parameters in the treatment of shock-wave data. <b>1987</b> , 8, 751-761	5
2038	Critical evaluation of the thermodynamic properties of cobalt. <b>1987</b> , 8, 481-510	84
2037	The elastic behaviour and vibrational anharmonicity of molybdenum phosphate glasses. <b>1987</b> , 22, 2113-2118	11
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2033	The Melting Laws. <b>1988</b> , 146, 105-110	18
2032	Phase Transition and Anharmonic Properties of Semimagnetic Semiconductors. <b>1988</b> , 146, 111-116	2
2031	Ground State and Electronic Properties of Silicon Carbide and Boron Nitride. <b>1988</b> , 146, 573-587	37
2030	Theoretical evidence for a new ultra-high-pressure phase of SiO <sub>2</sub> . <b>1988</b> , 336, 670-672	66
2029	A theoretical investigation of the electronic structure and some thermodynamic properties of $\beta$ -PbF <sub>2</sub> . <b>1988</b> , 21, 5351-5359	31
2028	Bandgap hydrostatic deformation potentials for epitaxial In <sub>0.52</sub> Al <sub>0.48</sub> As on InP(001). <b>1988</b> , 31, 383-387	1

2027	Measurement of the pressure dependence of the direct band gap of $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$ using stimulated emission. <b>1988</b> , 52, 2124-2126	10
2026	Local-density-pseudofunction theory of bulk Si. <b>1988</b> , 38, 2176-2178	19
2025	Elastic behavior of magnetic oxides from acoustic and static compression studies. <b>1988</b> , 51, 86-92	3
2024	Theory of electronic, vibrational, and superconducting properties of fcc silicon. <b>1988</b> , 37, 6344-6348	26
2023	Elastic constants of NbC and MoN: Instability of B1-MoN. <b>1988</b> , 37, 3295-3298	67
2022	Electronic and structural properties of $\text{MgH}_2$ . <b>1988</b> , 37, 8730-8737	122
2021	Hydrostatic-pressure dependencies of deep impurity levels in zinc-blende semiconductors. <b>1988</b> , 38, 12549-12555	17
2020	Universality relationships in condensed matter: Bulk modulus and sound velocity. <b>1988</b> , 37, 4351-4357	30
2019	Proposed universal interatomic potential for elemental tetrahedrally bonded semiconductors. <b>1988</b> , 38, 3318-3322	104
2018	Ground-state and electronic properties of covalent solids. <b>1988</b> , 38, 12675-12678	18
2017	Possibility of $\text{LiBeH}_3$ being metallic. <b>1988</b> , 38, 3576-3579	24
2016	Structural and electronic properties of spinel semiconductors: An ab initio pseudopotential study of $\text{MgIn}_2\text{S}_4$ . <b>1988</b> , 38, 8258-8263	26
2015	Local-density-approximation study of LaS and SmS. <b>1988</b> , 37, 10045-10049	25
2014	Structural and electronic properties of WC. <b>1988</b> , 38, 9483-9489	106
2013	Electronic and structural properties of elemental copper: A pseudopotential-local-orbital calculation. <b>1988</b> , 38, 7966-7971	41
2012	Local-density description of antiferromagnetic Cr. <b>1988</b> , 38, 12834-12836	33
2011	Theoretical model for the hcp-bcc transition in Mg. <b>1988</b> , 37, 5571-5576	51
2010	Effect of Pressure on the Direct Energy Gap of LiH. <b>1988</b> , 57, 367-371	41

2009	Samarium-ion valence instability in a glassy matrix. <b>1988</b> , 57, 49-53	16
2008	Some Elastic Constant Data on Minerals Relevant to Geophysics. <b>1988</b> , 237-270	
2007	Elasticity and Constitution of the Earth's Interior. <b>1988</b> , 31-90	
2006	Solid Solutions of AB <sub>2</sub> C <sub>4</sub> Defect Semiconductors. <b>1988</b> , 141, 195	1
2005	Elastic Constants of Single-Crystal Forsterite as a Function of Temperature and Pressure. <b>1988</b> , 271-282	1
2004	The Use of Ultrasonic Measurements Under Modest Compression to Estimate Compression at High Pressure. <b>1988</b> , 134-152	
2003	Bulk modulus and its pressure derivative of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7-x</sub> . <b>1989</b> , 39, 2872-2875	50
2002	Effect of relaxation of the second-nearest neighbors on the thermodynamic properties of semiconducting alloys: Application to GaAs <sub>y</sub> Sb <sub>1-y</sub> . <b>1989</b> , 39, 5987-5997	20
2001	Ab initio calculation of pressure coefficients of band gaps of silicon: Comparison of the local-density approximation and quasiparticle results. <b>1989</b> , 39, 7840-7847	91
2000	Ground-state properties of fcc and bcc lanthanum. <b>1989</b> , 39, 4921-4925	21
1999	Theory of high-pressure phases of hydrogen. <b>1989</b> , 62, 1150-1153	137
1998	Optical properties of gallium selenide under high pressure. <b>1989</b> , 40, 3837-3854	91
1997	Pressure effects on self-diffusion in silicon. <b>1989</b> , 40, 10643-10646	111
1996	Properties of hydrogen in crystalline silicon under compression and tension. <b>1989</b> , 63, 1090-1093	12
1995	Direct-band-gap absorption in germanium under pressure. <b>1989</b> , 39, 12921-12924	35
1994	Pressure dependence of the band gaps of semiconductors. <b>1989</b> , 40, 12516-12519	38
1993	Total-energy study of the equation of state of HgTe and HgSe. <b>1989</b> , 39, 10154-10161	31
1992	High-Pressure Studies of Absorption and Luminescence Spectra in 3CβiC. <b>1989</b> , 58, 2673-2676	11

1991	Photoluminescence of AlInAs under hydrostatic pressure. <b>1989</b> , 4, 243-245	5
1990	The pressure variation in the electronic charge density of LiH. <b>1989</b> , 1, 1601-1612	8
1989	Tests of the Harris energy functional. <b>1989</b> , 1, 7565-7576	82
1988	The dependences of the elastic stiffness moduli and the Poisson ratio of natural iron pyrites FeS <sub>2</sub> upon pressure and temperature. <b>1989</b> , 22, 670-675	33
1987	Graphite under pressure: Equation of state and first-order Raman modes. <b>1989</b> , 39, 12598-12603	470
1986	Inverted isothermal equations of state and determination of B <sub>0</sub> , B' <sub>0</sub> and B <sub>0</sub> . <b>1989</b> , 50, 263-268	58
1985	Geobarothermometric properties of growth twins and mathematical analysis of quartz data for a broad range of temperatures and pressures. <b>1989</b> , 16, 783-789	7
1984	Experimental and theoretical equation of state of cubic boron nitride. <b>1989</b> , 337, 349-352	278
1983	Extended x-ray-absorption fine-structure study of copper under high pressure. <b>1989</b> , 39, 12537-12547	42
1982	First-principles calculation of alloy phase diagrams: The renormalized-interaction approach. <b>1989</b> , 40, 3197-3231	244
1981	A five-parameter temperature-corrected Murnaghan equation for P-V-T surfaces. <b>1989</b> , 94, 9477	37
1980	Shock wave equation of state and finite strain theory. <b>1989</b> , 94, 5873	124
1979	Non-empirical pseudopotentials in the HF-LCAO approach to crystalline solids. <b>1989</b> , 67, 891-901	21
1978	Microscopic structure of the hydrogen-boron complex in crystalline silicon. <b>1989</b> , 39, 10809-10824	142
1977	Prediction of new low compressibility solids. <b>1989</b> , 245, 841-2	2307
1976	Theoretical study of cubic versus tetragonal structures of defect zinc-blende semiconductors: CdIn <sub>2</sub> Se <sub>4</sub> . <b>1989</b> , 40, 1725-1731	23
1975	Hydrogen in Crystalline Silicon under Compression and Tension. <b>1989</b> , 163, 425	
1974	High Pressure Phase of Arsenic and Antimony. <b>1989</b> , 58, 924-929	3



1973	Compression ratio and red shift of the R1 line for YAG : Cr. <b>1990</b> , 3, 153-155	5
1972	Theoretical Study of High Pressure Metallic Hydrogen. <b>1990</b> , 193, 15	
1971	Theoretical Studies of the Electronic Properties of Ceramic Materials. <b>1990</b> , 73, 3135-3160	240
1970	Thermoelastic stability of multiple growth twins in quartz and general geobarothermometric implications. <b>1990</b> , 23, 253-287	8
1969	Invar properties in Fe-Ni system from band theory. <b>1990</b> , 161, 115-120	18
1968	The elastic behaviour of natural single crystals of the high-spin compound MnS <sub>2</sub> . <b>1990</b> , 2, 3713-3721	4
1967	Effects of gradient corrections on electronic structure in metals. <b>1990</b> , 2, 7597-7611	85
1966	Equilibrium properties of zinc. <b>1990</b> , 42, 8885-8889	26
1965	Martensitic transformation of Ca. <b>1990</b> , 42, 4563-4567	21
1964	Theory of local bond-length relaxation in Hg <sub>1-x</sub> Cd <sub>x</sub> Te alloys. <b>1990</b> , 41, 7744-7748	20
1963	Room-temperature densification of a-SiO <sub>2</sub> versus pressure. <b>1990</b> , 41, 6086-6087	90
1962	Total energy, lattice dynamics, and structural phase transitions in silicon by the orthogonalized linear combination of atomic orbitals method. <b>1990</b> , 41, 12162-12179	40
1961	Variational quantum Monte Carlo nonlocal pseudopotential approach to solids: Formulation and application to diamond, graphite, and silicon. <b>1990</b> , 42, 3503-3522	170
1960	Magnetism of hexagonal 3d transition metals. <b>1990</b> , 42, 6683-6693	30
1959	Equations of state of alkali hydrides at high pressures. <b>1990</b> , 41, 7883-7886	42
1958	Surface and thermodynamic interatomic force fields for silicon clusters and bulk phases. <b>1990</b> , 41, 5735-5745	63
1957	Stability of DX centers in Al <sub>x</sub> Ga <sub>1-x</sub> As alloys. <b>1990</b> , 42, 7174-7177	69
1956	Ab initio Hartree-Fock calculations for periodic compounds: application to semiconductors. <b>1990</b> , 2, 7769-7789	181

1955	Cubic ZnS under pressure: Optical-absorption edge, phase transition, and calculated equation of state. <b>1990</b> , 42, 9113-9118	188
1954	Interatomic potentials and the structural properties of silicon dioxide under pressure. <b>1990</b> , 41, 10866-10869	20
1953	Structural and electronic properties of narrow-band-gap semiconductors: InP, InAs, and InSb. <b>1990</b> , 41, 12079-12085	86
1952	First-principles calculation of temperature-composition phase diagrams of semiconductor alloys. <b>1990</b> , 41, 8240-8269	232
1951	Structural properties and electronic structure of low-compressibility materials: beta -Si <sub>3</sub> N <sub>4</sub> and hypothetical beta -C <sub>3</sub> N <sub>4</sub> . <b>1990</b> , 41, 10727-10734	897
1950	Effect of pressure on the refractive index of Ge and GaAs. <b>1990</b> , 41, 10104-10110	75
1949	Rhombohedral to simple-cubic phase transition in arsenic under pressure. <b>1990</b> , 41, 5535-5543	75
1948	Pressure-dependent phonon properties of III-V compound semiconductors. <b>1990</b> , 41, 12129-12139	19
1947	High-pressure metallic phases of boron. <b>1990</b> , 42, 9033-9039	59
1946	Calculation of ground-state and optical properties of boron nitrides in the hexagonal, cubic, and wurtzite structures. <b>1991</b> , 44, 7787-7798	376
1945	Elastic constants and electronic structure of fluorite (CaF <sub>2</sub> ): an ab initio Hartree-Fock study. <b>1991</b> , 3, 4151-4164	93
1944	Analysis of thermodynamic properties of molybdenum and tungsten at high temperatures. <b>1991</b> , 44, 4332-4340	43
1943	Electronic structure of the ordered phases of Pt-Fe alloys. <b>1991</b> , 43, 11300-11318	94
1942	Structural phase transitions and optical absorption of LiInSe <sub>2</sub> under pressure. <b>1991</b> , 43, 9635-9642	34
1941	Efficient pseudopotentials for plane-wave calculations. II. Operators for fast iterative diagonalization. <b>1991</b> , 43, 8861-8869	584
1940	Atmospheric-pressure stability of energetic phases of carbon. <b>1991</b> , 44, 11578-11591	78
1939	Precise density-functional method for periodic structures. <b>1991</b> , 44, 7888-7903	391
1938	Pseudopotential plane-wave calculations for ZnS. <b>1991</b> , 43, 2213-2217	134

1937	A Hugoniot theory for solid and powder mixtures. <b>1991</b> , 69, 710-716	33
1936	Efficient pseudopotentials for plane-wave calculations. <b>1991</b> , 43, 1993-2006	13225
1935	Ground-state properties of lanthanum: Treatment of extended-core states. <b>1991</b> , 43, 6388-6392	508
1934	Pseudopotential Hartree-Fock study of seventeen III-V and IV-IV semiconductors. <b>1991</b> , 43, 11937-11943	168
1933	First-principles statistical mechanics of structural stability of intermetallic compounds. <b>1991</b> , 44, 512-544	274
1932	Predicting new solids and their properties. <b>1991</b> , 334, 501-513	14
1931	Relativistic effects on the structural and magnetic properties of iron. <b>1991</b> , 79, 121-124	10
1930	On the elastic properties of lithium, sodium and potassium oxide. An ab initio study. <b>1991</b> , 156, 11-19	219
1929	Pressure dependence of the Raman phonon spectrum in 6h-silicon carbide. <b>1991</b> , 247, 373-384	14
1928	Equilibrium properties of the layer $\text{ZnIn}_2\text{S}_4$ . <b>1991</b> , 13, 291-299	2
1927	Calculation of the state parameters of condensed substances at high pressures and temperatures. <b>1991</b> , 27, 426-432	3
1926	Compressibility of liquids: Theoretical basis for a century of empiricism. <b>1991</b> , 12, 855-868	16
1925	Calculation of the equation of state and elastic moduli of MgO using molecular orbital theory. <b>1991</b> , 17, 622	1
1924	Pressure dependence of photoluminescence in CdTe/Cd $_{1-x}$ Zn $_x$ Te strained-layer heterostructures. <b>1991</b> , 6, 454-460	16
1923	On the tests of universality for isothermal equations of state. <b>1991</b> , 3, 775-780	7
1922	Tellurium-based II-VI compound semiconductors and heterostructures under strain. <b>1991</b> , 6, 428-438	38
1921	Pressure dependences of band gaps and optical-phonon frequency in cubic SiC. <b>1991</b> , 44, 1053-1056	42
1920	Extended x-ray-absorption fine-structure study of alkali-metal halides under high pressure. <b>1991</b> , 43, 9894-9905	21

1919	Gradient-corrected density functionals: Full-potential calculations for iron. <b>1991</b> , 43, 11628-11634	157
1918	Theory of high-pressure phases of Pb. <b>1991</b> , 43, 1795-1798	34
1917	First-principles study of the structural properties of Sn under pressure. <b>1991</b> , 44, 4103-4108	52
1916	Influence of the local-spin-density correlation functional on the stability of bcc ferromagnetic iron. <b>1991</b> , 44, 7701-7703	22
1915	Pseudopotential plane-wave calculation of the structural properties of yttrium. <b>1991</b> , 44, 10339-10342	9
1914	Pressure tuning of strains in semiconductor heterostructures: (ZnSe epilayer)/(GaAs epilayer). <b>1991</b> , 44, 11307-11314	73
1913	Adequacy of the local-spin-density approximation for Gd. <b>1991</b> , 44, 7451-7454	73
1912	H-point phonon in molybdenum: Superlinearized augmented-plane-wave calculations. <b>1991</b> , 43, 1441-1445	22
1911	Theoretical equation of state for aluminized nitromethane. <b>1991</b> , 69, 3893-3900	20
1910	Quasiparticle calculation of the dielectric response of silicon and germanium. <b>1991</b> , 43, 4187-4207	199
1909	Structural and electronic properties of alpha -Sn, CdTe, and their. <b>1991</b> , 43, 8951-8961	10
1908	Theoretical study of atomic phases of metallic hydrogen. <b>1991</b> , 44, 11563-11568	19
1907	The effect of hydrostatic pressure on the band structure of the monolayer superlattice GaAs-Ga <sub>1-x</sub> Al <sub>x</sub> As(001). <b>1991</b> , 3, 6553-6558	1
1906	Electronic, structural, and mechanical properties of possible metastable phases of beryllium hydride. <b>1991</b> , 6, 291-299	
1905	High pressure phase transition in gallium nitride. <b>1991</b> , 7, 96-98	29
1904	Investigation of the hydrostatic pressure dependence of the E <sub>0</sub> gap, the excitonic binding energy and the refractive index of MOCVD-grown ZnTe layers. <b>1992</b> , 4, 6401-6416	27
1903	InP under high pressures. <b>1992</b> , 7, 2205-2210	5
1902	Theoretical investigation of (111) stacking faults in aluminium. <b>1992</b> , 66, 387-404	25

1901	Volume effects on the magnetic properties of cubic isostructural intermetallics of Ce. <b>1992</b> , 46, 6217-6224	12
1900	Theoretical determination of the pressure dependence of the electronic and the optical properties of fcc C60. <b>1992</b> , 46, 4241-4245	34
1899	Energetics and stability of diamondlike amorphous carbon. <b>1992</b> , 68, 1854-1857	63
1898	Superconductivity in arsenic at high pressures. <b>1992</b> , 46, 5523-5527	26
1897	Exciton photoluminescence in strained and unstrained ZnSe under hydrostatic pressure. <b>1992</b> , 46, 13371-13378	44
1896	Structural and electronic properties of KnC60. <b>1992</b> , 46, 1766-1772	102
1895	Electronic structure, lattice stability, and superconductivity of CrC. <b>1992</b> , 46, 14969-14974	27
1894	Raman scattering from cubic boron nitride up to 1600 K. <b>1992</b> , 72, 1955-1956	23
1893	Polymeric nitrogen. <b>1992</b> , 46, 14419-14435	364
1892	Short-range order and energetics of disordered silicon-carbon alloys. <b>1992</b> , 46, 10048-10061	42
1891	Electronic structure, magnetism, and stability of Co-doped NiAl. <b>1992</b> , 46, 14392-14397	19
1890	General trends in changing epilayer strains through the application of hydrostatic pressure. <b>1992</b> , 45, 11929-11935	37
1889	High-pressure atomic phases of solid nitrogen. <b>1992</b> , 46, 11117-11120	39
1888	Pressure dependence of the exciton absorption and the electronic subband structure of a Ga <sub>0.47</sub> In <sub>0.53</sub> As/Al <sub>0.48</sub> In <sub>0.52</sub> As multiple-quantum-well system. <b>1992</b> , 45, 6809-6818	13
1887	Native defects and self-compensation in ZnSe. <b>1992</b> , 45, 10965-10978	253
1886	First-principles study of the atomic structure and local vibrational modes of the DX center in GaAs under pressure. <b>1992</b> , 46, 13131-13135	12
1885	Structural and electronic properties of titanium dioxide. <b>1992</b> , 46, 1284-1298	335
1884	First-principles pseudopotential calculations of magnetic iron. <b>1992</b> , 45, 8887-8893	65

- 1883 Raman scattering and x-ray-absorption spectroscopy in gallium nitride under high pressure. **1992**, 45, 83-89 498
- 1882 Electronic structures, total energies, and optical properties of alpha -rhombohedral B12 and alpha -tetragonal B50 crystals. **1992**, 45, 5895-5905 46
- 1881 Cohesive properties of iron obtained by use of the generalized gradient approximation. **1992**, 46, 13599-13602 98
- 1880 Band gaps of diamond under anisotropic stress. **1992**, 45, 8239-8247 59
- 1879 First-principles determination of the Ni-Al phase diagram. **1992**, 4, 945-959 63
- 1878 Structural and electronic properties of C60. **1992**, 46, 1754-1765 253
- 1877 Ab initio Hartree-Fock study of tetragonal and cubic phases of zirconium dioxide. **1992**, 45, 592-601 83
- 1876 Temperature dependence of the acoustic-mode vibrational anharmonicity of quartz from 243 to 393 K. **1992**, 45, 10242-10254 9
- 1875 Magnetism in bcc cobalt. **1992**, 45, 2258-2261 38
- 1874 Near-Hartree-Fock wave functions for solids: The case of crystalline silicon. **1992**, 42, 5-33 43
- 1873 Anisotropy in the compressibility of molybdenum disulphide up to pressures of 90 kbar. **1992**, 53, 147-151 1
- 1872 Ab initio Hartree-Fock study of solid beryllium oxide: structure and electronic properties. **1992**, 164, 383-394 47
- 1871 Equation of state of compressed liquids: statistical-mechanical basis. **1993**, 88, 25-34 1
- 1870 Relaxation and electronic structure of surfaces in lithium sulphide: A Hartree-Fock ab initio approach. **1993**, 54, 1603-1611 27
- 1869 Equation-of-state measurements for crude oils at pressures up to 1 GPa. **1993**, 14, 215-220 5
- 1868 Thermische Dilatation und Hochdruckverhalten der Zintl-Phasen CaSn und BaSn. **1993**, 619, 897-900 11
- 1867 Mechanical Properties of LiF and LiCl Crystals Under High Pressure. **1993**, 175, K1-K4 1
- 1866 Quantum Mechanical Hartree-Fock Study of the Elastic Properties of Li<sub>2</sub>S and Na<sub>2</sub>S. **1993**, 177, 157-163 70

1865	Thermodynamic Approximations in High-pressure and High-Temperature Physics of Solids. <b>1993</b> , 179, 351-356	53
1864	pV-curves in the dynamic-static compression method. <b>1993</b> , 29, 646-648	2
1863	Electronic structure and bonding in epitaxially stabilized cubic iron silicides. <b>1993</b> , 48, 4364-4372	65
1862	Optimized and transferable nonlocal separable ab initio pseudopotentials. <b>1993</b> , 47, 4174-4180	872
1861	Static lattice and electron properties of MgCO <sub>3</sub> (magnesite) calculated by ab initio periodic Hartree-Fock methods. <b>1993</b> , 47, 9189-9198	86
1860	Calculation of pseudoatom information in gallium arsenide. <b>1993</b> , 5, 2511-2520	1
1859	Structural properties and energetics of amorphous forms of carbon. <b>1993</b> , 47, 1829-1839	84
1858	Electronic, optical, and structural properties of some wurtzite crystals. <b>1993</b> , 48, 4335-4351	538
1857	Thermal expansivity, bulk modulus, and melting curve of H <sub>2</sub> O ice VII to 20 GPa. <b>1993</b> , 99, 5369-5373	145
1856	Pressure and Temperature Evolution of the Structure of Solid C 70. <b>1993</b> , 22, 611-618	79
1855	Photoluminescence of ZnSe/ZnMnSe superlattices under hydrostatic pressure. <b>1993</b> , 73, 7730-7738	8
1854	Generalized-gradient-approximation study of the magnetic and cohesive properties of bcc, fcc, and hcp Mn. <b>1993</b> , 47, 15992-15995	73
1853	A theoretical study of selenium I under high pressure. <b>1993</b> , 5, 8065-8074	17
1852	Energetics and electronic structure of the hypothetical cubic zincblende form of GeC. <b>1993</b> , 1, 741-754	45
1851	High-pressure, low-temperature structural studies of orientationally ordered C60. <b>1993</b> , 5, 7923-7928	48
1850	Equations of state and a tight-binding model for strained layers: Application to a ZnSe-GaAs epilayer. <b>1993</b> , 48, 2452-2459	16
1849	Theoretical study of Raman modes in high-pressure phases of Si, Ge, and Sn. <b>1993</b> , 48, 3646-3653	28
1848	Ultrasonic study of the temperature and pressure dependences of the elastic properties of a Mn <sub>78</sub> Pt <sub>22</sub> -alloy single crystal. <b>1993</b> , 48, 3216-3223	4

1847	Structural and electronic properties of InSb under pressure. <b>1993</b> , 47, 4841-4848	22
1846	Application of gradient corrections to density-functional theory for atoms and solids. <b>1993</b> , 48, 14944-14952	78
1845	ZnTe at high pressure: X-ray-absorption spectroscopy and x-ray-diffraction studies. <b>1993</b> , 48, 8683-8693	64
1844	Pseudopotential study of the structural properties of bulk Li. <b>1993</b> , 47, 14020-14022	9
1843	Bulk structural properties of Mo: Plane-wave-basis pseudopotential study with a partial-core-correction scheme. <b>1993</b> , 47, 2979-2982	1
1842	Pressure dependence of the band structure, density of states, Fermi surfaces, and optical properties of superconducting K3C60. <b>1993</b> , 47, 8249-8259	16
1841	Crystal binding energies from atomic-cluster calculations. <b>1993</b> , 47, 4025-4028	6
1840	Ab initio calculations of Si, As, S, Se, and Cl adsorption on Si(001) surfaces. <b>1993</b> , 47, 1898-1910	178
1839	Influence of pressure on (001)GaAs surfaces. <b>1993</b> , 47, 1412-1418	
1838	Optical studies of strained pseudomorphic semiconductor heterostructures under external pressure. <b>1994</b> , 70, 369-380	21
1837	An ab initio pseudopotential calculation of ground-state and excited-state properties of gallium nitride. <b>1994</b> , 6, 8781-8794	19
1836	Pressure-induced band gap reduction, orientational ordering and reversible amorphization in single crystals of C70: Photoluminescence and Raman studies. <b>1994</b> , 70, 347-358	15
1835	Universal equation of state for compressed solids. <b>1994</b> , 49, 3049-3060	72
1834	Ordering in BxC1-x compounds with the graphite structure. <b>1994</b> , 49, 2805-2812	33
1833	Optical properties of beta -C3N4 and its pressure dependence. <b>1994</b> , 50, 11231-11234	46
1832	Reversible pressure-induced amorphization in solid C70: Raman and photoluminescence study. <b>1994</b> , 73, 3411-3414	36
1831	Energetics and lattice contraction of beta -phase YH2+x. <b>1994</b> , 49, 10731-10734	23
1830	Electronic and geometrical structure of rutile surfaces. <b>1994</b> , 50, 12015-12024	114



1829	Quantum-mechanical calculation of the solid-state equilibrium MgO+ alpha -Al <sub>2</sub> O <sub>3</sub> . <b>1994</b> , 49, 14179-14187	150
1828	Raman and modulated-reflectivity spectra of a strained pseudomorphic ZnTe epilayer on InAs under pressure. <b>1994</b> , 49, 2181-2184	17
1827	Ab initio structural study of the silicon/nickel disilicide interfaces. <b>1994</b> , 49, 2927-2930	6
1826	Pseudopotential plane-wave study of alpha -YH <sub>x</sub> . <b>1994</b> , 49, 13357-13365	20
1825	Effects of pressure on the optical absorption and photoluminescence of WBIler siloxene. <b>1994</b> , 49, 5362-5367	6
1824	Theoretical studies of the stability of ordered A <sub>8</sub> B compounds. <b>1994</b> , 50, 5962-5970	9
1823	Lattice-constant dependence of the dynamical effective charge in AlAs and GaAs. <b>1994</b> , 50, 14125-14130	14
1822	Magnetic structures of hcp bulk gadolinium. <b>1994</b> , 49, 4348-4351	40
1821	Electronic structure of platinum at ultrahigh pressure. <b>1994</b> , 12, 161-170	6
1820	Electronic bonding and optical properties of the H <sub>2</sub> -H <sub>2</sub> O phase at high pressure. <b>1994</b> , 50, 17709-17712	3
1819	First-principles study of hydrogen ordering in beta -YH <sub>2+x</sub> . <b>1994</b> , 49, 6481-6489	25
1818	Anisotropy of the elastic and nonlinear acoustic properties of dense textured Bi <sub>2</sub> Sr <sub>2</sub> CaCu <sub>2</sub> O <sub>8+y</sub> . <b>1994</b> , 49, 9862-9873	18
1817	Comment on "Local exchange-correlation functional: Numerical test for atoms and ions". <b>1994</b> , 49, 5152-5155	3
1816	Thermal conductivity and heat capacity per unit volume of poly(methyl methacrylate) under high pressure. <b>1994</b> , 15, 949-962	10
1815	Pressure-volume-temperature behavior of Fe <sub>2</sub> SiO <sub>4</sub> (spinel) based on static compression measurements at 400° C. <b>1994</b> , 21, 413	7
1814	Birch Equation of State for Alkali Halide Crystals. <b>1994</b> , 181, 387-395	10
1813	Pressure Dependent Properties of Boron Phosphide. <b>1994</b> , 185, 379-388	3
1812	Compressibility and Moelwyn-Hughes Parameter of NaBr Crystals under High Pressure. <b>1994</b> , 185, K57-K60	

1811	Contrasting effects of lanthanum and samarium modifiers on the elastic and non-linear acoustic properties of phosphate glasses. <b>1994</b> , 29, 562-568	4
1810	Crystal chemical estimation of polymorphic transformation pressures of covalent compounds. <b>1994</b> , 34, 588-592	1
1809	Optical and ultrasonic properties of europium phosphate glasses. <b>1994</b> , 29, 2847-2859	16
1808	Analysis of cohesive energies and equation of state for high-temperature superconductors. <b>1994</b> , 227, 109-112	3
1807	Magnetic and structural properties of MnSi. <b>1994</b> , 131, 321-328	17
1806	Ab initio calculation of thermodynamic data and phase diagram of binary transition metal based alloys. <b>1994</b> , 15, 330-338	4
1805	First-Principles Calculation of Electronic, Optical, and Structural Properties of $\text{Al}_2\text{O}_3$ . <b>1994</b> , 77, 404-411	123
1804	Structure of SAPO-31 refined from single-crystal diffraction data: substitution of P by Si established by diffraction methods. <b>1994</b> , 50, 290-294	26
1803	Ab initio Hartree-Fock study of lithium and sodium sulfides: electronic and scattering properties. <b>1994</b> , 50, 279-290	17
1802	Ab initio calculation of the structural and electronic properties of carbon and boron nitride using ultrasoft pseudopotentials. <b>1994</b> , 50, 15606-15622	326
1801	First-principles study of stability and local order in bcc-based Fe-Cr and Fe-V alloys. <b>1994</b> , 50, 15542-15558	48
1800	Explicit treatment of the gallium 3d electrons in GaN using the plane-wave pseudopotential method. <b>1994</b> , 50, 2159-2165	158
1799	Energetics and electronic structure of silver chloride. <b>1994</b> , 49, 17420-17423	34
1798	Influence of atomic relaxations on the structural properties of SiC polytypes from ab initio calculations. <b>1994</b> , 50, 17037-17046	122
1797	First-principles calculation of the Mg(0001) surface relaxation. <b>1994</b> , 302, 215-222	47
1796	C60 under pressure-bulk modulus and equation of state. <b>1994</b> , 96, 179-183	47
1795	Phase transformation of AlAs to NiAs structure at high pressure. <b>1994</b> , 72, 2045-2048	62
1794	Pressure- and laser-tuned Raman scattering in II-VI semiconductor nanocrystals: Electron-phonon coupling. <b>1994</b> , 50, 15108-15112	15

1793	Structural and electronic properties of cubic, 2H, 4H, and 6H SiC. <b>1994</b> , 49, 4485-4493	264
1792	X-ray absorption and diffraction spectroscopy of icosahedral Al-Cu-Fe quasicrystals under high pressure. <b>1994</b> , 70, 855-866	31
1791	Pressure Effects on Electronic Structure and Electron-Lattice Interaction of Cubic Phase of Solid Iodine. <b>1995</b> , 64, 3860-3870	10
1790	Theory of some Carbon Solids. <b>1995</b> , 383, 33	
1789	Prediction of a Very Hard Triclinic form of Diamond. <b>1995</b> , 408, 351	1
1788	High Pressure Equation of State for Fe <sub>2</sub> O <sub>3</sub> . <b>1995</b> , 418, 421	
1787	Thermodynamic properties of the generalized Murnaghan equation of state of solids. <b>1995</b> , 16, 1009-1026	8
1786	Total energy calculations in the DFT on binary compounds. <b>1995</b> , 55, 339-345	20
1785	Equations of State and Pressure Dependence of Bulk Modulus for NaCl Crystals. <b>1995</b> , 189, 363-369	12
1784	Calculation of the Ground State Properties of Diamond and Cubic Boron Nitride. <b>1995</b> , 191, 369-385	31
1783	Study of the Electronic Structure and the Role of Gallium 3d Electrons in Gallium Nitride. <b>1995</b> , 191, 387-394	9
1782	Electronic and optical properties of three phases of titanium dioxide: Rutile, anatase, and brookite. <b>1995</b> , 51, 13023-13032	781
1781	Theoretical study of the Si(100) surface reconstruction. <b>1995</b> , 51, 14504-14523	353
1780	Theory of structural, electronic, vibrational, and superconducting properties of high-pressure phases of sulfur. <b>1995</b> , 52, 12572-12578	35
1779	Symmetric stress tensor in the local-density-functional framework using a separable nonlocal pseudopotential. <b>1995</b> , 51, 14697-14700	7
1778	Temperature dependence of strain in ZnSe(epilayer)/GaAs(epilayer). <b>1995</b> , 78, 6569-6573	15
1777	Use of the generalized gradient approximation in pseudopotential calculations of solids. <b>1995</b> , 51, 9521-9525	58
1776	Calculated structural and electronic properties of CdSe under pressure. <b>1995</b> , 51, 4926-4930	43

1775	Pressure-induced phase transformations in AlAs: Comparison between ab initio theory and experiment. <b>1995</b> , 51, 5678-5681	17
1774	Optical investigation of the DX centers in GaAs under hydrostatic pressure. <b>1995</b> , 51, 17551-17560	5
1773	Ab initio Hartree-Fock study of structural and electronic properties of beta -Si <sub>3</sub> N <sub>4</sub> and beta -C <sub>3</sub> N <sub>4</sub> compounds. <b>1995</b> , 52, 6293-6300	40
1772	Ab initio total-energy pseudopotential calculations for polymorphic B <sub>2</sub> O <sub>3</sub> crystals. <b>1995</b> , 51, 1447-1455	32
1771	Self-interaction corrections in semiconductors. <b>1995</b> , 52, 16567-16574	32
1770	Band structure in adaptive curvilinear coordinates. <b>1995</b> , 51, 9508-9514	30
1769	Extension of a local-orbital density-functional method to transition metals: Application to Pt(110) surface relaxation. <b>1995</b> , 52, 16420-16427	8
1768	Pressure evolution of the cinnabar phase of HgTe. <b>1995</b> , 51, 8731-8736	48
1767	Ab initio pseudopotential calculations of the atomic and electronic structure of the Ta (100) and (110) surfaces. <b>1995</b> , 52, 11784-11792	14
1766	Recovery of an N-body potential from a universal cohesion equation. <b>1995</b> , 51, 15856-15860	9
1765	DDX diffraction system: A combined diffraction system with EDX and ADX for high-pressure structure studies. <b>1995</b> , 66, 1335-1337	7
1764	First-principles study on electronic structure of the (001) surface of SrTiO <sub>3</sub> . <b>1995</b> , 51, 11049-11054	88
1763	High-pressure low-symmetry phases of cesium halides. <b>1995</b> , 51, 8060-8068	22
1762	Application of adaptive curvilinear coordinates to the electronic structure of solids. <b>1995</b> , 51, 7337-7340	82
1761	Fundamental studies on the structures and properties of some B <sub>12</sub> -based crystals. <b>1995</b> , 52, 17073-17083	28
1760	Theoretical study on the high-pressure phase transformation in ZnSe. <b>1995</b> , 52, 4658-4661	46
1759	Theoretical study of cubic structures based on fullerene carbon clusters: C <sub>28</sub> C and (C <sub>28</sub> ) <sub>2</sub> . <b>1995</b> , 52, 2125-2130	9
1758	Valley mixing in resonant tunnelling diodes with applied hydrostatic pressure. <b>1995</b> , 10, 1673-1679	16

1757	The pressure-induced ferroelastic phase transition of SiO <sub>2</sub> stishovite. <b>1995</b> , 7, 3693-3698	26
1756	Boron nitride phase diagram. State of the art. <b>1995</b> , 13, 199-214	44
1755	Electronic structure and phase stability study in the Ni-Ti system. <b>1995</b> , 52, 15176-15190	64
1754	Ab initio study of antiferromagnetic rutile-type FeF <sub>2</sub> . <b>1995</b> , 52, 2422-2427	45
1753	The size dependence of the high-pressure phase stability of II-VI semiconductor nanocrystals. <b>1995</b> , 7, 8519-8527	26
1752	Plane-wave-basis pseudopotential study of the ground-state properties of Ni. <b>1995</b> , 52, 9159-9161	18
1751	Theoretical study of electronic, magnetic, and structural properties of alpha -Fe <sub>2</sub> O <sub>3</sub> (hematite). <b>1995</b> , 51, 7441-7450	242
1750	Consistent structural properties for AlN, GaN, and InN. <b>1995</b> , 51, 7866-7869	235
1749	Role of d electrons in the zinc-blende semiconductors ZnS, ZnSe, and ZnTe. <b>1995</b> , 52, 1459-1462	76
1748	Universal compressibility behavior of dense phases. <b>1995</b> , 51, 28-37	75
1747	Studies on Fullerenes Using Positron Annihilation Spectroscopy. <b>1995</b> , 3, 661-679	4
1746	Application of generalized gradient approximations: The diamond- beta -tin phase transition in Si and Ge. <b>1995</b> , 52, 2550-2556	121
1745	Ab initio calculations of structural and electronic properties of gallium solid-state phases. <b>1995</b> , 52, 9988-9998	133
1744	Elastic and anelastic properties, vibrational anharmonicity, and fractal bond connectivity of superionic glasses. <b>1996</b> , 53, 5287-5300	15
1743	A Comparison of Pressure-Induced Structural Transformations in CdSe, InP, and Si Nanocrystals. <b>1996</b> , 331-342	5
1742	Optical properties of wurtzite GaN grown by low-pressure metalorganic chemical-vapor deposition. <b>1996</b> , 79, 3691-3696	43
1741	Pressure-induced phase transition in icosahedral Al <sub>70</sub> Pt <sub>30</sub> quasicrystals. <b>1996</b> , 74, 629-639	11
1740	Ab initio pseudopotential study of the structural phase transformations of ZnS under high pressure. <b>1996</b> , 53, 8262-8266	40

1739	Generalized Kohn-Sham schemes and the band-gap problem. <b>1996</b> , 53, 3764-3774	906
1738	An ab Initio Hartree-Fock Study of the Cubic and Tetragonal Phases of Bulk Tungsten Trioxide. <b>1996</b> , 118, 12174-12182	99
1737	Unusual Chemical Behavior for Potassium under Pressure: Potassium-Silver Compounds. <b>1996</b> , 118, 12104-12108	30
1736	Effects of Pressure on the Azafullerene (C <sub>59</sub> N) <sub>2</sub> Molecular Solid to 22 GPa. <b>1996</b> , 118, 8715-8716	37
1735	Application of a simple relation for describing wave velocity as a function of pressure in rocks containing microcracks. <b>1996</b> , 101, 5643-5652	22
1734	Ab initio pseudopotential study of Fe, Co, and Ni employing the spin-polarized LAPW approach. <b>1996</b> , 53, 10685-10689	49
1733	Nonlinear piezoelectricity: The effect of pressure on CdTe. <b>1996</b> , 53, 6951-6954	28
1732	Total-energy study of electronic structure and mechanical behavior of C15 Laves phase compounds: NbCr <sub>2</sub> and HfV <sub>2</sub> . <b>1996</b> , 54, 12753-12762	72
1731	Electrical and optical properties of Zn/sub x/Mg/sub 1-x/Se/ZnTe and Zn/sub x/Mg/sub 1-x/Se/GaAs heterojunctions.	
1730	Elastic Constants of A Laves Phase Compound: C15 NbCr <sub>2</sub> . <b>1996</b> , 460, 623	3
1729	Structural, elastic, and high-pressure properties of cubic TiC, TiN, and TiO. <b>1996</b> , 53, 3072-3079	243
1728	Ab initio Hartree-Fock study of the electronic charge density of the cubic boron nitride and its comparison with experiments. <b>1996</b> , 52, 586-595	15
1727	Electronic and geometrical structure of bulk rutile studied with Hartree-Fock and density functional methods. <b>1996</b> , 58, 297-306	29
1726	Bulk modulus and equation of state of High-Temperature superconductors. <b>1996</b> , 196, 209-212	4
1725	A comparative study of birch and kumar equations of state under high pressure NaCl as an example. <b>1996</b> , 196, 303-307	12
1724	Determination of the Linear Pressure Coefficients of Semiconductor Bandgaps. <b>1996</b> , 198, 57-60	13
1723	Zn <sub>1-x</sub> Mg <sub>x</sub> Se Samples and a ZnSe/Zn <sub>0.93</sub> Mg <sub>0.07</sub> Se Quantum Well under Pressure: Optical Absorption and Photoluminescence. <b>1996</b> , 198, 355-361	9
1722	Pressure-Induced Amorphization of LiInGe. <b>1996</b> , 198, 509-514	2

1721	Dynamical Charge and Force Constant Calculations in c-BN under Pressure. <b>1996</b> , 198, 721-728	1
1720	The search for a universal equation of state correct up to very high pressures. <b>1996</b> , 8, 67-81	108
1719	Pressure dependence of the photoluminescence of strained (001) and (111) In <sub>x</sub> Ga <sub>1-x</sub> As quantum wells. <b>1996</b> , 53, 10116-10120	8
1718	Plasmon Raman scattering and photoluminescence of heavily doped n-type InP near the Gamma-X crossover. <b>1996</b> , 53, 1287-1293	37
1717	Structural, magnetic, and electronic properties of Fe/Au monatomic multilayers. <b>1996</b> , 54, 3030-3032	23
1716	Lattice distortion of NiO under high pressure. <b>1996</b> , 54, R9581-R9584	19
1715	Ab initio analysis of structural stability in the compound Ni <sub>3</sub> V. <b>1996</b> , 53, 6203-6208	12
1714	Structure and electronic properties of quinizarin chemisorbed on alumina. <b>1996</b> , 104, 8143-8150	17
1713	Fe, Ru, and Os disilicides: Electronic structure of ordered compounds. <b>1996</b> , 54, 7897-7908	27
1712	Generalized gradient theory for silica phase transitions. <b>1996</b> , 76, 660-663	271
1711	Pressure dependence of Born effective charges, dielectric constant, and lattice dynamics in SiC. <b>1996</b> , 53, 5430-5437	42
1710	Total-energy study of hydrogen ordering in PdH <sub>x</sub> (0 < x < 1). <b>1996</b> , 53, 1-4	78
1709	Semiempirical methodology for simulating covalently bonded materials: Application to silicon. <b>1996</b> , 104, 4632-4641	5
1708	First-principles study on energetics of c-BN(001) reconstructed surfaces. <b>1996</b> , 54, 5586-5603	435
1707	Electronic structure and optical properties of the B <sub>12</sub> O <sub>2</sub> crystal. <b>1996</b> , 54, 1451-1454	40
1706	Compressibility of C <sub>60</sub> in the temperature range 150-335 K up to a pressure of 1 GPa. <b>1996</b> , 53, 8329-8336	33
1705	Structure of solid-state systems from embedded-cluster calculations: A divide-and-conquer approach. <b>1996</b> , 53, 12713-12724	21
1704	Electronic structure of normal, inverse, and partially inverse spinels in the MgAl <sub>2</sub> O <sub>4</sub> system. <b>1996</b> , 54, 16555-16561	59

1703	Adsorption of CO on TiO <sub>2</sub> (110) studied by means of a cluster model surrounded by multipoles obtained from slab calculations. <b>1996</b> , 54, 14812-14821	33
1702	The high-pressure phase transitions of silicon and gallium nitride: a comparative study of Hartree - Fock and density functional calculations. <b>1996</b> , 8, 3993-4000	34
1701	Pressure effects on the electronic properties of PrAg in the ferromagnetic phase. <b>1996</b> , 8, 10457-10466	2
1700	The pressure-induced transition between shallow and deep states of an Si donor in GaAs. <b>1996</b> , 11, 17-21	1
1699	Harris functional densities: from solid to atom. <b>1996</b> , 8, 7379-7391	4
1698	First-principles studies of the thermodynamic properties of bulk Li. <b>1997</b> , 9, 2135-2148	18
1697	First-principles calculation of the Coulomb pseudopotential for the simple hexagonal phase of Si. <b>1997</b> , 9, 6351-6358	4
1696	Compared electron charge densities for the series of solid phosphide compounds; anab initiostudy. <b>1997</b> , 9, 3139-3149	9
1695	Carbon nitride compounds with 1:1 stoichiometry. <b>1997</b> , 55, 5684-5688	25
1694	Transition in Ce from temperature-dependent band-structure calculations. <b>1997</b> , 55, 1288-1291	45
1693	Nonorthogonal tight-binding Hamiltonians for defects and interfaces in silicon. <b>1997</b> , 56, 10488-10496	46
1692	LDA simulations of pressure-induced anomalies in $c/a$ and electric-field gradients for Zn and Cd. <b>1997</b> , 56, 7206-7214	64
1691	Adaptive-coordinate electronic structure of 3d bands: TiO <sub>2</sub> . <b>1997</b> , 56, 14979-14984	14
1690	SiO <sub>2</sub> stishovite under high pressure: Dielectric and dynamical properties and the ferroelastic phase transition. <b>1997</b> , 56, 7321-7330	28
1689	Crystal structure of CuGeO <sub>3</sub> under pressure. <b>1997</b> , 56, R11357-R11360	14
1688	B <sub>2</sub> O <sub>3</sub> crystals investigated by plane-wave pseudopotential calculations using the generalized-gradient approximation. <b>1997</b> , 55, 2824-2830	11
1687	First-principles calculations on the atomic and electronic structure of Al <sub>2</sub> O <sub>3</sub> . <b>1997</b> , 56, 8553-8558	34
1686	Lattice dynamical theory of thermal expansion and mode Grüneisen parameters in cubic BP. <b>1997</b> , 55, 11293-11299	13



1685	First-principles calculations of the thermal expansion of metals. <b>1997</b> , 56, 7767-7770	90
1684	Ultrasonic study of the temperature and pressure dependences of the elastic properties of fcc Co-Mn alloy single crystals. <b>1997</b> , 55, 11181-11190	10
1683	Phase-stability study of the Al-Nb system. <b>1997</b> , 56, 552-565	38
1682	Direct subsurface absorption of hydrogen on Pd(111): Quantum mechanical calculations on a new two-dimensional potential energy surface. <b>1997</b> , 106, 9286-9296	39
1681	Electronic, Structural and Magnetic Properties of Transition-Metal Mononitrides. <b>1997</b> , 66, 3147-3152	53
1680	Temperature-dependent electronic structure: from heavy fermion behaviour to phase stability. <b>1997</b> , 60, 1305-1349	14
1679	Chapter 13 Phonons and Phase Transitions in GaN. <b>1997</b> , 409-429	3
1678	High Pressure Study of III-Nitrides and Related Heterostructures. <b>1997</b> , 499, 361	1
1677	High-Pressure Raman Scattering of Biaxially Strained GaN on GaAs. <b>1997</b> , 468, 225	3
1676	Theory of Ga, N and H terminated GaN (0001)/( $\overline{1}00$ ) surfaces. <b>1997</b> , 482, 940	3
1675	Band offsets in near-GaAs alloys. <b>1997</b> ,	
1674	Young Modulus of Crystalline Polyethylene from ab initio Molecular Dynamics. <b>1997</b> , 30, 5953-5957	44
1673	Theoretical study of boron nitride modifications at hydrostatic pressures. <b>1997</b> , 55, 6203-6210	116
1672	Transition Metal Oxide Chemistry: Electronic Structure Study of WO <sub>3</sub> , ReO <sub>3</sub> , and NaWO <sub>3</sub> . <b>1997</b> , 101, 3945-3952	93
1671	Structural, dynamical, electronic, and bonding properties of laser-heated silicon: An ab initio molecular-dynamics study. <b>1997</b> , 56, 3806-3812	81
1670	Ab initio study of silicon in the R8 phase. <b>1997</b> , 56, 6662-6668	91
1669	Prediction of hexagonal Ta <sub>2</sub> O <sub>5</sub> structure by first-principles calculations. <b>1997</b> , 55, 11155-11160	73
1668	Comparison of the projector augmented-wave, pseudopotential, and linearized augmented-plane-wave formalisms for density-functional calculations of solids. <b>1997</b> , 55, 2005-2017	185

1667	Ultrasoft pseudopotentials applied to magnetic Fe, Co, and Ni: From atoms to solids. <b>1997</b> , 56, 15629-15646	302
1666	High-pressure phases of PbF <sub>2</sub> : A joint experimental and theoretical study. <b>1997</b> , 56, 543-551	22
1665	Atomic structure of the surface reconstructions of zincblende GaN(001). <b>1997</b> , 385, 178-186	15
1664	Elastic properties of zinc-blende and wurtzite AlN, GaN, and InN. <b>1997</b> , 82, 2833-2839	871
1663	The p - d hybridization in the electronic structure of. <b>1997</b> , 9, 6031-6048	15
1662	Electronic, structural, and optical properties of crystalline yttria. <b>1997</b> , 56, 14993-15000	126
1661	The equation-of-states of Jilin ordinary chondrite and Nandan iron meteorite. <b>1997</b> , 40, 403-410	3
1660	Thermal conductivity, heat capacity, and compressibility of atactic poly(propylene) under high pressure. <b>1997</b> , 18, 845-864	6
1659	Thermal conductivity of amorphous Teflon (AF 1600) at high pressure. <b>1997</b> , 18, 209-219	6
1658	Estimation of thermodynamic stability conditions and perspectives for synthesis of covalent carbon nitride. <b>1997</b> , 22, 34-37	2
1657	Equation of state and pressure derivatives of bulk modulus for NaCl crystal. <b>1997</b> , 239, 337-344	33
1656	Relaxation of Crystals with the Quasi-Newton Method. <b>1997</b> , 131, 233-240	1913
1655	Single Crystal Diffraction Studies of WO <sub>3</sub> at High Pressures and the Structure of a High-Pressure WO <sub>3</sub> Phase. <b>1997</b> , 132, 123-130	39
1654	Ab-Initio Total Energy Calculation of $\beta$ -Silicon Nitride and the Derivation of Effective Pair Potentials with Application to Lattice Dynamics. <b>1998</b> , 81, 3189-3196	68
1653	Modeling the structure of zircon (ZrSiO <sub>4</sub> ): empirical potentials, ab initio electronic structure. <b>1998</b> , 257, 282-286	51
1652	A comparative study of the electronic structure of $\beta$ -MnS (alabandite) calculated at the Hartree-Fock and Density Functional levels of theory. <b>1998</b> , 236, 97-105	20
1651	Pressure-Induced Phase Transformation of LiIn and LiCd: From NaTl-Type Phases to $\beta$ -Brass-Type Alloys. <b>1998</b> , 137, 104-111	6
1650	Remarks on the Kumar isothermal equation. <b>1998</b> , 253, 138-141	5

1649	Equation of state of cementitious materials by ultrasonic methodology. <b>1998</b> , 251, 121-128	8
1648	Study on momentum density in narrow-gap mixed IIIIV alloys by positron annihilation under pressure. <b>1998</b> , 54, 161-167	2
1647	Lattice deformation potential from the variation of the unit cell volume and band gap of oxygen doped CuInSe <sub>2</sub> . <b>1998</b> , 37, 107-110	6
1646	Electronic structure, cohesive properties and phase stability in Ni <sub>3</sub> V, Pd <sub>3</sub> V, and Pt <sub>3</sub> V compounds. <b>1998</b> , 264, 31-37	15
1645	Structural phase transition of HoGa <sub>2</sub> at high pressure. <b>1998</b> , 268, 161-165	18
1644	Pressure dependence of optical transitions in In <sub>0.15</sub> Ga <sub>0.85</sub> N/GaN multiple quantum wells. <b>1998</b> , 58, R10191-R10194	17
1643	Pressure dependence of the direct band gap in tetrahedral semiconductors. <b>1998</b> , 58, 12579-12582	28
1642	First-principles band-structure calculation of yttrium oxysulfide. <b>1998</b> , 57, 8939-8944	43
1641	An Analytical Free Energy and the Temperature-Pressure Superposition Principle for Pure Polymeric Liquids. <b>1998</b> , 31, 6650-6661	32
1640	Trends in band-gap pressure coefficients in chalcopyrite semiconductors. <b>1998</b> , 58, R1710-R1713	54
1639	Pressure-induced phase transitions in silver halides. <b>1998</b> , 57, 5098-5105	45
1638	Elastic and high pressure properties of ZnO. <b>1998</b> , 83, 8065-8067	90
1637	Equations of state for solids under strong compression. <b>1998</b> , 16, 81-126	93
1636	High-pressure X-ray diffraction of icosahedral Al-Cu-Ru and Al-Pd-Re quasicrystals. <b>1998</b> , 77, 115-128	15
1635	Chapter 4 Optical Properties of Semiconductors under Pressure. <b>1998</b> , 54, 247-425	53
1634	Phonons, Strains, and Pressure in Semiconductors. <b>1998</b> , 55, 117-233	35
1633	Electronic structure of possible 3d 'heavy-fermion' compound. <b>1998</b> , 10, L119-L126	102
1632	Ab initio study of structural, dielectric, and dynamical properties of GaN. <b>1998</b> , 57, 7043-7049	156

1631	Pseudopotential study of binding properties of solids within generalized gradient approximations: The role of core-valence exchange correlation. <b>1998</b> , 57, 2134-2145	174
1630	The phase transition in alkaline-earth oxides: a comparison of ab initio Hartree-Fock and density functional calculations. <b>1998</b> , 10, 6897-6909	87
1629	Large-Scale Electronic-Structure Calculations Based on the Adaptive Finite-Element Method. <b>1998</b> , 67, 3844-3858	96
1628	Verification of Tersoff's Potential for Static Structural Analysis of Solids of Group-IV Elements. <b>1998</b> , 37, 414-422	26
1627	Raman and absorption spectroscopy of InP under high pressure. <b>1998</b> , 10, 8611-8618	11
1626	Ab initio local-orbital density-functional method for transition metals and semiconductors. <b>1998</b> , 58, 1832-1838	5
1625	Pressure-induced phase transitions in solid Si, SiO <sub>2</sub> , and Fe: Performance of local-spin-density and generalized-gradient-approximation density functionals. <b>1998</b> , 58, 11266-11272	69
1624	Inverse versus Normal NiAs Structures as High-Pressure Phases of FeO and MnO. <b>1998</b> , 81, 1027-1030	60
1623	Site preferences and formation energies of substitutional Si, Nb, Mo, Ta, and W solid solutions in L10 Ti-Al. <b>1998</b> , 57, 13459-13470	69
1622	Cohesive properties of the lanthanides: Effect of generalized gradient corrections and crystal structure. <b>1998</b> , 58, 4345-4351	53
1621	Total energy calculations of the lattice properties of cubic and hexagonal diamond. <b>1998</b> , 57, 13355-13358	30
1620	Possible high-pressure phase of diamond. <b>1998</b> , 57, 5661-5667	11
1619	Extension of the universal equation of state for solids in high-pressure phases. <b>1998</b> , 58, 20-22	16
1618	First-principles theory of Ta up to 10 Mbar pressure: Structural and mechanical properties. <b>1998</b> , 57, 10340-10350	85
1617	DX-center formation in wurtzite and zinc-blende Al <sub>x</sub> Ga <sub>1-x</sub> N. <b>1998</b> , 57, R2033-R2036	131
1616	Direct comparison of the pressure-induced band-gap shifts in cubic and hexagonal GaN. <b>1998</b> , 84, 2971-2973	8
1615	Electronic structure of pyrite-type manganese disulphide (pMnS <sub>2</sub> ): An ab initio study. <b>1998</b> , 58, 1236-1242	7
1614	Full potential linearized-augmented-plane-wave calculations for 5d transition metals using the relativistic generalized gradient approximation. <b>1998</b> , 33, 209-223	26

1613	High-pressure investigation of InGaN quantum wells. <b>1998</b> , 512, 399	2
1612	Pressure Dependence of Optical Transitions in InGaN/GaN Multiple Quantum Wells. <b>1998</b> , 537, 1	
1611	First-Principles Total Energy Study of NbCr <sub>2</sub> + V Laves Phase Ternary System. <b>1998</b> , 552, 1	2
1610	High Pressure Phases and the Structural Phase Transition of Selenium. <b>1998</b> , 67, 3141-3146	14
1609	Pressure Dependence of Optical Transitions in InGaN/GaN Multiple Quantum Wells. <b>1999</b> , 4, 191-196	
1608	Ground-state properties of cubic C-BN solid solutions. <b>1999</b> , 11, 927-935	57
1607	Structural Analysis of SiGe and SiGeC Alloys by Ab Initio Total-Energy Calculations. <b>1999</b> , 38, 2566-2568	3
1606	Electronic structure of Ti <sub>2</sub> AlNb (O phase). <b>1999</b> , 11, 6179-6186	7
1605	Elastic constants and their pressure dependence of Zr <sub>41</sub> Ti <sub>14</sub> Cu <sub>12.5</sub> Ni <sub>9</sub> Be <sub>22.5</sub> C <sub>1</sub> bulk metallic glass. <b>1999</b> , 74, 1803-1805	89
1604	Atomic and molecular hydrogen interacting with Pt(111). <b>1999</b> , 111, 11155-11163	176
1603	Dependence of the fundamental band gap of Al <sub>x</sub> Ga <sub>1-x</sub> N on alloy composition and pressure. <b>1999</b> , 85, 8505-8507	100
1602	Bulk modulus of C <sub>60</sub> studied by single-crystal neutron diffraction. <b>1999</b> , 59, 11020-11026	35
1601	Detailed investigation of the magnetic phase diagram of CeRu <sub>2</sub> Ge <sub>2</sub> up to 11 GPa. <b>1999</b> , 59, 3651-3660	52
1600	Raman linewidths of optical phonons in 3C <sub>2</sub> BiC under pressure: First-principles calculations and experimental results. <b>1999</b> , 59, 6774-6783	57
1599	Theoretical study of the structural phase transformation of BeO under pressure. <b>1999</b> , 59, 13501-13504	48
1598	Silylated carbodiimides in molecular and extended structures. <b>1999</b> , 60, 3126-3139	30
1597	Electronic structure of a grain-boundary model in SrTiO <sub>3</sub> . <b>1999</b> , 60, 2416-2424	84
1596	Transformation mechanism for the pressure-induced phase transition in shocked CdS. <b>1999</b> , 59, 11704-11715	79

1595	Wavelets in all-electron density-functional calculations. <b>1999</b> , 60, 1437-1440	18
1594	Pseudopotential study of bonding and ionicity in InP at various pressures. <b>1999</b> , 40, 117-121	12
1593	Synthesis of cubic silicon nitride. <b>1999</b> , 400, 340-342	549
1592	Extending the methodology of X-ray crystallography to allow imaging of micrometre-sized non-crystalline specimens. <b>1999</b> , 400, 342-344	1437
1591	Cohesive, structural, and electronic properties of Fe-Si compounds. <b>1999</b> , 59, 12860-12871	190
1590	The Fe <sub>4</sub> N system revisited: an ab initio calculation study of the magnetic interactions. <b>1999</b> , 191, 234-240	58
1589	Molecular and solid-state tests of density functional approximations: LSD, GGAs, and meta-GGAs. <b>1999</b> , 75, 889-909	519
1588	Ab initio calculation of the lattice dynamics and phase diagram of boron nitride. <b>1999</b> , 59, 8551-8559	303
1587	The equation of state of supercritical HF, HCl, and reactive supercritical mixtures containing the elements H, C, F, and Cl. <b>1999</b> , 110, 12023-12032	13
1586	Ab initio study of structural and electronic properties of yttria-stabilized cubic zirconia. <b>1999</b> , 59, 797-810	246
1585	High Pressure Polymerization of the Li-Intercalated Fulleride Li <sub>3</sub> CsC <sub>60</sub> . <b>1999</b> , 11, 2960-2965	15
1584	Temperature and pressure dependence of orientational disorder and bonding in Li <sub>2</sub> CsC <sub>60</sub> . <b>1999</b> , 1, 157-163	3
1583	Predicted band-gap pressure coefficients of all diamond and zinc-blende semiconductors: Chemical trends. <b>1999</b> , 60, 5404-5411	480
1582	First-principles study on electronic structures and phase stability of MnO and FeO under high pressure. <b>1999</b> , 59, 762-774	103
1581	Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. <b>1999</b> , 59, 5521-5535	564
1580	Structural transformations and metastability in semiconductor nanocrystals. <b>1999</b> , 68, 1-25	14
1579	Transition metals and their carbides and nitrides: Trends in electronic and structural properties. <b>1999</b> , 60, 6343-6347	218
1578	Electronic structure of yttrium aluminum garnet (Y <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> ). <b>1999</b> , 59, 10530-10535	142

1577	An equation of state applied to solid up to 1 TPa. <b>1999</b> , 11, 10375-10391	25
1576	Solvothermal synthesis of the graphitic form of C <sub>3</sub> N <sub>4</sub> as macroscopic sample. <b>1999</b> , 8, 1707-1710	62
1575	An analytic model for the prediction of incoherent shaped charge jets. <b>1999</b> , 86, 1255-1265	4
1574	Comparison of the Bulk and Surface Properties of Ceria and Zirconia by ab Initio Investigations. <b>1999</b> , 103, 10158-10170	125
1573	First-principles calculation of the thermal properties of silver. <b>1999</b> , 59, 965-969	109
1572	Electronic structure, phase stability, and cohesive properties of Ti <sub>2</sub> XAl (X=Nb,V,Zr). <b>1999</b> , 60, 15683-15690	35
1571	High-pressure x-ray absorption study of InSe. <b>1999</b> , 60, 3757-3763	26
1570	Full-potential KKR calculations for metals and semiconductors. <b>1999</b> , 60, 5202-5210	103
1569	Ab initio full-potential study of the structural and magnetic phase stability of iron. <b>1999</b> , 60, 3839-3848	302
1568	In situ high pressure X-ray diffraction and EXAFS spectroscopy of icosahedral Al-Cu-Ru quasicrystals. <b>2000</b> , 80, 2057-2071	5
1567	High Pressure Studies of Quasicrystals. <b>2000</b> , 643, 551	
1566	First-Principles Calculations of Electronic Structure and Structural Properties for MoV, MoNb, and MoTa. <b>2000</b> , 646, 365	2
1565	Electronic structure of Ge <sub>3</sub> N <sub>4</sub> possible structures. <b>2000</b> , 80, 249-257	36
1564	Pressure-Induced Structural Phase Transitions in Ln <sub>2</sub> Nd <sub>x</sub> CuO <sub>4</sub> for Ln=La (0.6 ≤ x) and Ln=Pr (x=0). <b>2000</b> , 151, 231-240	6
1563	New Experimental Results on the Phase Diagram of Boron Nitride. <b>2000</b> , 154, 280-285	32
1562	Optical Absorption of Zinc Selenide Doped with Cobalt (Zn <sub>1-x</sub> CoxSe) under Hydrostatic Pressure. <b>2000</b> , 180, 561-568	6
1561	Inadequacy of linear pressure dependence of vibrational frequency. <b>2000</b> , 114, 637-641	4
1560	Hartree-Fock and density functional calculations of the elastic constants of the alkaline-earth oxides: comparison with experiment. <b>2000</b> , 116, 543-546	19

1559	The effect of hydrostatic pressure on the electronic and optical properties of InP. <b>2000</b> , 44, 2193-2198	55
1558	Comparison of elastic constants and electronic structures in the series of the alkaline-earth selenides: a quantum chemical approach. <b>2000</b> , 61, 1707-1715	44
1557	Ab initio calculations of elastic properties and electronic structure of calcium selenide. <b>2000</b> , 61, 603-608	3
1556	High pressure Brillouin scattering and energy dispersive X-ray diffraction study of (NH <sub>4</sub> ) <sub>2</sub> ZnCl <sub>4</sub> . <b>2000</b> , 61, 719-726	10
1555	Analysis of temperature dependence of elastic constants and bulk modulus for ionic solids. <b>2000</b> , 291, 373-378	29
1554	Author's reply on the remark of Prieto and Renero on Kumar equation of state. <b>2000</b> , 292, 173-175	11
1553	Vacancies in SiC nanopowders. <b>2000</b> , 77, 147-158	13
1552	Development of glue-type potentials for the AlBb system: phase diagram calculation. <b>2000</b> , 48, 1753-1761	65
1551	Description of structural and electronic properties of TiC and ZrC by generalized gradient approximation. <b>2000</b> , 285, 392-396	34
1550	Positron behaviour in GaSb under pressure. <b>2000</b> , 61, 109-114	20
1549	Investigation of the possible ternary nitrides in the system Li <sub>3</sub> N/Na <sub>3</sub> N. <b>2000</b> , 2, 449-456	18
1548	The behaviour of electron valence and conduction charge densities in InP under pressure. <b>2000</b> , 65, 107-112	34
1547	Electronic structure of (Na <sup>+</sup> Bi <sup>3+</sup> )TiO <sub>3</sub> and its solid solution with BaTiO <sub>3</sub> . <b>2000</b> , 80, 1141-1151	18
1546	High-pressure thermodynamic, electronic and magnetic properties of Ni. <b>2000</b> , 12, 8953-8962	15
1545	Rubidium at high pressure and temperature. <b>2000</b> , 12, 921-931	7
1544	Theory of the anomalously low band-gap pressure coefficients in strained-layer semiconductor alloys. <b>2000</b> , 62, 13612-13616	33
1543	Structural properties and energetics of oxygen impurities in GaAs. <b>2000</b> , 61, 5326-5331	12
1542	C incorporation in epitaxial Ge <sub>1-x</sub> Cy layers grown on Ge(001): An ab initio study. <b>2000</b> , 62, R7723-R7726	19



1541	Analysis of dislocation mechanism for melting of elements: Pressure dependence. <b>2000</b> , 88, 6294-6301	70
1540	First-principles formation energies of monovacancies in bcc transition metals. <b>2000</b> , 61, 2579-2586	85
1539	First-principles study on the high-pressure behavior of the zone-center modes of lonsdaleite silicon. <b>2000</b> , 61, 5-8	30
1538	First-principles calculations of the thermodynamic and structural properties of strained $\text{In}_x\text{Ga}_{1-x}\text{N}$ and $\text{Al}_x\text{Ga}_{1-x}\text{N}$ alloys. <b>2000</b> , 62, 2475-2485	172
1537	Extreme softening of Vanderbilt pseudopotentials: General rules and case studies of first-row and d-electron elements. <b>2000</b> , 61, 4576-4587	98
1536	Structural and thermodynamic properties of diamond: A path-integral Monte Carlo study. <b>2000</b> , 63,	50
1535	Superexchange via cluster states: Calculations of spin-phonon coupling constants for $\text{CuGeO}_3$ . <b>2000</b> , 62, 3816-3823	4
1534	Structural, electronic, and magnetic properties of thin $\text{Mn}/\text{Cu}(100)$ films. <b>2000</b> , 61, 11492-11505	63
1533	Electronic theory of phase stability in substitutional alloys: application to the $\text{AuNi}$ system. <b>2000</b> , 296, 6-19	14
1532	Full ab initio geometry optimization of all known crystalline phases of $\text{Si}_3\text{N}_4$ . <b>2000</b> , 61, 8696-8700	74
1531	Relative energetics and structural properties of zirconia using a self-consistent tight-binding model. <b>2000</b> , 61, 6617-6630	76
1530	Pressure-induced structural transition in intermetallic compounds $\text{MnRhP}$ and $\text{MnRhAs}$ . <b>2000</b> , 307, 96-100	2
1529	Pressure dependence of band gaps in $\text{PbS}$ , $\text{PbSe}$ and $\text{PbTe}$ . <b>2000</b> , 18, 127-131	29
1528	Optical absorption of zinc selenide doped with cobalt ( $\text{Zn}_{1-x}\text{Co}_x\text{Se}$ ) under hydrostatic pressure. <b>2000</b> , 18, 89-94	1
1527	Explicit Gibbs free energy equation of state applied to the carbon phase diagram. <b>2000</b> , 61, 8734-8743	121
1526	Dynamics and polarization of group-III nitride lattices: A first-principles study. <b>2000</b> , 62, 8003-8011	98
1525	Clathrates as effective p-type and n-type tetrahedral carbon semiconductors. <b>2000</b> , 61, 12689-12692	28
1524	High-pressure phase transformation of the silicon clathrate $\text{Si}_{136}$ . <b>2000</b> , 12, 4013-4020	42

1523	Theoretical study of the relative stability of structural phases in group-III nitrides at high pressures. <b>2000</b> , 62, 16612-16623	183
1522	Volume and composition dependence of direct and indirect band gaps in ordered ternary III-V semiconductor compounds: A screened-exchange LDA study. <b>2000</b> , 61, 4677-4684	11
1521	LDA and GGA calculations for high-pressure phase transitions in ZnO and MgO. <b>2000</b> , 62, 1660-1665	370
1520	Bond Scission in a Perfect Polyethylene Chain and the Consequences for the Ultimate Strength. <b>2000</b> , 33, 9098-9108	25
1519	Electronic structure, structural properties, and dielectric functions of IV-VI semiconductors: PbSe and PbTe. <b>2000</b> , 61, 16589-16595	108
1518	O/N Ordering in Y <sub>2</sub> Si <sub>3</sub> O <sub>3</sub> N <sub>4</sub> with the Melilite-type Structure from First-Principles Calculations. <b>2000</b> , 12, 1071-1075	27
1517	Energetics of silicon suboxides. <b>2000</b> , 61, 9899-9901	61
1516	Electronic structure and bonding in garnet crystals Gd <sub>3</sub> Sc <sub>2</sub> Ga <sub>3</sub> O <sub>12</sub> , Gd <sub>3</sub> Sc <sub>2</sub> Al <sub>3</sub> O <sub>12</sub> , and Gd <sub>3</sub> Ga <sub>3</sub> O <sub>12</sub> compared to Y <sub>3</sub> Al <sub>3</sub> O <sub>12</sub> . <b>2000</b> , 61, 1817-1824	75
1515	Intrinsic stress and local rigidity in tetrahedral amorphous carbon. <b>2000</b> , 62, 15686-15694	51
1514	First-principles elastic constants and electronic structure of Pt <sub>2</sub> Si and PtSi. <b>2001</b> , 63,	336
1513	Comprehensiveab initiostudy of properties of monovacancies and antisites in 4H-SiC. <b>2001</b> , 13, 6203-6231	122
1512	Structure and energetics of stoichiometric TiO <sub>2</sub> anatase surfaces. <b>2001</b> , 63,	1143
1511	High-pressure phases of group IV and III-V semiconductors. <b>2001</b> , 64, 483-516	190
1510	Phase stability and electronic structure of the HfAl <sub>3</sub> compound. <b>2001</b> , 64,	21
1509	Effect of pressure on optical phonon modes and transverse effective charges in GaN and AlN. <b>2001</b> , 64,	195
1508	Structural phase transition of GdGa <sub>2</sub> at high pressure. <b>2001</b> , 216,	14
1507	Piezoelectric field and its influence on the pressure behavior of the light emission from GaN/AlGaN strained quantum wells. <b>2001</b> , 79, 1483-1485	64
1506	Electronic structure, bonding, and ground-state properties of AlB <sub>2</sub> -type transition-metal diborides. <b>2001</b> , 63,	375

1505	Structural, electronic, and effective-mass properties of silicon and zinc-blende group-III nitride semiconductor compounds. <b>2001</b> , 63,	111
1504	First-principles study of the stability of BN and C. <b>2001</b> , 64,	96
1503	Compressibility of the MgB <sub>2</sub> superconductor. <b>2001</b> , 64,	55
1502	Numerical atomic orbitals for linear-scaling calculations. <b>2001</b> , 64,	864
1501	Energy and pressure versus volume: Equations of state motivated by the stabilized jellium model. <b>2001</b> , 63,	116
1500	Design and Synthesis of Energetic Materials. <b>2001</b> , 31, 291-321	350
1499	Comparative study of the electronic structure of two laser crystals: BeAl <sub>2</sub> O <sub>4</sub> and LiYF <sub>4</sub> . <b>2001</b> , 63,	27
1498	Equations of state for solids under strong compression. <b>2001</b> , 216,	62
1497	Interdot interactions and band gap changes in CdSe nanocrystal arrays at elevated pressure. <b>2001</b> , 89, 8127-8140	96
1496	Pressure-induced structural phase transition in a ferromagnet CrTe. <b>2001</b> , 315, 16-21	20
1495	Phase stability and electronic structure in ZrAl <sub>3</sub> compound. <b>2001</b> , 319, 154-161	44
1494	Direct wide band gap material: a Hartree-Fock study of $\beta$ -Be <sub>3</sub> N <sub>2</sub> . <b>2001</b> , 21, 95-100	23
1493	Elastic and non-linear acoustic properties and thermal expansion of cerium metaphosphate glasses. <b>2001</b> , 282, 291-305	47
1492	Influence of disorder on the magnetic properties of FeAl alloys: theory. <b>2001</b> , 287, 302-307	25
1491	Electron correlation in the Si(1 0 0) surface. <b>2001</b> , 482-485, 458-463	15
1490	Investigation of vinyl phosphonic acid/hydroxylated $\gamma$ -Al <sub>2</sub> O <sub>3</sub> ( $\gamma$ ) reaction enthalpies. <b>2001</b> , 494, 1-20	43
1489	A combined ab initio and photoelectron study of galena (PbS). <b>2001</b> , 491, 226-238	34
1488	Electronic and optical properties of the cubic spinel phase of $\alpha$ -Si <sub>3</sub> N <sub>4</sub> , $\alpha$ -Ge <sub>3</sub> N <sub>4</sub> , $\alpha$ -SiGe <sub>2</sub> N <sub>4</sub> , and $\alpha$ -GeSi <sub>2</sub> N <sub>4</sub> . <b>2001</b> , 63,	51

1487	Equation of state of bulk metallic glasses studied by an ultrasonic method. <b>2001</b> , 79, 3947-3949	40
1486	Equation of state of turbostratic boron nitride. <b>2001</b> , 21, 115-120	12
1485	Density of constitutional and thermal point defects in L12 Al <sub>3</sub> Sc. <b>2001</b> , 63,	54
1484	Bulk and surface properties of hexagonal-close-packed Be and Mg. <b>2001</b> , 13, 10767-10776	81
1483	First-principles density-functional study of metal-carbonitride interface adhesion: Co/TiC(001) and Co/TiN(001). <b>2001</b> , 64,	104
1482	Pressure evolution of the structure of (NH <sub>3</sub> ) <sub>3</sub> K <sub>3</sub> C <sub>60</sub> . <b>2001</b> , 56, 61-66	7
1481	Applications of Ultrasonics on Tellurite Glasses. <b>2001</b> ,	
1480	Determination, prediction, and understanding of structures, using the energy landscapes of chemical systems [Part II. <b>2001</b> , 216, 361-383	50
1479	Full-Potential KKR Calculations for Point Defect Energies in Metals, based on the Generalized-Gradient Approximation: I. Vacancy Formation Energies in fcc and bcc Metals. <b>2001</b> , 42, 2206-2215 <sup>38</sup>	
1478	Raman-Scattering Study of Doping Effects on the Structural Phase Transitions under Hydrostatic Pressures in CuGeO <sub>3</sub> . <b>2001</b> , 70, 290-296	2
1477	Lattice dynamics of magnesium fluoride from a semiempirical two-body potential model. <b>2001</b> , 7, 33-37	1
1476	The ground state and the bonding properties of the hypothetical cubic zinc-blende-like GeC and SnC compounds. <b>2001</b> , 282, 299-308	39
1475	Hartree-Fock and density functional calculations of the elastic constants of CaO. <b>2001</b> , 62, 661-663	4
1474	Bonding structure analysis of carbon nitride films by Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). <b>2001</b> , 70, 239-246	11
1473	Deposition of calcium ions on rutile (110): a first-principles investigation. <b>2001</b> , 49, 2169-2177	78
1472	Ab initio investigation of elastic constants of superconducting MgB <sub>2</sub> . <b>2001</b> , 363, 189-193	34
1471	First-principles calculations for point-defect energies in metals and phase diagrams of binary alloys. <b>2001</b> , 312, 72-76	6
1470	Pressure dependence of photoluminescence of ZnTe/Zn <sub>1-x</sub> CdxTe strained-layer superlattice. <b>2001</b> , 32, 847-851	1

1469	Pressure and Temperature Dependent Studies of GaN <sub>x</sub> As <sub>1-x</sub> /GaAs Quantum Well Structures. <b>2001</b> , 223, 163-169	29
1468	Theory of the Anomalous Low Band-Gap Pressure Coefficients of Semiconductor Strained Layers. <b>2001</b> , 223, 205-211	2
1467	An Isothermal Equation of State of Solid. <b>2001</b> , 226, 125-132	11
1466	A Projector Augmented Wave (PAW) code for electronic structure calculations, Part I: atompaw for generating atom-centered functions. <b>2001</b> , 135, 329-347	274
1465	Electronic, magnetic structures and neutron diffraction in B1 and B3 phases of MnS: a density functional approach. <b>2001</b> , 335, 449-457	22
1464	Correlation between core-level shift and bulk modulus in transition-metal carbides and nitrides. <b>2001</b> , 64,	21
1463	Pressure-induced quenching of the Jahn-Teller distortion and insulator-to-metal transition in LaMnO <sub>3</sub> . <b>2001</b> , 87, 125501	230
1462	Structure and electrical levels of point defects in monoclinic zirconia. <b>2001</b> , 64,	271
1461	Geometry Optimization and Ground-State Properties of Complex Ceramic Oxides. <b>2001</b> , 84, 801-805	21
1460	Structure Models for Aluminum Oxynitride from Ab Initio Calculations. <b>2001</b> , 84, 2633-2637	38
1459	Monatomic structures of B, C, N, and O: first-principle study of relative stabilities and bulk moduli. <b>2001</b> , 72, 136-140	
1458	Ab initio investigation of mechanical behaviour of MgB <sub>2</sub> superconductor under pressure. <b>2001</b> , 13, L641-L645	27
1457	High-pressure synchrotron radiation diffraction studies of icosahedral Ti-Zr-Ni and hydrogenated Ti-Zr-Ni quasicrystals. <b>2001</b> , 13, 8527-8536	9
1456	First-Principle Studies on Elastic Properties and Spontaneous Polarizations of PbTiO <sub>3</sub> . <b>2001</b> , 40, 5806-5808	5
1455	MgB <sub>2</sub> under pressure: phonon calculations, Raman spectroscopy, and optical reflectance. <b>2001</b> , 13, 9945-9962	60
1454	Quantum atomistic simulations of silicon and germanium. <b>2001</b> , 16, 2505-2512	5
1453	The structural and electronic properties of (AlN) <sub>x</sub> (C <sub>2</sub> ) <sub>1-x</sub> and (AlN) <sub>x</sub> (BN) <sub>1-x</sub> alloys. <b>2001</b> , 13, 5295-5311	15
1452	Degree of localization of the exchange-correlation hole and its influence on the ground-state (structural and magnetic) properties of d metals. <b>2001</b> , 13, 9463-9470	16

1451	Vibrational modes in epitaxial $Ti_{1-x}Sc_xN(001)$ layers: An ab initio calculation and Raman spectroscopy study. <b>2001</b> , 64,	45
1450	Accurate total energies without self-consistency. <b>2001</b> , 87, 226401	22
1449	X-ray diffraction and theoretical studies of the high-pressure structures and phase transitions in magnesium fluoride. <b>2001</b> , 64,	95
1448	Ab initio determination of the atomistic structure of $Si_xGe_{1-x}$ alloy. <b>2001</b> , 64,	56
1447	Structure-compressibility relationships in layered cuprate materials. <b>2001</b> , 65,	8
1446	Pressure-induced phase transformation and structural resilience of single-wall carbon nanotube bundles. <b>2001</b> , 63,	90
1445	Electronic band structure and structural stability of LaBiPt. <b>2001</b> , 63,	38
1444	Ab initio simulation of ammonia monohydrate ( $NH_3 \cdot H_2O$ ) and ammonium hydroxide ( $NH_4OH$ ). <b>2001</b> , 115, 7006-7014	41
1443	Structure and physical properties of $Na_4C_{60}$ under ambient and high pressures. <b>2001</b> , 63,	14
1442	First-principles study on structural, dielectric, and dynamical properties for three BN polytypes. <b>2001</b> , 63,	120
1441	Comparison of global and local adaptive coordinates for density-functional calculations. <b>2001</b> , 63,	60
1440	Structural and superconducting transition in selenium at high pressure. <b>2001</b> , 63,	15
1439	Prediction of spinel structure and properties of single and double nitrides. <b>2001</b> , 63,	84
1438	Pressure dependence of local vibrational modes in InP. <b>2001</b> , 63,	9
1437	Epitaxial $Sc_{1-x}Ti_xN(001)$ : Optical and electronic transport properties. <b>2001</b> , 89, 401-409	78
1436	Magnetic behavior of epitaxial $SrRuO_3$ thin films under pressure up to 23 GPa. <b>2002</b> , 80, 2338-2340	26
1435	Cohesive properties of group-III nitrides: A comparative study of all-electron and pseudopotential calculations using the generalized gradient approximation. <b>2002</b> , 65,	118
1434	Photoluminescence from $Zn_{1-x}Te_x$ alloys under hydrostatic pressure. <b>2002</b> , 66,	8

1433	Delocalization and phase transitions in Pr: Theory. <b>2002</b> , 65,	29
1432	Ab initio calculations of bulk moduli and comparison with experiment. <b>2002</b> , 66,	33
1431	Crystal structure and lattice dynamics of AlB <sub>2</sub> under pressure and implications for MgB <sub>2</sub> . <b>2002</b> , 66,	58
1430	The Co/sub 2/MnGe Heusler compound: a first principles study of the bulk phase and of the interface with GaAs. <b>2002</b> , 38, 2895-2897	14
1429	Density-functional investigation of magnetism in EPu. <b>2002</b> , 66,	118
1428	Ab initio studies of structural stability and magnetism in Ni <sub>3</sub> In. <b>2002</b> , 66,	9
1427	First-principles study of the ferroelastic phase transition in CaCl <sub>2</sub> . <b>2002</b> , 65,	14
1426	Pressure-volume relationship of Ta. <b>2002</b> , 91, 4143-4148	29
1425	A photon echo study of two-level systems in polyisobutylene under high pressure. <b>2002</b> , 116, 1737-1743	7
1424	Experimental and theoretical study of the electronic structures of Ni <sub>3</sub> Al, Ni <sub>3</sub> Ga, Ni <sub>3</sub> In, and NiGa. <b>2002</b> , 92, 1419-1424	24
1423	Experimental and theoretical study of the electronic structure of Fe <sub>3</sub> Al, Fe <sub>2</sub> VAl, and Fe <sub>2</sub> VGa. <b>2002</b> , 66,	21
1422	Electronic structure of cubic and orthorhombic phases of ZrW <sub>2</sub> O <sub>8</sub> . <b>2002</b> , 65,	18
1421	First-principles study of transparent p-type conductive SrCu <sub>2</sub> O <sub>2</sub> and related compounds. <b>2002</b> , 65,	83
1420	First-principles studies of the structural and electronic properties of pyrite FeS <sub>2</sub> . <b>2002</b> , 65,	56
1419	THE BAND STRUCTURE AND BULK MODULUS OF CUBIC (3C) AND HEXAGONAL (2H) POLYTYPES OF SILICON CARBIDE. <b>2002</b> , 16, 383-392	2
1418	Equations of state for barium in high-pressure phases. <b>2002</b> , 14, 5129-5134	3
1417	High-pressure effects on the Raman spectrum and the force constants of the rare-earth aluminium garnets (RE <sub>3</sub> Al <sub>5</sub> O <sub>12</sub> ). <b>2002</b> , 14, 3875-3890	9
1416	First-Principles Investigation of L10-Disorder Phase Equilibrium in Fe-Pt System. <b>2002</b> , 43, 2104-2109	51

1415 Cohesive Energy. **2002**,

1414 Plane-wave pseudopotential study on mechanical and electronic properties for group III-V binary phases. **2002**, 743, L11.38.1

1413 Adhesion, atomic structure, and bonding at the Al(111)/Al<sub>2</sub>O<sub>3</sub>(0001) interface: A first principles study. **2002**, 65, 191

1412 Electronic and dielectric properties of insulating Zr<sub>3</sub>N<sub>4</sub>. **2002**, 66, 40

1411 Density-functional study of Fe<sub>3</sub>Al: LSDA versus GGA. **2002**, 65, 105

1410 Nephelauxetic effect in LiNbO<sub>3</sub>:Cr<sup>3+</sup> crystals. **2002**, 81, 442-444 17

1409 First-principles simulations of metal-ceramic interface adhesion: Co/WC versus Co/TiC. **2002**, 65, 129

1408 Plane-wave pseudopotential study on mechanical and electronic properties for IV and III-V crystalline phases with zinc-blende structure. **2002**, 66, 153

1407 Ab initio calculation of the thermal properties of Cu: Performance of the LDA and GGA. **2002**, 65, 91

1406 Structure and properties of spinel Fe<sub>3</sub>N<sub>4</sub> and comparison to zinc blende FeN. **2002**, 80, 2904-2906 28

1405 Ab initio investigation of phonon modes in the MgAl<sub>2</sub>O<sub>4</sub> spinel. **2002**, 14, 3543-3552 51

1404 Sodium under pressure: bcc to fcc structural transition and pressure-volume relation to 100 GPa. **2002**, 65, 103

1403 First-principles elastic and structural properties of uranium metal. **2002**, 66, 108

1402 Effective elastic stiffnesses of InAs under uniform strain. **2002**, 92, 3027-3033 41

1401 Co<sub>2</sub>MnX (X=Si, Ge, Sn) Heusler compounds: An ab initio study of their structural, electronic, and magnetic properties at zero and elevated pressure. **2002**, 66, 513

1400 Electronic and optical properties of SnTe and GeTe. **2002**, 14, 8625-8637 32

1399 Elastic stability and electronic structure of fcc Ti, Zr, and Hf: A first-principles study. **2002**, 65, 90

1398 Vibrational properties of ZnTe at high pressures. **2002**, 14, 739-757 35



1397	A plane-wave pseudopotential study on III V zinc-blende and wurtzite semiconductors under pressure. <b>2002</b> , 14, 9579-9587	98
1396	Energetically favourable sites of iodine atoms in zirconium: An ab initio approach. <b>2002</b> , 82, 73-83	2
1395	First-principles study for ordering and phase separation in the Fe-Pd system. <b>2002</b> , 14, 1903-1913	40
1394	The calculation of structural, elastic and phase stability properties of minerals using first principles techniques: A comparison of HF, DFT and Hybrid functional treatments of exchange and correlation. <b>2002</b> , 28, 903-915	14
1393	Crystal structure and chemical bonding of the high-pressure phase of MgAl <sub>2</sub> O <sub>4</sub> from first-principles calculations. <b>2002</b> , 82, 2885-2894	2
1392	Systematic generation of finite-range atomic basis sets for linear-scaling calculations. <b>2002</b> , 66,	228
1391	Bipolar doping and band-gap anomalies in delafossite transparent conductive oxides. <b>2002</b> , 88, 066405	280
1390	Density functional calculations on hydrogen in palladium-silver alloys. <b>2002</b> , 330-332, 332-337	51
1389	First-principles electronic structure calculations of BaSi <sub>7</sub> N <sub>10</sub> with both corner- and edge-sharing SiN <sub>4</sub> tetrahedra. <b>2002</b> , 336, 1-4	12
1388	Elastic properties of a polycrystalline sample of the L1 <sub>2</sub> Al <sub>5</sub> CrTi <sub>2</sub> intermetallic compound under hydrostatic pressure up to 1 GPa at room temperature. <b>2002</b> , 337, 58-63	3
1387	Effect of pressure on the magnetic properties of MnRh <sub>1-x</sub> CoxAs. <b>2002</b> , 345, 59-67	4
1386	Ab initio calculation of the formation energies of L1 <sub>2</sub> , D0 <sub>22</sub> , D0 <sub>23</sub> and one dimensional long period structures in TiAl <sub>3</sub> compound. <b>2002</b> , 10, 751-764	42
1385	Ab initio calculations of elastic constants and thermodynamic properties of bcc, fcc, and hcp Al crystals under pressure. <b>2002</b> , 14, 6989-7005	512
1384	Phonon spectrum of ZnAl <sub>2</sub> O <sub>4</sub> spinel from inelastic neutron scattering and first-principles calculations. <b>2002</b> , 66,	49
1383	Prediction of ferromagnetic cubic spinel phase of Fe <sub>3</sub> N <sub>4</sub> . <b>2002</b> , 91, 7352	6
1382	Pressure dependence of optoelectronic properties of GaN in the zinc-blende structure. <b>2002</b> , 73, 51-56	50
1381	Electron and Positron Energy Levels and Deformation Potentials in Group-III Nitrides. <b>2002</b> , 231, 391-402	48
1380	Energetic and Electronic Structure of the Hypothetical Cubic Zincblende-Like Semiconductors GeC and SnC. <b>2002</b> , 231, 411-422	14

1379	Full-Potential Study of the Electronic Structure of Silver Halides. <b>2002</b> , 234, 580-589	10
1378	First principles calculations of the hypothetical interface BN/XC (X = Si, Ge, Sn). <b>2002</b> , 31, 219-228	3
1377	A new form of the Sutton-Chen potential for the Cu-Ag alloys. <b>2002</b> , 31, 297-313	5
1376	Electronic and optical properties of CdTe under hydrostatic pressure effect. <b>2002</b> , 32, 25-34	7
1375	High pressure study of the C <sub>84</sub> fullerene. <b>2002</b> , 318, 372-377	9
1374	Electronic and magnetic structures of Ni/Fe(0 0 1) overlayers: first-principles study. <b>2002</b> , 321, 222-229	4
1373	Charge density distribution with pressure in Y-123. <b>2002</b> , 321, 360-364	12
1372	Electronic and structural properties of $\beta$ -Be <sub>3</sub> N <sub>2</sub> . <b>2002</b> , 324, 305-311	53
1371	Structural and electronic properties of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> under high pressures. <b>2002</b> , 370, 85-93	21
1370	High pressure dependence of positron states in zinc-blende boron nitride. <b>2002</b> , 94, 54-61	7
1369	Effect of chromium addition on the ordering behaviour of Ni-Mo alloy: experimental results vs. electronic structure calculations. <b>2002</b> , 50, 3301-3315	46
1368	Theoretical study on the lattice dynamics and electron-phonon interaction of vanadium under high pressures. <b>2002</b> , 14, 10869-10872	32
1367	Vacancy and interstitial defects in hafnia. <b>2002</b> , 65,	493
1366	LDA and GGA investigations of some ground state properties of aluminium with the all electron MAPW method. <b>2003</b> , 37, 405-411	11
1365	Theory for structure and bulk modulus determination. <b>2003</b> , 68,	39
1364	Pathways of atomistic processes on TiN(001) and (111) surfaces during film growth: an ab initio study. <b>2003</b> , 93, 9086-9094	292
1363	Formation and stability of radiation defect complexes in Si and Si:Ge: Composition and pressure effects. <b>2003</b> , 202, 107-113	7
1362	Elastic constants and electronic structure of alkaline-earth chalcogenides. Performances of various hamiltonians. <b>2003</b> , 367, 430-438	73

1361	Structural, electronic and elastic properties of some fluoride crystals: an ab initio study. <b>2003</b> , 368, 7-11	46
1360	The structure, ordering and equation of state of ammonia dihydrate ( $\text{nh}_3 \cdot 2\text{h}_2\text{o}$ ). <b>2003</b> , 162, 59-73	29
1359	First-principle study of structural, electronic and elastic properties of SrS, SrSe and SrTe under pressure. <b>2003</b> , 339, 208-215	79
1358	Pressure derivatives of bulk and shear modulus of rare gas solids. <b>2003</b> , 64, 1125-1130	6
1357	Pressure dependence of TC of the layered superconductor $\text{Y}_2\text{C}_2\text{I}_2$ : lattice versus electronic effects. <b>2003</b> , 171, 367-370	6
1356	Nephelauxetic effect in luminescence of $\text{Cr}^{3+}$ -doped lithium niobate and garnets. <b>2003</b> , 102-103, 571-574	19
1355	Zinc-blende ZnS under pressure: predicted electronic properties. <b>2003</b> , 47, 1335-1338	41
1354	Density functional study of alkali metals adsorption on the $\text{MgO}(111)$ surface. <b>2003</b> , 538, 240-248	8
1353	Stress-dependence tight binding study of tellurium-based III-VI semiconductors. <b>2003</b> , 315, 143-149	16
1352	FP-LAPW investigations of electronic structure and bonding mechanism of NbC and NbN compounds. <b>2003</b> , 325, 46-56	103
1351	First-principles study of the electronic and optical properties of zincblende zinc selenide. <b>2003</b> , 337, 1-9	28
1350	Full potential linearized augmented plane wave calculations of structural and electronic properties of GeC, SnC and GeSn. <b>2003</b> , 336, 321-328	42
1349	Ab initio calculations of the electronic structure of the silver palladium oxide $\text{Ag}_2\text{PdO}_2$ . <b>2003</b> , 337, 102-110	3
1348	Ab initio calculations of the electronic and structural properties of beryllium-, magnesium- and calcium-nitrides. <b>2003</b> , 337, 122-129	46
1347	Ab initio study of the structural and electronic properties of the complex structures of $\text{RuO}_2$ . <b>2003</b> , 339, 1-10	15
1346	Calculated band structures and optical properties of lead chalcogenides $\text{PbX}$ ( $\text{X}=\text{S}, \text{Se}, \text{Te}$ ) under hydrostatic pressure. <b>2003</b> , 337, 394-403	21
1345	Full potential calculation of structural, electronic and optical properties of $\text{CdSiP}_2$ and $\text{CdGeP}_2$ . <b>2003</b> , 98, 81-88	22
1344	Properties of simple metals beyond the local density approximation of density functional theory. <b>2003</b> , 91, 224-229	7

1343	Pressure-induced Changes of the Crystal Structure of Eu <sub>4</sub> P <sub>3</sub> . <b>2003</b> , 629, 454-458	3
1342	Exploiting Covalency to Enhance Metal-Oxide and Oxide-Oxide Adhesion at Heterogeneous Interfaces. <b>2003</b> , 86, 373-386	31
1341	Electronic Structure and Bonding in Crystalline Y <sub>10</sub> [SiO <sub>4</sub> ] <sub>6</sub> N <sub>2</sub> . <b>2003</b> , 86, 1424-1426	8
1340	Local structure and electronic properties of BaTaO <sub>2</sub> N with perovskite-type structure. <b>2003</b> , 64, 281-286	59
1339	Mechanical behaviour of AgB <sub>2</sub> in comparison to MgB <sub>2</sub> — first principle study. <b>2003</b> , 390, 16-20	12
1338	Applicability of three-parameter equation of state of solids: compatibility with first principles approaches and application to solids. <b>2003</b> , 15, 1643-1663	5
1337	Electronic and optical properties of Y <sub>2</sub> SiO <sub>5</sub> and Y <sub>2</sub> Si <sub>2</sub> O <sub>7</sub> with comparisons to HfSiO <sub>2</sub> and Y <sub>2</sub> O <sub>3</sub> . <b>2003</b> , 67,	65
1336	First-principles study on structures and energetics of intrinsic vacancies in SrTiO <sub>3</sub> . <b>2003</b> , 68,	178
1335	Theoretical study of the electronic structure, chemical bonding and optical properties of KNbO <sub>3</sub> in the paraelectric cubic phase. <b>2003</b> , 15, 5945-5958	240
1334	Elasticity of carbon allotropes. III. Hexagonal graphite: Review of data, previous calculations, and a fit to a modified anharmonic Keating model. <b>2003</b> , 67,	25
1333	Bond switching from two- to three-dimensional polymers of C <sub>60</sub> at high pressure. <b>2003</b> , 68,	24
1332	Understanding the complex metallic element Mn. II. Geometric frustration in $\beta$ -Mn, phase stability, and phase transitions. <b>2003</b> , 68,	115
1331	Electronic phase transition and superconductivity of vanadium under high pressure. <b>2003</b> , 67,	28
1330	Structural and electronic properties of lithium intercalated graphite LiC <sub>6</sub> . <b>2003</b> , 68,	126
1329	A modified empirical potential for energetic calculations of planar defects in GaN. <b>2003</b> , 27, 43-49	39
1328	Electronic structure of magnesium nitride-fluorides from first-principles calculations. <b>2003</b> , 351, 72-76	22
1327	Stability of $\beta$ -Pu alloys from first-principles theory. <b>2003</b> , 354, 99-103	20
1326	First-principles study on the lonsdaleite phases of C, Si and Ge. <b>2003</b> , 15, L197-L202	50

1325	Phonon spectrum and thermal properties of cubic Si <sub>3</sub> N <sub>4</sub> from first-principles calculations. <b>2003</b> , 93, 5175-5180	44
1324	Co-phase penetration of WC(101̄0)/WC(101̄0) grain boundaries from first principles. <b>2003</b> , 67,	76
1323	Structural changes in single-walled carbon nanotubes under non-hydrostatic pressures: x-ray and Raman studies. <b>2003</b> , 5, 143-143	25
1322	Equation of state and phonon frequency calculations of diamond at high pressures. <b>2003</b> , 68,	69
1321	Understanding the complex metallic element Mn. I. Crystalline and noncollinear magnetic structure of $\beta$ Mn. <b>2003</b> , 68,	205
1320	High pressure x-ray study on anthracene. <b>2003</b> , 119, 1078-1084	49
1319	Pressure-induced phonon instabilities in copper chloride. <b>2003</b> , 67,	26
1318	Lattice relaxation by atomic hydrogen irradiation of IIĪV semiconductor alloys. <b>2003</b> , 68,	36
1317	Quantum design and synthesis of a boron̄oxygen̄ttrium phase. <b>2003</b> , 82, 4286-4288	1
1316	Electronic structure and energetics of RCo <sub>5</sub> H <sub>4</sub> and RCo <sub>5</sub> (R=La,Pr). <b>2003</b> , 82, 1042-1044	9
1315	Noble-gas solids at negative pressure. <b>2003</b> , 68,	16
1314	First-principles study of the structural phase transformation of hafnia under pressure. <b>2003</b> , 68,	128
1313	Pressure-induced structural phase transition in fullerides doped with rare-earth metals. <b>2003</b> , 67,	2
1312	Elastic modulus of amorphous boron suboxide thin films studied by theoretical and experimental methods. <b>2003</b> , 93, 940-944	17
1311	First-principles study of the solubility, diffusion, and clustering of C in Ni. <b>2003</b> , 68,	67
1310	Pressure dependence of electron-phonon coupling and superconductivity in hcp Fe: A linear response study. <b>2003</b> , 67,	32
1309	Vacancy hardening in single-crystal TiN <sub>x</sub> (001) layers. <b>2003</b> , 93, 6025-6028	131
1308	Effect of composition on vacancy mediated diffusion in random binary alloys: First principles study of the Si <sub>1-x</sub> Gex system. <b>2003</b> , 94, 174-185	37

1307	Thermal expansion of the Ag(110) surface studied by low-energy electron diffraction and density-functional theory. <b>2003</b> , 68,	17
1306	Ab initio simulation of water interaction with the (100) surface of pyrite. <b>2003</b> , 118, 8917-8926	92
1305	Theoretical analysis of clock-reconstructed PdCu surface alloy. <b>2003</b> , 67,	10
1304	MgB <sub>2</sub> : Superconductivity and Pressure. <b>2003</b> , 17, 3785-3806	6
1303	Optical properties of the antiperovskite superconductor MgCNi <sub>3</sub> . <b>2003</b> , 15, 833-841	18
1302	Chain-length-dependent intermolecular packing in polyphenylenes: a high pressure study. <b>2003</b> , 15, 3375-3389	39
1301	Elastic behaviour and microstructural characteristics of Nd <sub>60</sub> Al <sub>10</sub> Fe <sub>20</sub> Co <sub>10</sub> bulk metallic glass investigated by ultrasonic measurement under pressure. <b>2003</b> , 15, 4503-4509	20
1300	Orbital-free density functional theory calculations of the properties of Al, Mg and Al/Mg crystalline phases. <b>2003</b> , 11, 339-348	36
1299	Models of defects in wide-gap oxides. <b>2003</b> , 151-222	15
1298	Lattice vibrations and thermal properties of carbon nitride with defect ZnS structure from first-principles calculations. <b>2004</b> , 16, 3027-3034	6
1297	Electronic Structures and Magnetic Properties of CoN, NiN and CuN. <b>2004</b> , 21, 1612-1615	14
1296	Electron-phonon coupling of $\alpha$ boron. <b>2004</b> , 70,	51
1295	High-pressure study of layered nitride superconductors. <b>2004</b> , 70,	13
1294	Stability of reduced V <sub>2</sub> O <sub>5</sub> (001) surfaces. <b>2004</b> , 70,	110
1293	Electronic structures of rocksalt, litharge, and herzenbergite SnO by density functional theory. <b>2004</b> , 70,	105
1292	Full potential linearized augmented plane wave investigations of structural and electronic properties of pyrochlore systems. <b>2004</b> , 96, 6482-6487	31
1291	Transferable local pseudopotentials derived via inversion of the Kohn-Sham equations in a bulk environment. <b>2004</b> , 69,	66
1290	First-principles phase diagram of the Ce-Th system. <b>2004</b> , 70,	10

1289	Effect of atomic displacements on the ground state of $\text{FeO}_2$ . <b>2004</b> , 69,	14
1288	Search for metal hydrides with short hydrogen-hydrogen separation: Ab initio calculations. <b>2004</b> , 70,	19
1287	Phosphorus under pressure: Ba-IV-type structure as a candidate for P-IV. <b>2004</b> , 69,	19
1286	Stability of corundum- versus rutile-type structures of ruthenium and rhodium oxides. <b>2004</b> , 70,	18
1285	Weak itinerant ferromagnetism and electronic and crystal structures of alkali-metal iron antimonides: $\text{NaFe}_4\text{Sb}_{12}$ and $\text{KFe}_4\text{Sb}_{12}$ . <b>2004</b> , 70,	76
1284	Wetting of TiC and TiN by metals. <b>2004</b> , 69,	85
1283	First-principles calculation of the structure and magnetic phases of hematite. <b>2004</b> , 69,	356
1282	Metamagnetic behavior of $\text{Fe}_3\text{M}$ (M=Al and Si) alloys at high pressure. <b>2004</b> , 70,	14
1281	Quasiparticle band structures and optical spectra of cristobalite $\text{SiO}_2$ . <b>2004</b> , 69,	37
1280	Structure and stability of rare-earth and transition-metal oxides. <b>2004</b> , 69,	110
1279	Theoretical study of structural and electronic properties of $\text{EMoN}$ . <b>2004</b> , 70,	13
1278	Optical properties of correlation-induced paramagnetic FeAl alloy. <b>2004</b> , 96, 7018-7021	4
1277	Structure Prediction of Solids: Heuristic Algorithms for Local Optimization on Hartree-Fock Level. <b>2004</b> , 453-454, 71-76	16
1276	Pressure dependence of metallization and superconducting transition in AgCl and AgBr. <b>2004</b> , 16, 1577-1592	25
1275	First Principle Calculation of Oxidation of Metals. <b>2004</b> , 461-464, 161-168	
1274	From configuration space to thermodynamic space: Predicting new inorganic solids via global exploration of their energy landscapes. <b>2004</b> , 848, 23	4
1273	The Non-Linear Field Theories of Mechanics. <b>2004</b> , 1-579	31
1272	V B2 and ZrB2: a density functional study. <b>2004</b> , 16, 2335-2344	33

1271	BULK MODULUS CALCULATIONS FOR GROUP-IV CARBIDES AND GROUP-III NITRIDES. <b>2004</b> , 18, 1247-1254	2
1270	Electronic Structure and Bonding of $\beta$ -SiAlON. <b>2004</b> , 83, 780-786	31
1269	Theoretical Prediction of the Structure and Properties of Cubic Spinel Nitrides. <b>2004</b> , 85, 75-80	86
1268	The influence of hydrostatic pressure on the static and dynamic properties of an InSe crystal: A first-principles study. <b>2004</b> , 46, 179-187	8
1267	The mechanism of ionic conductivity in stabilized cubic zirconia. <b>2004</b> , 46, 453-457	35
1266	Predicted electronic properties of GaAs under hydrostatic pressure. <b>2004</b> , 84, 375-379	46
1265	Structure of amorphous iron-based coatings processed by HVOF and APS thermally spraying. <b>2004</b> , 85, 113-119	39
1264	Structural, electronic, and optical properties of beryllium monochalcogenides. <b>2004</b> , 39, 5-17	63
1263	Numerical atomic basis orbitals from H to Kr. <b>2004</b> , 69,	567
1262	Effects of additives in $\beta$ - and $\delta$ -alumina: an ab initio study. <b>2004</b> , 16, 8971-8980	30
1261	High-pressure X-ray diffraction study of $UMn_2Ge_2$ . <b>2004</b> , 344, 255-259	8
1260	High pressure electrical transport measurements of $Cs_2MoS_4$ and $KTbP_2Se_6$ and X-ray diffraction study of $Cs_2MoS_4$ . <b>2004</b> , 129, 511-514	2
1259	Pressure-induced amorphization in $Y_2(WO_4)_3$ : in situ X-ray diffraction and Raman studies. <b>2004</b> , 177, 4087-4092	32
1258	FeNb and FeSi thermal spraying coatings: microstructure and first principle calculations. <b>2004</b> , 107, 27-32	5
1257	Empirical molecular dynamics study of structural, elastic and thermodynamic properties of zinc-blende-like SiGe compound. <b>2004</b> , 111, 207-213	5
1256	Ab initio Study of the Si Adsorption on Mo(110). <b>2004</b> , 13, 327-330	1
1255	Enthalpy Landscapes of the Earth Alkaline Metal Oxides. <b>2004</b> , 630, 2354-2366	46
1254	Structural, electronic and optical calculations of $Cu(In,Ga)Se_2$ ternary chalcopyrites. <b>2004</b> , 241, 2516-2528	42



1253	Band structure, metallization and superconductivity of GaP and GaN under high pressure. <b>2004</b> , 241, 2489-2500	4
1252	Electronic and structural properties of strontium chalcogenides SrS, SrSe and SrTe. <b>2004</b> , 241, 2529-2537	38
1251	High-pressure polymorphism in phosphorus nitrides. <b>2004</b> , 241, 2319-2325	12
1250	High pressure Raman study of Y3Al5O12. <b>2004</b> , 241, 3149-3154	21
1249	High pressure phase transition and variation of elastic constants of diluted magnetic semiconductors. <b>2004</b> , 241, 3374-3380	13
1248	Magnetism of Ni overlayers on Fe(111). <b>2004</b> , 1, 1760-1764	2
1247	Stability and magnetism of NiBe alloyed overlayers on Fe(001). <b>2004</b> , 1, 1765-1768	
1246	Advances in the theory of electronic structure of semiconductors. <b>2004</b> , 1, 2003-2027	39
1245	Bulk metallic glasses. <b>2004</b> , 44, 45-89	1949
1244	Full potential calculation of structural, electronic and elastic properties of alkaline earth oxides MgO, CaO and SrO. <b>2004</b> , 344, 334-342	102
1243	An isothermal equation of state for solids. <b>2004</b> , 350, 375-388	5
1242	Electronic structures of filled tetrahedral semiconductors LiMgN and LiZnN: conduction band distortion. <b>2004</b> , 353, 278-286	33
1241	Calculation of surface properties of bcc iron. <b>2004</b> , 74, 179-183	64
1240	High pressure phase transition in metallic LaB6: Raman and X-ray diffraction studies. <b>2004</b> , 129, 791-796	37
1239	High-pressure behavior of red mercuric iodide: in situ X-ray diffraction and optical absorption studies. <b>2004</b> , 131, 473-478	7
1238	Superconductivity of Li under pressure. <b>2004</b> , 131, 671-675	6
1237	Pressure dependence of elastic constants in zinc-blende GaN and InN and their influence on the pressure coefficients of the light emission in cubic InGaN/GaN quantum wells. <b>2004</b> , 131, 763-767	26
1236	Structural phase transition of boron nitride compound. <b>2004</b> , 132, 465-470	24

1235	High pressure X-ray diffraction and electrical resistance study of the quasi-one-dimensional sulfide InV <sub>6</sub> S <sub>8</sub> . <b>2004</b> , 132, 731-736	3
1234	Prediction study of elastic properties under pressure effect for zincblende BN, AlN, GaN and InN. <b>2004</b> , 48, 1601-1606	57
1233	Structural and electronic properties of matlockite MFX (MSr, Ba, Pb; XCl, Br, I) compounds. <b>2004</b> , 65, 1871-1878	56
1232	Calculation of bulk modulus for highly anisotropic materials. <b>2004</b> , 326, 442-448	23
1231	Prediction of structural and thermodynamic properties of zinc-blende AlN: molecular dynamics simulation. <b>2004</b> , 302, 135-141	45
1230	Elastic property and its response to pressure in a typical bulk metallic glass. <b>2004</b> , 52, 715-719	26
1229	Structure prediction of high-pressure phases for alkali metal sulfides. <b>2004</b> , 121, 2289-304	80
1228	Adhesion and adhesive transfer at aluminum/diamond interfaces: A first-principles study. <b>2004</b> , 69,	105
1227	Structural and Electronic Characterizations of Two Isomers of Ce@C <sub>82</sub> . <b>2004</b> , 108, 7580-7585	27
1226	Ab initio study of the $\beta$ -tin-bmna-bh phase transitions in silicon and germanium. <b>2004</b> , 69,	25
1225	Design of Potential Hydrogen-Storage Materials Using First-Principle Density-Functional Calculations. <b>2004</b> , 4, 471-477	50
1224	Pressure dependence of the fundamental band-gap energy of CdSe. <b>2004</b> , 84, 67-69	58
1223	Structural and electronic properties of YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> and YSr <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub> under mechanical and strontium chemical pressures. <b>2004</b> , 70,	16
1222	Generalized-stacking-fault energy and dislocation properties in bcc Fe: A first-principles study. <b>2004</b> , 70,	93
1221	Equations of State and Thermophysical Properties of Solids Under Pressure. <b>2004</b> , 217-236	6
1220	Crystal structure of LaTiO <sub>3.41</sub> under pressure. <b>2004</b> , 69,	19
1219	Ab initio calculations of structure and lattice dynamics in NiMnAl shape memory alloys. <b>2004</b> , 70,	51
1218	Hybrid density functional theory study of vanadium monoxide. <b>2004</b> , 69,	30

1217	Lattice Dynamics of Defects and Thermal Properties of 3C-SiC. <b>2004</b> , 161-208	1
1216	Metal-insulator and magnetic transition of NiO at high pressures. <b>2004</b> , 69,	54
1215	Physical trends in amorphous carbon: A tight-binding molecular-dynamics study. <b>2004</b> , 70,	45
1214	High-pressure band structure and superconductivity of bcc and fcc lithium. <b>2004</b> , 70,	10
1213	Constant pressure reactive molecular dynamics simulations of phase transitions under pressure: The graphite to diamond conversion revisited. <b>2004</b> , 39, 41-47	24
1212	Zinc-blende AlN and GaN under pressure: structural, electronic, elastic and piezoelectric properties. <b>2004</b> , 19, 1220-1231	61
1211	First-principles electronic structure of spinel LiCr <sub>2</sub> O <sub>4</sub> : A possible half-metal. <b>2004</b> , 69,	17
1210	First-principles study of the mechanisms for the pressure-induced phase transitions in zinc-blende CuBr and CuI. <b>2004</b> , 69,	30
1209	Theoretical study of structural and electronic properties of Ba <sub>2</sub> O <sub>5</sub> and La <sub>2</sub> O <sub>5</sub> . <b>2004</b> , 69,	60
1208	B1-to-B2 phase transition of transition-metal monoxide CdO under strong compression. <b>2004</b> , 70,	60
1207	Electronic structure and electron energy-loss spectroscopy of ZrO <sub>2</sub> zirconia. <b>2004</b> , 70,	121
1206	Hardness and fracture toughness of brittle materials: A density functional theory study. <b>2004</b> , 70,	60
1205	Interaction of lithium with graphene: An ab initio study. <b>2004</b> , 70,	157
1204	First-principles elastic constants and phonons of Pu. <b>2004</b> , 70,	30
1203	Ab initio study of the enthalpy barriers of the high-pressure phase transition from the cubic-diamond to the $\beta$ structure of silicon and germanium. <b>2004</b> , 30, 1-7	14
1202	Ab-initio study of the Imma phase in silicon. <b>2004</b> , 30, 8-15	7
1201	Properties of strained zinc-blende GaN: first-principles study. <b>2004</b> , 366, 86-93	37
1200	High pressure studies of GdMn <sub>2</sub> and its hydrides. <b>2004</b> , 375, 62-66	6

1199	Optical properties of Ni <sub>3</sub> Al, Ni <sub>3</sub> Ga, and Ni <sub>3</sub> In. <b>2004</b> , 377, 29-33	6
1198	Electronic and elastic properties of RCo <sub>5</sub> and RCo <sub>5</sub> H <sub>n</sub> (R = La, Ce, Pr). <b>2004</b> , 379, 41-53	21
1197	HVOF-sprayed Tribaloy <sup>®</sup> -400: microstructure and first principle calculations. <b>2004</b> , 58, 2433-2436	19
1196	The Performance of Hybrid Density Functionals in Solid State Chemistry. <b>2004</b> , 171-232	164
1195	Electronic structure of ZnCNi <sub>3</sub> . <b>2004</b> , 70,	38
1194	Efficient hybrid density functional calculations in solids: assessment of the Heyd-Scuseria-Ernzerhof screened Coulomb hybrid functional. <b>2004</b> , 121, 1187-92	1520
1193	Ab initio study of structural, electronic and optical properties of ordered group-IV binary alloy Ge <sub>0.5</sub> Sn <sub>0.5</sub> . <b>2004</b> , 29, 131-137	4
1192	An ab initio study of structural properties and single vacancy defects in Wurtzite AlN. <b>2004</b> , 120, 4890-6	25
1191	Tests of a ladder of density functionals for bulk solids and surfaces. <b>2004</b> , 69,	313
1190	Effect of the Order-Disorder Transition of the bcc Structure on the Solubility of Be in the Fe-Be Binary System. <b>2004</b> , 45, 1499-1506	9
1189	First-Principles Calculation of L10-Disorder Phase Boundary in Fe-Pd System. <b>2004</b> , 45, 1478-1484	27
1188	Study of Elastic Properties and Their Pressure Dependence of Semi Magnetic Semiconductors. <b>2005</b> , 74, 382-388	33
1187	Point defects in uranium dioxide: Ab initio pseudopotential approach in the generalized gradient approximation. <b>2005</b> , 347, 44-51	113
1186	Mössbauer effect and first principle calculations of the electronic structure and hyperfine interaction parameters of Hf <sub>2</sub> Fe. <b>2005</b> , 66, 1815-1819	1
1185	Full potential investigations of structural and electronic properties of ZrSiO <sub>4</sub> . <b>2005</b> , 81, 514-523	125
1184	First-principles investigation of BN <sub>x</sub> P <sub>1-x</sub> , BN <sub>x</sub> As <sub>1-x</sub> and BP <sub>x</sub> As <sub>1-x</sub> ternary alloys. <b>2005</b> , 121, 170-177	107
1183	Full-potential calculations of structural, elastic and electronic properties of MgAl <sub>2</sub> O <sub>4</sub> and ZnAl <sub>2</sub> O <sub>4</sub> compounds. <b>2005</b> , 344, 271-279	58
1182	First-principles calculations of optical properties of GeC, SnC and GeSn under hydrostatic pressure. <b>2005</b> , 355, 392-400	32

1181	First-principles study of structural, elastic and high-pressure properties of cerium chalcogenides. <b>2005</b> , 363, 255-261	33
1180	Occurrence of superconductivity in diboride of Zr. <b>2005</b> , 426-431, 464-468	2
1179	High pressure electronic properties and elastic stability criteria of AlAs. <b>2005</b> , 123, 87-93	17
1178	Theoretical studies on band structure and optical properties of 3CBiC by FPLAPW. <b>2005</b> , 144-147, 593-596	6
1177	The first principle study on the atomic and electronic structure of GaN() surface. <b>2005</b> , 144-147, 597-600	2
1176	Structure, stability, and stress properties of amorphous and nanostructured carbon films. <b>2005</b> , 482, 56-62	10
1175	Equation of state of aluminum carbide Al <sub>4</sub> C <sub>3</sub> . <b>2005</b> , 133, 385-388	32
1174	Electronic band structures of filled tetrahedral semiconductor LiMgP and zinc-blende AlP. <b>2005</b> , 135, 124-128	34
1173	Equation of state of aluminum silicon carbide Al <sub>4</sub> SiC <sub>4</sub> . <b>2005</b> , 135, 87-89	11
1172	P $\nu$ relation for cuprous halides: Pseudopotential approach. <b>2005</b> , 136, 157-162	
1171	Theoretical investigation of electronic structure and optical properties of paramagnetic non-oxide perovskite AlCNi <sub>3</sub> . <b>2005</b> , 136, 605-610	30
1170	First-principles calculation of structural energetics of Al <sub>3</sub> TM (TM=Ti, Zr, Hf) intermetallics. <b>2005</b> , 53, 3225-3252	171
1169	Electronic structure and optical properties of TaC from the first principles calculation. <b>2005</b> , 44, 281-286	17
1168	Structural, electronic and optical properties of fluorite-type compounds. <b>2005</b> , 47, 63-70	30
1167	Computational DFT Study of ZrSiO <sub>4</sub> Polymorphs: Potential Microelectronic, Nuclear Safety and Geological Implications. <b>2005</b> , 894, 1	1
1166	A comprehensive review of ZnO materials and devices. <b>2005</b> , 98, 041301	8776
1165	Geometry of {001} Surfaces of Spinel (MgAl <sub>2</sub> O <sub>4</sub> ): First-Principles Simulations and Experimental Measurements. <b>2005</b> , 88, 1544-1548	30
1164	Phase Equilibria and Thermodynamics in the Al <sub>2</sub> O <sub>3</sub> -Bi <sub>2</sub> O <sub>3</sub> System Modeling of Mullite and Liquid. <b>2005</b> , 88, 2544-2551	45

1163	Full potential calculation of structural, electronic and optical properties of KMgF3. <b>2005</b> , 91, 185-191	50
1162	Cubic binary compounds MnN and MnAs and diluted magnetic semiconductor alloys: a first-principle study. <b>2005</b> , 288, 384-396	16
1161	Some physical properties of GaX (X=P, As and Sb) semiconductor compounds using higher-order perturbation theory. <b>2005</b> , 357, 305-311	4
1160	First-principle calculations of structural, electronic and optical properties of BaTiO3 and BaZrO3 under hydrostatic pressure. <b>2005</b> , 136, 120-125	83
1159	First-principles study of sulfur overlayers on Pd(1 1 1) surface. <b>2005</b> , 596, 229-241	37
1158	Pressure induced metallization of Cu3N. <b>2005</b> , 40, 4661-4664	9
1157	Effects of hydrostatic pressure and temperature on electronic band parameters in Al <sub>x</sub> Ga <sub>1-x</sub> As. <b>2005</b> , 55, 65-72	9
1156	First-principles calculations on the origins of the gap bowing in BeS <sub>x</sub> Se <sub>1-x</sub> , BeS <sub>x</sub> Te <sub>1-x</sub> and BeS <sub>x</sub> Te <sub>1-x</sub> alloys. <b>2005</b> , 242, 909-915	57
1155	Full potential calculation of structural, elastic and electronic properties of BaZrO3 and SrZrO3. <b>2005</b> , 242, 1054-1062	95
1154	How do electronic properties of conventional III-V semiconductors hold for the III-V boron bismuth BBi compound?. <b>2005</b> , 242, 2856-2863	22
1153	First-principles study of BN <sub>x</sub> Sb <sub>1-x</sub> , BP <sub>x</sub> Sb <sub>1-x</sub> and BAs <sub>x</sub> Sb <sub>1-x</sub> alloys. <b>2005</b> , 242, 3129-3137	34
1152	First-principles calculations of the structural, electronic and optical properties of IIA-IV antiferroite compounds. <b>2005</b> , 242, 2022-2032	30
1151	Effect of Ordering on the Elastic Parameters of Multicomponent Ni-Based Systems. <b>2005</b> , 482, 147-150	1
1150	Relativistic effects on the equation of state of the light actinides. <b>2005</b> , 893, 1	2
1149	Pressure-induced phase transition of nanocrystalline ZnSe. <b>2005</b> , 17, 5187-5200	14
1148	Orientation and Composition Dependences of the Surface Energy and Work Function Observed by First-Principles Calculation for the MoBiF System. <b>2005</b> , 74, 1766-1771	8
1147	Using ONETEP for accurate and efficient density functional calculations. <b>2005</b> , 17, 5757-5769	34
1146	Influence of pressure on the structure and electronic properties of the layered superconductor Y2C2I2. <b>2005</b> , 17, S3121-S3130	6

1145	Effects of pressure on the electric field gradient in USn3. <b>2005</b> , 17, 2407-2418	4
1144	A model for heterogeneous materials including phase transformations. <b>2005</b> , 97, 083509	4
1143	Scalar relativistic all-electron density functional calculations on periodic systems. <b>2005</b> , 122, 84108	23
1142	Improving the orbital-free density functional theory description of covalent materials. <b>2005</b> , 122, 44103	71
1141	Electronic properties of the binary noble metal nitride PtN: First-principles calculations. <b>2005</b> , 72,	49
1140	Organic-inorganic hybrid semiconductor ZnSe(C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> ) <sub>10</sub> under hydrostatic pressure. <b>2005</b> , 72,	4
1139	Response of acoustic and elastic properties to pressure and crystallization of Ce-based bulk metallic glass. <b>2005</b> , 72,	27
1138	First-principles study of electron-phonon coupling in hole- and electron-doped diamonds in the virtual crystal approximation. <b>2005</b> , 72,	89
1137	Experimental and theoretical study of the electronic structure of AuAl <sub>2</sub> , AuGa <sub>2</sub> , and AuIn <sub>2</sub> . <b>2005</b> , 72,	22
1136	PtN: A zinc-blende metallic transition-metal compound. <b>2005</b> , 71,	45
1135	Vibrational properties of GaAs <sub>0.915</sub> N <sub>0.085</sub> under hydrostatic pressures up to 20GPa. <b>2005</b> , 71,	14
1134	Core energy levels of Sc and N and their variation with coordination number in ScN. <b>2005</b> , 72,	8
1133	First-principles calculation of intrinsic defect formation volumes in silicon. <b>2005</b> , 72,	68
1132	Crystal stability and equation of state for Am: Theory. <b>2005</b> , 72,	46
1131	High-pressure phases of FeTiO <sub>3</sub> from first principles. <b>2005</b> , 72,	35
1130	Ab initio phonon calculations for the layered compound TiOCl. <b>2005</b> , 71,	19
1129	First principles local pseudopotential for silver: towards orbital-free density-functional theory for transition metals. <b>2005</b> , 122, 184108	30
1128	Water adsorption at metal surfaces: A first-principles study of the p(3B)R30° H <sub>2</sub> O bilayer on Ru(0001). <b>2005</b> , 71,	57

1127	FIRST PRINCIPLES CALCULATION OF THE ELECTRONIC AND STRUCTURAL PROPERTIES OF $USn_3$ USING LDA+U METHOD. <b>2005</b> , 19, 3049-3061	2
1126	High-pressure characteristics of $\beta\text{-Fe}_2\text{O}_3$ using DFT+U. <b>2005</b> , 78, 251-258	19
1125	Phase stability in heavy f-electron metals from first-principles theory. <b>2005</b> , 893, 1	1
1124	Influence of high pressure on the luminescence transitions of $Mn^{4+}$ -doped gadolinium gallium garnet. <b>2005</b> , 17, 7185-7197	48
1123	The performance of hybrid density functionals in solid state chemistry: the case of $BaTiO_3$ . <b>2005</b> , 103, 2483-2496	127
1122	Influence of the anion on lone pair formation in $Sn(II)$ monochalcogenides: a DFT study. <b>2005</b> , 109, 18868-75	149
1121	Band structures and optical spectra of $InN$ polymorphs: Influence of quasiparticle and excitonic effects. <b>2005</b> , 72,	102
1120	First-Principles Study of Bipolar Dopability in the $CuInO_2$ Transparent Semiconductor. <b>2005</b> , 17, 5529-5537	12
1119	Effective elastic constants in nonlinear elasticity. <b>2005</b> , 97, 103505	9
1118	Pressure-dependent photoluminescence study of $ZnO$ nanowires. <b>2005</b> , 86, 153117	80
1117	. <b>2005</b> ,	5
1116	Structural and magnetic phase transitions in simple oxides using hybrid functionals. <b>2005</b> , 31, 367-377	26
1115	Electronic Structure of Novel Carbon Allotrope, the Simple Cubic Fullerite SCF-C24 (Cubic Graphite) as Prospective Low-Dielectric Molecular Semiconductor. <b>2005</b> , 13, 415-426	3
1114	Full-potential LAPW electronic structure study of $\beta$ -plutonium and the (001) surface. <b>2005</b> , 72,	28
1113	First-Principles Study on the Elastic Properties of Platinum Nitride. <b>2005</b> , 22, 2637-2638	26
1112	Band structure and bulk modulus calculations of germanium carbide. <b>2005</b> , 20, 1101-1106	27
1111	Reduction of the (001) surface of $\gamma\text{-V}_2\text{O}_5$ compared to $\alpha\text{-V}_2\text{O}_5$ . <b>2005</b> , 109, 374-80	17
1110	Low-temperature polymorphs of $ZrO_2$ and $HfO_2$ : A density-functional theory study. <b>2005</b> , 72,	163



1109	Structural and electronic properties of the in situ impurity AsHg in Hg <sub>0.5</sub> Cd <sub>0.5</sub> Te: First-principles study. <b>2005</b> , 71,	17
1108	Effect of chemical bonding on the magnetic stability and magnetic moment in Mn-based binary compounds. <b>2005</b> , 72,	25
1107	Structural and electronic properties of the wide-gap Zn <sub>1-x</sub> Mg <sub>x</sub> S, Zn <sub>1-x</sub> Mg <sub>x</sub> Se and Zn <sub>1-x</sub> Mg <sub>x</sub> Te ternary alloys. <b>2005</b> , 17, 7077-7088	48
1106	Electronic and crystal structures of osmium under high pressure. <b>2005</b> , 72,	33
1105	First-principles investigation of electronic structure and magnetic properties in ferromagnetic Ga <sub>x</sub> Mn <sub>1-x</sub> N and Al <sub>x</sub> Mn <sub>1-x</sub> N. <b>2005</b> , 38, 1853-1859	29
1104	Ab initio all-electron periodic Hartree-Fock study of hydrostatic compression of pentaerythritol tetranitrate. <b>2005</b> , 109, 13668-75	13
1103	Ab initio calculations on the effects of additives on alumina phase stability. <b>2005</b> , 71,	22
1102	FP-LAPW investigation of electronic structure of TaN and TaC compounds. <b>2005</b> , 33, 175-183	69
1101	Local vibrational modes of Zn <sub>2</sub> As defects in GaAs, ZnSe and ZnTe. <b>2005</b> , 33, 145-147	2
1100	Implementation of a new model for pressure dependence of condensed phases in Thermo-Calc. <b>2005</b> , 29, 49-55	50
1099	Pressure-induced Superconductivity in Elemental Materials. <b>2005</b> , 74, 1345-1357	57
1098	Analytic potential energy functions for simulating aluminum nanoparticles. <b>2005</b> , 109, 3915-20	35
1097	Functional designed to include surface effects in self-consistent density functional theory. <b>2005</b> , 72,	457
1096	Shock properties of H <sub>2</sub> O ice. <b>2005</b> , 110, n/a-n/a	61
1095	Phase stability, phase transformations, and elastic properties of Cu <sub>6</sub> Sn <sub>5</sub> : Ab initio calculations and experimental results. <b>2005</b> , 20, 3102-3117	105
1094	Pressure-induced phase transition in ZnO and ZnO/MgO pseudobinary system: A first-principles lattice dynamics study. <b>2005</b> , 72,	91
1093	Thermodynamics of structural vacancies in titanium monoxide from first-principles calculations. <b>2005</b> , 71,	40
1092	Ab initio study of structural parameters and gap bowing in zinc-blende Al <sub>x</sub> Ga <sub>1-x</sub> N and Al <sub>x</sub> In <sub>1-x</sub> N alloys. <b>2005</b> , 98, 063710	23

1091	Influence of hydrostatic pressure on radiative transition probability of the intrashell 4f transitions in Yb <sup>3+</sup> ions in lithium niobate crystals. <b>2005</b> , 72,	16
1090	First-principles calculations of the electrical properties of LaAlO <sub>3</sub> and its interface with Si. <b>2005</b> , 72,	45
1089	Deformation potentials of the semimetal HgTe. <b>2005</b> , 71,	11
1088	Characterization of cathodic arc deposited titanium aluminium nitride films prepared using plasma immersion ion implantation. <b>2005</b> , 17, 2791-2800	6
1087	Ab initio calculations in the virtual-crystal approximation of the structural and the elastic properties of Be <sub>x</sub> Se <sub>1-x</sub> alloys under high pressure. <b>2005</b> , 13, 1153-1162	23
1086	Structure and properties of ilmenite from first principles. <b>2005</b> , 71,	82
1085	Structural phase transition of CeAuGe at high pressure. <b>2005</b> , 220,	11
1084	Nonequivalence of the generalized gradient approximations PBE and PW91. <b>2006</b> , 73,	96
1083	First principles study of gallium atom adsorption on the alpha-Al <sub>2</sub> O <sub>3</sub> (0001) surface. <b>2006</b> , 110, 9608-18	13
1082	Structural and electronic properties of III-V bismuth compounds. <b>2006</b> , 73,	133
1081	Structural properties of hexagonal boron nitride. <b>2006</b> , 14, 515-535	62
1080	Pressure dependence of vibrational, thermal, and elastic properties of ZnSe: An ab initio study. <b>2006</b> , 73,	37
1079	High-pressure studies of optical dephasing in polymer glasses. <b>2006</b> , 110, 227-33	
1078	Magnetism of close packed Fe <sub>147</sub> clusters. <b>2006</b> , 79, 701-707	4
1077	Pressure-induced phase transformations in the Ba <sub>8</sub> Si <sub>46</sub> clathrate. <b>2006</b> , 74,	23
1076	Valence band x-ray emission spectra of compressed germanium. <b>2006</b> , 96, 137402	9
1075	THE ELECTRONIC BAND STRUCTURE OF AlN, AlSb, AlAs AND THEIR TERNARY ALLOYS WITH In. <b>2006</b> , 20, 3199-3221	4
1074	Fermi surfaces and electronic structure of the Heusler alloy Co <sub>2</sub> TiSn. <b>2006</b> , 18, 2897-2903	15

1073	Electronic structure of the $\Gamma$ and $L$ phases of $\text{Bi}_2\text{O}_3$ : A combined ab initio and x-ray spectroscopy study. <b>2006</b> , 73,	168
1072	The p-type conduction mechanism in $\text{Cu}_2\text{O}$ : a first principles study. <b>2006</b> , 8, 5350-8	247
1071	Cubic $(\text{BN})_x\text{C}_2(1-x)$ ordered alloys: a first-principles study of the structural, electronic, and effective mass properties. <b>2006</b> , 18, 3509-3516	5
1070	Mechanism of the increase in bulk modulus of perovskite $\text{ScRh}_3\text{B}_x$ by vacancies. <b>2006</b> , 73,	17
1069	Optical properties of the filled tetrahedral semiconductors $\text{LiMgX}$ ( $X = \text{N}, \text{P}$ and $\text{As}$ ). <b>2006</b> , 18, 7237-7247	25
1068	First-principles study of ground- and excited-state properties of $\text{MgO}$ , $\text{ZnO}$ , and $\text{CdO}$ polymorphs. <b>2006</b> , 73,	325
1067	Density functional study of diamond epitaxy on the (111) and (100) surfaces of copper. <b>2006</b> , 15, 1201-1205	2
1066	Influence of pressure on the structural, dynamical, and electronic properties of the $\text{SnP}_2\text{S}_6$ layered crystal. <b>2006</b> , 73,	16
1065	Assessment of metageneralized gradient approximation and screened Coulomb hybrid density functionals on bulk actinide oxides. <b>2006</b> , 73,	146
1064	Stability of alkali-metal oxides as a function of pressure: Theoretical calculations. <b>2006</b> , 73,	40
1063	Laser ablation condensation of polymorphic $\text{ZrO}_2$ nanoparticles: Effects of laser parameters, residual stress, and kinetic phase change. <b>2006</b> , 99, 054302	14
1062	Crystalline, electronic, and magnetic structures of $\Gamma\text{Fe}_3\text{C}$ , $\Gamma\text{Fe}_5\text{C}_2$ , and $\Gamma\text{Fe}_2\text{C}$ from first principle calculation. <b>2006</b> , 99, 093508	113
1061	Structural, electronic and magnetic properties of $\text{Gd}$ investigated by DFT+U methods: bulk, clean and H-covered (0001) surfaces. <b>2006</b> , 18, 7021-7043	51
1060	The CALPHAD Method. <b>2006</b> , 1001-1030	2
1059	Characterization of the structural and electronic properties of crystalline lithium silicates. <b>2006</b> , 110, 22346-52	56
1058	Pressure-induced phase transitions in cobalt-filled multiwalled carbon nanotubes. <b>2006</b> , 73,	9
1057	Ferromagnetism in tetrahedrally coordinated compounds of I/II-V elements: Ab initio calculations. <b>2006</b> , 73,	141
1056	A theoretical and experimental study of the distorted pyrochlore $\text{Bi}_2\text{Sn}_2\text{O}_7$ . <b>2006</b> , 16, 3452	27

1055	Perturbation of adsorbed CO by amine derivatives coadsorbed on the gamma-Al <sub>2</sub> O <sub>3</sub> surface: FTIR and first principles studies. <b>2006</b> , 110, 4742-50	11
1054	Ground state properties and structural phase transition of beryllium chalcogenides. <b>2006</b> , 35, 423-431	78
1053	Ab initio simulation of diamond epitaxial growth on copper. <b>2006</b> , 36, 139-142	4
1052	First-principle study of structural, electronic and elastic properties of beryllium chalcogenides BeS, BeSe and BeTe. <b>2006</b> , 37, 292-299	71
1051	Murnaghan's equation of state for the electronic ground state energy. <b>2006</b> , 38, 350-353	92
1050	Energetics of phase transitions in BaO through DFT calculations with norm-conserving pseudopotentials: LDA vs. GGA results. <b>2006</b> , 37, 349-354	17
1049	Elastic, electronic and optical properties of ZnS, ZnSe and ZnTe under pressure. <b>2006</b> , 38, 29-38	230
1048	Ab initio study of structural, electronic, elastic and high pressure properties of barium chalcogenides. <b>2006</b> , 38, 263-270	97
1047	The calculation of ternary miscibility gaps using the linear contributions method: Problems, benchmark systems and an application to (K, Li, Na)Br. <b>2006</b> , 30, 185-190	3
1046	Magnetic instability within the series TCu <sub>3</sub> N (T=Pd, Rh, and Ru): A first-principles study. <b>2006</b> , 74,	29
1045	Screened hybrid density functionals applied to solids. <b>2006</b> , 124, 154709	1591
1044	Computation of densities, bulk moduli and glass transition temperatures of vinylic polymers from atomistic simulation. <b>2006</b> , 32, 1187-1193	34
1043	Distinct magnetic states of metastable fcc structured Fe and FeCu alloys studied by ab initio calculations. <b>2006</b> , 414, 36-41	21
1042	Valence behaviour of ytterbium in YbNiGa <sub>4</sub> . <b>2006</b> , 416, 35-42	14
1041	Influence of alloying on the thermodynamic stability of FeAl B2 phase. <b>2006</b> , 14, 1245-1251	12
1040	Density functional study of Zn <sub>1-x</sub> MgxSeyTe <sub>1-y</sub> quaternary semiconductor alloys. <b>2006</b> , 73,	41
1039	First-Principles Calculation of Point Defects in Uranium Dioxide. <b>2006</b> , 47, 2651-2657	88
1038	Alkali Metal Carbonates at High Pressure. <b>2006</b> , 632, 1437-1448	23

1037	Pressure-induced optoelectronic properties of InP nanocrystals: Tight-binding approach. <b>2006</b> , 3, 3832-3835	1
1036	FP-LAPW investigations of Zn <sub>1-x</sub> Bex S, Zn <sub>1-x</sub> Bex Se and Zn <sub>1-x</sub> Bex Te ternary alloys. <b>2006</b> , 243, 1296-1305	49
1035	Equation of state and high-pressure irreversible amorphization in Y <sub>3</sub> Fe <sub>5</sub> O <sub>12</sub> . <b>2006</b> , 83, 37-41	18
1034	Phase stability and cohesive properties of Ti <sub>1-x</sub> Zn intermetallics: First-principles calculations and experimental results. <b>2006</b> , 54, 4977-4997	83
1033	First-principles vibrational studies of pentaerythritol crystal under hydrostatic pressure. <b>2006</b> , 422, 397-401	14
1032	YNi <sub>4</sub> Cu: XPS measurements and electronic structure calculation. <b>2006</b> , 151, 1-3	
1031	Structural, electronic, elastic and high-pressure properties of some alkaline-earth chalcogenides: An ab initio study. <b>2006</b> , 371, 12-19	64
1030	First-principles study of structural and electronic properties of different phases of GaAs. <b>2006</b> , 373, 16-22	24
1029	Analysis of temperature dependence of thermal pressure and thermoelastic properties of MgO. <b>2006</b> , 373, 258-261	6
1028	First-principles calculations of elastic properties of LiBC. <b>2006</b> , 381, 139-143	18
1027	Diatomic substitutionals in superconducting Nb(1-x)B <sub>2</sub> . <b>2006</b> , 449, 1-8	6
1026	First-principles optical calculations of AsNMg <sub>3</sub> and SbNMg <sub>3</sub> . <b>2006</b> , 130, 101-107	39
1025	NbB <sub>2</sub> : a density functional study. <b>2006</b> , 350, 288-292	33
1024	Volume changes in <sup>238</sup> Plutonium from helium and other decay products. <b>2006</b> , 355, 21-29	11
1023	Structural and elastic properties of the filled tetrahedral semiconductors LiZnX (X=N, P, and As). <b>2006</b> , 67, 846-850	35
1022	Elastic properties and high-pressure behavior of MgAl <sub>2</sub> O <sub>4</sub> from ab initio calculations. <b>2006</b> , 67, 1477-1483	40
1021	High pressure study of structural and electronic properties of magnesium telluride. <b>2006</b> , 67, 1668-1673	10
1020	First-principles investigation of Mg(AlH <sub>4</sub> ) <sub>2</sub> complex hydride. <b>2006</b> , 159, 111-115	22

1019	Crystal structure and high-pressure properties of $\text{EMo}_2\text{N}$ determined by neutron powder diffraction and X-ray diffraction. <b>2006</b> , 179, 1762-1767	53
1018	Deposition and characterization of ternary thin films within the $\text{TiAlTi}$ system by DC magnetron sputtering. <b>2006</b> , 291, 290-300	187
1017	Equation of state of graphite-like BC. <b>2006</b> , 137, 268-271	22
1016	Superconducting $\text{NbB}_2$ : An ab initio study of elastic constants. <b>2006</b> , 137, 253-256	15
1015	Equation of state for group $\text{IVIV}$ semiconductors. <b>2006</b> , 139, 132-137	1
1014	Elastic and electronic properties of $\text{BeB}_2$ in comparison to superconducting $\text{MgB}_2$ and $\text{NbB}_2$ . <b>2006</b> , 139, 315-320	15
1013	Pressure induced phase transition in $\text{ZnS}$ . <b>2006</b> , 139, 246-249	56
1012	Pressure behaviour and thermal expansion of $\text{NiMnSb}$ from first principles calculations. <b>2006</b> , 140, 251-255	7
1011	Elastic and optical properties of $\text{BeS}$ , $\text{BeSe}$ and $\text{BeTe}$ under pressure. <b>2006</b> , 50, 1382-1388	63
1010	Structural phase stability and elastic properties of lanthanum monochalcogenides at high pressure. <b>2006</b> , 777, 5-10	43
1009	Fundamental state quantities and high-pressure phase transition in beryllium chalcogenides. <b>2006</b> , 18, 10365-75	33
1008	Advances in data reduction of high-pressure x-ray powder diffraction data from two-dimensional detectors: a case study of schafarikite ( $\text{FeSb}_2\text{O}_4$ ). <b>2006</b> , 18, S1021-37	10
1007	Electronic properties and bulk moduli of new boron nitride polymorphs, i.e., hyperdiamond $\text{B}_{12}\text{N}_{12}$ and simple cubic $\text{B}_{24}\text{N}_{24}$ , $\text{B}_{12}\text{N}_{12}$ fulborenites. <b>2006</b> , 40, 636-641	8
1006	Electronic structure and elastic moduli of the simple cubic fullerite $\text{C}_{24}$ a new allotropic carbon modification. <b>2006</b> , 48, 1405-1410	14
1005	The $5f$ localization/delocalization in square and hexagonal americium monolayers: a FP-LAPW electronic structure study. <b>2006</b> , 50, 497-503	12
1004	Magnetic properties, Mössbauer effect and first principle calculations study of laves phase $\text{HfFe}_2$ . <b>2006</b> , 50, 425-430	11
1003	Ab initio computation of low-temperature phase diagrams exhibiting miscibility gaps. <b>2006</b> , 8, 1778-84	39
1002	First-principles investigation of the structural, electronic and optical properties of olivine- $\text{Si}_3\text{N}_4$ and olivine- $\text{Ge}_3\text{N}_4$ . <b>2006</b> , 18, 10663-10676	10

1001	Atomistic calculations of structural and elastic properties of serpentine minerals: the case of lizardite. <b>2006</b> , 33, 266-275	43
1000	First-principles study on the structural, elastic and electronic properties of platinum carbide. <b>2006</b> , 381, 174-178	25
999	Adhesion at metal- $\text{TiO}_2$ interfaces. <b>2006</b> , 61, 303-344	156
998	Ab initio study of $\text{Ti}_3\text{Si}_0.5\text{Ge}_0.5\text{C}_2$ under pressure. <b>2006</b> , 67, 2149-2153	5
997	Ab initio calculations of elastic constants of the bcc V-Nb system at high pressures. <b>2006</b> , 67, 2056-2064	39
996	Electronic origin of elastic properties of titanium carbonitride alloys. <b>2006</b> , 37, 3391-3396	31
995	Composition-dependent band gap in $\text{ZnS}_x\text{Se}_{1-x}$ : a combined experimental and theoretical study. <b>2006</b> , 8, 44-49	49
994	Temperature dependence of volume expansion for solids. <b>2006</b> , 8, 573-576	6
993	Electronic structure of some mono-, semi-titanium boride and diboride. <b>2006</b> , 60, 1433-1436	15
992	Cohesive properties and energy band-gap of cubic $\text{Al}_x\text{Ga}_y\text{In}_{1-x-y}\text{N}$ quaternary alloys. <b>2006</b> , 74, 104-107	6
991	Electronic Structures of the Filled Tetrahedral Semiconductor $\text{Li}_3\text{AlN}_2$ . <b>2006</b> , 23, 186-188	3
990	Crystallographic properties of the $\text{MnGa}_2\text{Se}_4$ compound under high pressure. <b>2006</b> , 100, 093513	17
989	Orbital-corrected orbital-free density functional theory. <b>2006</b> , 124, 081107	16
988	Self-consistent embedding theory for locally correlated configuration interaction wave functions in condensed matter. <b>2006</b> , 125, 084102	112
987	Structural and thermodynamic properties of $\text{AlB}_2$ compound. <b>2006</b> , 15, 3014-3018	21
986	Prediction of unusual stable ordered structures of Au-Pd alloys via a first-principles cluster expansion. <b>2006</b> , 74,	66
985	Model of annealing-induced short-range order effects in $(\text{GaIn})_n(\text{NP})$ alloys. <b>2006</b> , 74,	8
984	Effects of Fe substitution on the electronic, transport, and magnetic properties of $\text{ZnGa}_2\text{O}_4$ : A systematic ab initio study. <b>2006</b> , 73,	31

983	Crystal structure of oligoacenes under high pressure. <b>2006</b> , 74,	52
982	Electronic structure and magnetic properties of cubic and hexagonal SrMnO <sub>3</sub> . <b>2006</b> , 74,	130
981	Theoretical study of the molecular and electronic structure of one-dimensional crystals of potassium iodide and composites formed upon intercalation in single-walled carbon nanotubes. <b>2006</b> , 73,	35
980	Electronic structure and magnetic coupling in FeSbO <sub>4</sub> : A DFT study using hybrid functionals and GGA+U methods. <b>2006</b> , 73,	37
979	General trend of the mechanical properties of the ternary carbides M <sub>3</sub> SiC <sub>2</sub> (M=transition metal). <b>2006</b> , 74,	42
978	Electron correlation, reference states and empirical potentials. <b>2006</b> , 86, 2683-2711	16
977	Mechanical stability of possible structures of PtN investigated using first-principles calculations. <b>2006</b> , 73,	149
976	Lattice dynamics of metal-organic frameworks: Neutron inelastic scattering and first-principles calculations. <b>2006</b> , 74,	66
975	Relaxations and bonding mechanism in Hg <sub>1-x</sub> CdxTe with mercury vacancy defect: First-principles study. <b>2006</b> , 73,	15
974	Density-functional-theory calculations for the silicon vacancy. <b>2006</b> , 74,	56
973	Ab initio study of CsI and its surface. <b>2006</b> , 74,	12
972	Structural and electronic properties of OsB <sub>2</sub> : A hard metallic material. <b>2006</b> , 74,	62
971	Coarse-grained model for a molecular crystal. <b>2006</b> , 89, 021919	14
970	Phase transition and electronic properties of fluorene: A joint experimental and theoretical high-pressure study. <b>2006</b> , 73,	24
969	Photoluminescence of wurtzite ZnO under hydrostatic pressure. <b>2006</b> , 99, 066102	19
968	First-principles electronic structure study of Sc-II. <b>2006</b> , 74,	18
967	Pressure dependence of exchange interactions in NiO. <b>2006</b> , 74,	34
966	PRESS-INDUCED PHASE TRANSITIONS OF KNbO <sub>3</sub> STUDIED FROM THE FIRST PRINCIPLE CALCULATION. <b>2006</b> , 20, 557-564	3



965	PRESSURE DEPENDENCE OF OPTO-ELECTRONIC PROPERTIES IN ZnS <sub>x</sub> Se <sub>1-x</sub> . <b>2006</b> , 20, 4807-4820	6
964	Fermi surface nesting and pre-martensitic softening in V and Nb at high pressures. <b>2006</b> , 18, 5079-5085	62
963	Structural distortion and electronic properties of NiO under high pressure: an ab initio GGA+U study. <b>2006</b> , 18, 9691-9701	8
962	THE ELECTRONIC BAND STRUCTURE OF GaN, GaAs AND In <sub>x</sub> Ga <sub>1-x</sub> As <sub>1-y</sub> N <sub>y</sub> ALLOYS. <b>2007</b> , 21, 4357-4375	2
961	BAND STRUCTURE, METALLIZATION, AND SUPERCONDUCTIVITY OF GaAs AND InAs UNDER HIGH PRESSURE. <b>2007</b> , 06, 833-843	3
960	Pressure-induced phase transitions in nanocrystalline ReO <sub>3</sub> . <b>2007</b> , 19, 4362-14	14
959	Prediction of MAX phases, VN <sub>1</sub> SiCN (N=1,2), from first-principles theory. <b>2007</b> , 101, 0135-11	14
958	Ab initio prediction of the low-temperature phase diagrams in the systems KBr-NaBr, KX-RbX, and LiX-RbX (X=Cl,Br). <b>2007</b> , 126, 1245-08	16
957	Brillouin-scattering determination of the acoustic properties and their pressure dependence for three polymeric elastomers. <b>2007</b> , 127, 1049-06	48
956	Effect of the Excess Volume of Lattice Defects on the Enthalpy of Formation and Desorption Temperature of Metal Hydrides. <b>2007</b> , 45	
955	Range separated hybrid density functional with long-range Hartree-Fock exchange applied to solids. <b>2007</b> , 127, 0541-01	86
954	Achieving plane wave accuracy in linear-scaling density functional theory applied to periodic systems: a case study on crystalline silicon. <b>2007</b> , 127, 1647-12	43
953	High pressure study of ZnSe:Cr <sup>2+</sup> crystals: the origin of the 1.25 eV luminescence. <b>2007</b> , 19, 0962-13	4
952	Ab initio studies of structural, elastic, and electronic properties of RRh <sub>3</sub> BX (R=Sc, Y, La, and Ce). <b>2007</b> , 91, 0819-01	14
951	First-principles calculations of the elastic, electronic, and optical properties of the filled skutterudites CeFe <sub>4</sub> P <sub>12</sub> and ThFe <sub>4</sub> P <sub>12</sub> . <b>2007</b> , 75,	62
950	Structural, magnetic, and electronic properties of the Co-Fe-Al oxide spinel system: Density-functional theory calculations. <b>2007</b> , 76,	134
949	Polygonization and anomalous graphene interlayer spacing of multi-walled carbon nanofibers. <b>2007</b> , 75,	22
948	Role of carbon in AlCNi <sub>3</sub> and GaCNi <sub>3</sub> : A density functional theory study. <b>2007</b> , 75,	34

947	Theoretical study of doped $Tl_2Mn_2O_7$ and $Tl_2Mn_2O_7$ under pressure. <b>2007</b> , 75,	1
946	Effect of Zr on the properties of $(TiZr)Ni$ alloys from first-principles calculations. <b>2007</b> , 76,	41
945	Bulk and nanoscale GaN: Role of Gad states. <b>2007</b> , 76,	9
944	Magnetic properties of CrSb: A first-principle study. <b>2007</b> , 101, 093912	29
943	Search for superconductivity in LiBC at high pressure: Diamond anvil cell experiments and first-principles calculations. <b>2007</b> , 75,	21
942	Semiempirical pressure-volume-temperature equation of state: $MgSiO_3$ perovskite is an example. <b>2007</b> , 102, 123506	7
941	Mechanical strengths of silicon nitrides studied by ab initio calculations. <b>2007</b> , 90, 191903	52
940	Optical properties of PbSe nanocrystal quantum dots under pressure. <b>2007</b> , 90, 043110	25
939	Implementation of ultrasoft pseudopotentials in large-scale grid-based electronic structure calculations. <b>2007</b> , 76,	19
938	Structural and electronic properties of p-doped silicon clathrates. <b>2007</b> , 75,	31
937	The temperature dependence of the isothermal bulk modulus at 1bar pressure. <b>2007</b> , 101, 023514	59
936	Low-temperature acoustic properties and quasiharmonic analysis for Cu-based bulk metallic glasses. <b>2007</b> , 76,	24
935	Pressure dependence of the charge-density-wave gap in rare-earth tritellurides. <b>2007</b> , 98, 026401	48
934	First-principles study of pressure-induced metal-insulator transition in $BiNiO_3$ . <b>2007</b> , 91, 101901	26
933	Cubic phases of BC2N: A first-principles study. <b>2007</b> , 75,	40
932	Lattice expansion, stability, and Mn solubility in substitutionally Mn-doped GaAs. <b>2007</b> , 75,	19
931	Theory of InP nanocrystals under pressure. <b>2007</b> , 75,	20
930	Electronic structure and transport properties of doped CoSi single crystal. <b>2007</b> , 101, 033715	31

929	Metallic state in cubic FeGe beyond its quantum phase transition. <b>2007</b> , 98, 047204	56
928	First principles studies of ideal strength and bonding nature of AlN polymorphs in comparison to TiN. <b>2007</b> , 91, 031906	62
927	B3LYP density functional calculations on the ground-state structure, elastic properties, and compression mechanism of $\text{ErW}_2\text{O}_8$ . <b>2007</b> , 75,	13
926	THEORETICAL INVESTIGATION OF THE ELASTIC PROPERTIES AND LATTICE DYNAMICS OF THE $\text{MgS}_x\text{Se}_{1-x}$ ALLOY. <b>2007</b> , 21, 249-259	13
925	Probability of $\text{Yb}^{3+} 4f^14f$ transitions in gadolinium gallium garnet crystals at high hydrostatic pressures. <b>2007</b> , 75,	21
924	Theoretical study of stability and electronic structure of $\text{Li}(\text{Mg,Zn})\text{N}$ alloys: A candidate for solid state lighting. <b>2007</b> , 76,	18
923	Structure and mechanical stability of molybdenum nitrides: A first-principles study. <b>2007</b> , 76,	56
922	First Principles Study of $\text{Al}(100)$ Twisted Interfaces. <b>2007</b> , 129, 131-136	0
921	Determination of symmetry reduced structures by a soft-phonon analysis in $\text{Ni}_2\text{MnGa}$ . <b>2007</b> , 1050, 1	1
920	Electronic and optical properties of zincblende AlN, GaN and InN compounds under pressure. <b>2007</b> , 75, 414-418	13
919	Electronic excitations: Ab initio calculations of electronic spectra and application to zirconia $\text{ZrO}_2$ , titania $\text{TiO}_2$ and cuprous oxide $\text{Cu}_2\text{O}$ . <b>2007</b> , 38, 482-493	16
918	Ab initio study of structural and electronic properties of III-arsenide binary compounds. <b>2007</b> , 39, 580-586	78
917	Electronic structure and transport properties of $\text{Co}(\text{Si}_{1-x}\text{M}_x)$ ( $\text{M} = \text{Al, P}$ ): First-principles study. <b>2007</b> , 39, 752-758	10
916	Atomistic study of structural, elastic, electronic and thermal properties of perovskites $\text{Ba}(\text{Ti,Zr,Nb})\text{O}_3$ . <b>2007</b> , 39, 896-902	36
915	Ab-initio calculation of electronic structure and electric field gradients in $\text{HfAl}_2$ and $\text{ZrAl}_2$ Laves phases. <b>2007</b> , 41, 164-167	9
914	Thermodynamic models for crystalline phases. Composition dependent models for volume, bulk modulus and thermal expansion. <b>2007</b> , 31, 28-37	42
913	Introduction of pressure in binary phase diagram calculations. Application to the $\text{AgCu}$ system. <b>2007</b> , 31, 380-389	16
912	Structural and electronic properties of lead chalcogenides from first principles. <b>2007</b> , 75,	166

911	Electronic structure, equilibrium and magnetic properties of Ni <sub>2</sub> MnGe: Ab initio study. <b>2007</b> , 427, 54-60	22
910	First-principles investigation of wide-gap quaternary alloys Zn <sub>1-x</sub> Mg <sub>x</sub> SyTe <sub>1-y</sub> . <b>2007</b> , 433, 306-312	9
909	Bonding and stability of the intermetallic compounds of hafnium with Ti <sub>2</sub> Ni structure. <b>2007</b> , 442, 252-254	9
908	Structural distortion of $\alpha$ -structured MnO and FeO. <b>2007</b> , 142, 6-9	18
907	Young's modulus as a function of composition for an n-type lead-antimony-silver-telluride (LAST) thermoelectric material. <b>2007</b> , 87, 4907-4934	27
906	Mechanical properties of cubic zinc carboxylate IRMOF-1 metal-organic framework crystals. <b>2007</b> , 76,	103
905	Raman and x-ray diffraction studies of Ba doped germanium clathrate Ba <sub>8</sub> Ge <sub>43</sub> at high pressures. <b>2007</b> , 101, 063549	18
904	Interaction potential for silicon carbide: A molecular dynamics study of elastic constants and vibrational density of states for crystalline and amorphous silicon carbide. <b>2007</b> , 101, 103515	208
903	Atomic and electronic structures of 4d transition-metal nitrides. <b>2007</b> , 75,	47
902	Structural and vibrational properties of the 6H diamond: First-principles study. <b>2007</b> , 16, 21-28	16
901	Structural, electronic and thermodynamic properties of magnesium chalcogenide ternary alloys. <b>2007</b> , 19, 386234	16
900	First-principles study of the structural, electronic, and elastic properties of RRh <sub>3</sub> BxC <sub>1-x</sub> (R=Sc and Y). <b>2007</b> , 76,	21
899	Origin of the hardness enhancement in superhard nc-TiN/a-Si <sub>3</sub> N <sub>4</sub> and ultrahard nc-TiN/a-Si <sub>3</sub> N <sub>4</sub> /TiSi <sub>2</sub> nanocomposites. <b>2007</b> , 87, 955-966	58
898	Ab Initio Study for Site Symmetry of Phosphorus-Doped Diamond. <b>2007</b> , 46, 315-317	8
897	Structural, electronic and optical properties of spinel oxides: cadmium gallate and cadmium indiate. <b>2007</b> , 38, 203-210	16
896	Route to a correct description of the fundamental properties of cubic InN. <b>2007</b> , 91, 182105	13
895	Electronic structure and magnetism of EuTiO(3): a first-principles study. <b>2007</b> , 19, 406217	53
894	Melting curve of tantalum from first principles. <b>2007</b> , 75,	94

893	CaCl <sub>2</sub> -type high-pressure phase of magnesium hydride predicted by ab initio phonon calculations. <b>2007</b> , 75,	33
892	The broken-symmetry phase of solid hydrogen: evidence from infrared and Raman active vibrons. <b>2007</b> , 19, 425237	6
891	Superconductivity and lattice instability in face-centered cubic lanthanum under high pressure. <b>2007</b> , 19, 425234	11
890	A first-principles study of electron-phonon coupling in electron-doped LiH. <b>2007</b> , 19, 425218	11
889	Energetics and kinetics of vacancy diffusion and aggregation in shocked aluminium via orbital-free density functional theory. <b>2007</b> , 9, 4951-66	57
888	Computational and Experimental Investigation of the Transformation of V <sub>2</sub> O <sub>5</sub> Under Pressure. <b>2007</b> , 19, 5262-5271	42
887	Ab initio study of the half-metal to metal transition in strained magnetite. <b>2007</b> , 9, 5-5	48
886	First-principles investigation of electronic and structural properties and bowing parameters in SrFCl <sub>x</sub> Br <sub>1-x</sub> alloy. <b>2007</b> , 19, 436213	2
885	Equation of State, Thermal Expansion Coefficient, and Isothermal Compressibility for Ices Ih, II, III, V, and VI, as Obtained from Computer Simulation. <b>2007</b> , 111, 15877-15888	35
884	High-pressure studies of cyclohexane to 40 GPa. <b>2007</b> , 111, 4103-8	30
883	Experimental and Atomistic Simulation Study of the Structural and Adsorption Properties of Faujasite Zeolite-Templated Nanostructured Carbon Materials. <b>2007</b> , 111, 15863-15876	48
882	Adsorption and Decomposition Pathways of Vinyl Phosphonic and Ethanoic Acids on the Al(111) Surface: a Density Functional Analysis. <b>2007</b> , 111, 7366-7375	10
881	Polymorphism in Bismuth Stannate: A First-Principles Study. <b>2007</b> , 19, 5158-5164	40
880	Adsorption of Al, O, Hf, Y, Pt, and S Atoms on $\alpha$ -Al <sub>2</sub> O <sub>3</sub> (0001). <b>2007</b> , 111, 7105-7126	92
879	Structural stability of thallium <sup>IV</sup> compounds. <b>2007</b> , 19, 106221	30
878	Half-metallic ferromagnetism in zinc-blende CaC, SrC, and BaC from first principles. <b>2007</b> , 75,	253
877	The effects of pressure on the electronic, transport and dynamical properties of AuX <sub>2</sub> (X = Al, Ga and In). <b>2007</b> , 19, 425224	14
876	Elastic Properties of Rutile TiO <sub>2</sub> at High Temperature. <b>2007</b> , 24, 2642-2645	14

875	Band-structure anomalies of the chalcopyrite semiconductors CuGaX <sub>2</sub> versus AgGaX <sub>2</sub> (X=S and Se) and their alloys. <b>2007</b> , 75,	111
874	Experimental and theoretical study of the electronic structures of $\text{PbO}$ and $\text{PbO}_2$ . <b>2007</b> , 17, 267-277	92
873	Structural, elastic and electronic properties of metastable diamond-like Ti, Fe and Zn monocarbides: Density functional-based tight binding calculations. <b>2007</b> , 16, 243-247	2
872	Probing the sp <sup>2</sup> dependence of elastic moduli in ultrahard diamond films. <b>2007</b> , 16, 1643-1647	13
871	Simulations on the elastic response of amorphous and nanocomposite carbon. <b>2007</b> , 16, 1676-1681	2
870	Ab initio study of the thermodynamic properties of nonmagnetic elementary fcc metals: Exchange-correlation-related error bars and chemical trends. <b>2007</b> , 76,	184
869	Ab initio computation of the low-temperature phase diagrams of the alkali metal iodide-bromides: $\text{MBr}(x)\text{I}_{1-x}$ (0 . <b>2007</b> , 111, 3943-52	14
868	Phonon and elastic instabilities in rocksalt alkali hydrides under pressure: First-principles study. <b>2007</b> , 75,	37
867	Density functional study of the actinide nitrides. <b>2007</b> , 76,	82
866	Why does the B3LYP hybrid functional fail for metals?. <b>2007</b> , 127, 024103	424
865	Surface Sensitivity in Lithium-Doping of MgO: A Density Functional Theory Study with Correction for on-Site Coulomb Interactions. <b>2007</b> , 111, 7971-7979	91
864	The role of the phonon anomaly in the superconductivity of vanadium and selenium under high pressures. <b>2007</b> , 19, 125206	13
863	Magnetic and structural properties of FeCr alloys. <b>2007</b> , 99, 237201	46
862	Possible existence of alkali metal orthocarbonates at high pressure. <b>2007</b> , 13, 7330-48	30
861	Pressure-induced structural phase transition in rare-earth trihydrides. Part III. Systematics: General and geometric approach. <b>2007</b> , 141, 354-358	28
860	Ground state structures in the polonium based $\text{IIIV}$ compounds. <b>2007</b> , 141, 523-528	8
859	Ab initio determination of crystal lattice constants and thermal expansion for germanium isotopes. <b>2007</b> , 143, 161-165	31
858	Electronic properties of the A-15 Nb-based intermetallics $\text{Nb}_3(\text{Os}, \text{Ir}, \text{Pt}, \text{Au})$ . <b>2007</b> , 144, 352-356	7

857	Theoretical study of phase separation in Cd <sub>1-x</sub> Zn <sub>x</sub> O alloys. <b>2007</b> , 144, 5-9	11
856	First-principles calculations of structural properties of GaN : V. <b>2007</b> , 144, 109-113	9
855	SixC <sub>1-x</sub> O <sub>2</sub> alloys: A possible route to stabilize carbon-based silica-like solids?. <b>2007</b> , 144, 273-276	14
854	Optical properties of alkaline-earth fluorohalides BaFX (X=Cl, Br, I) compounds. <b>2007</b> , 51, 1133-1138	6
853	Structural investigations of -FeGe at high pressure and low temperature. <b>2007</b> , 8, 416-419	15
852	Magnetic ordering of Vn/Mo(001) systems: Ab-initio calculations. <b>2007</b> , 601, 4944-4952	3
851	Structural and electronic properties calculations of BexZn <sub>1-x</sub> Se alloy. <b>2007</b> , 10, 6-13	20
850	Electronic and structural properties of zincblende AlxIn <sub>1-x</sub> N. <b>2007</b> , 274, 361-365	11
849	Electronic structure and electric field gradient calculations for Hf <sub>2</sub> Rh intermetallic compound. <b>2007</b> , 462, 294-296	3
848	Equation of state and thermal expansivity of NaCl under high pressure and high temperature. <b>2007</b> , 387, 352-357	13
847	Structural and elastic properties of AlB <sub>2</sub> compound via first-principles calculations. <b>2007</b> , 388, 213-218	19
846	Ab initio investigations of zinc chalcogenides semiconductor alloys. <b>2007</b> , 391, 363-370	26
845	Analysis of temperature and isobaric volume expansion dependence of elastic moduli of solids. <b>2007</b> , 393, 255-258	1
844	Theoretical study of FCC/HCP phase coexistence and phase stability in Al by FP-LAPW method with GGA for exchange and correlation. <b>2007</b> , 393, 278-284	15
843	PbSe vs. CdSe: Thermodynamic properties and pressure dependence of the band gap. <b>2007</b> , 394, 1-7	23
842	Electronic and structural properties of Sr <sub>2</sub> YSbO <sub>6</sub> . <b>2007</b> , 398, 248-251	21
841	First-principles calculations of structural properties of Sc <sub>1-x</sub> In <sub>x</sub> N compound. <b>2007</b> , 398, 385-388	2
840	First principles study of structural and electronic properties of different phases of boron nitride. <b>2007</b> , 400, 297-306	35

839	Structural property of platinum mononitride. <b>2007</b> , 399, 50-54	11
838	Ab initio study on structure and phase transition of A- and B-type rare-earth sesquioxides Ln <sub>2</sub> O <sub>3</sub> (Ln=La, Pr, Y, and Sc) based on density function theory. <b>2007</b> , 180, 3280-3287	86
837	Investigation of structural stability and electronic properties of CuN, AgN and AuN by first principles calculations. <b>2007</b> , 362, 73-83	24
836	First principle study on phase stability and electronic structure of YCu. <b>2007</b> , 368, 495-498	31
835	Nephelauxetic effect in high-pressure luminescence of transition-metal ion dopants. <b>2007</b> , 125, 266-270	5
834	Mercury telluride crystals encapsulated within single walled carbon nanotubes: A density functional study. <b>2007</b> , 108, 797-807	13
833	Effect of hydrogen on electronic structure of fcc iron in relation to hydrogen embrittlement of austenitic steels. <b>2007</b> , 204, 4249-4258	24
832	Semiempirical LUC-INDO calculations on the effect of pressure on the electronic structure of diamond. <b>2007</b> , 244, 1304-1317	10
831	Raman study of nano-crystalline Ge under high pressure. <b>2007</b> , 244, 1376-1380	11
830	Ab-initio investigation of structural, electronic and optical properties for three phases of ZnO compound. <b>2007</b> , 244, 3154-3167	77
829	High-pressure behavior of Ni-filled and Fe-filled multiwalled carbon nanotubes. <b>2007</b> , 244, 3612-3619	12
828	Lattice dynamics of CuAlO <sub>2</sub> under high pressure from ab initio calculations. <b>2007</b> , 244, 342-346	12
827	Effect of pressure on the structural properties and electronic band structure of GaSe. <b>2007</b> , 244, 244-255	28
826	High-pressure properties and phase diagram of boron. <b>2007</b> , 244, 303-308	34
825	Structural properties of ZnO polymorphs. <b>2007</b> , 244, 1538-1543	16
824	On the Occurrence of (Mg, Fe)SiO <sub>3</sub> in the Lower Mantle. <b>2007</b> , 42, 993-1009	44
823	Dependence of structural properties of ZnO on high pressure. <b>2007</b> , 106, 11-15	25
822	Structural and electronic properties of Zn <sub>1-x</sub> Mg <sub>x</sub> Se <sub>1-y</sub> S <sub>y</sub> alloys. <b>2007</b> , 61, 1178-1182	12



821	Electronic structure and energies of interatomic bonds in the TiSi <sub>2</sub> compound with a C49 crystal structure. <b>2007</b> , 49, 39-45	4
820	A New Class of Supramolecular Wires. <b>2007</b> , 111, 18912-18916	11
819	Simulations of the mechanical properties of crystalline, nanocrystalline, and amorphous SiC and Si. <b>2007</b> , 75,	68
818	Ab initio study of the structural and elastic properties of spinels MgX <sub>2</sub> O <sub>4</sub> (X = Al, Ga, In) under pressure. <b>2007</b> , 56, 1-5	35
817	Quantum size effects on the (0001) surface of double hexagonal close packed americium. <b>2007</b> , 55, 13-22	5
816	First-principles study of the optical properties of PbFX (X = Cl, Br, I) compounds in its matlockite-type structure. <b>2007</b> , 60, 463-468	26
815	Beyond a Hartree-Fock description of crystalline solids: the case of lithium hydride. <b>2007</b> , 117, 781-791	29
814	Electronic and structural properties of zincblende Al <sub>x</sub> Ga <sub>1-x</sub> N. <b>2007</b> , 86, 539-543	7
813	Tuning catalytic properties of bimetallic surfaces: Oxygen adsorption on pseudomorphic Pt/Ru overlayers. <b>2007</b> , 52, 2219-2228	85
812	An Eulerian-Lagrangian approach for simulating explosions of energetic devices. <b>2007</b> , 85, 660-674	78
811	Electronic band structure of thorium hydrides: ThH <sub>2</sub> and Th <sub>4</sub> H <sub>15</sub> . <b>2007</b> , 389, 296-301	19
810	Ab initio study of structural and electronic properties of BiAlO <sub>3</sub> and BiGaO <sub>3</sub> . <b>2007</b> , 390, 96-100	46
809	Electronic structures and shape-memory behavior of Ti <sub>50</sub> Ni <sub>50-x</sub> Cu <sub>x</sub> (x=0, 6.25, 12.5, 18.75 and 25.0at%) by density functional theory. <b>2007</b> , 393, 18-23	16
808	Structural and electronic properties of the A-15 compounds and. <b>2007</b> , 393, 105-109	7
807	Ab initio study of structural phase stability and elastic properties of ScSb and YSb under pressure effect. <b>2007</b> , 362, 476-479	46
806	Electronic structure of half-Heusler semiconductor LiBeN. <b>2007</b> , 367, 389-393	13
805	Pressure effect on the optical properties of the filled tetrahedral semiconductors LiZnX. <b>2007</b> , 68, 2286-2292	13
804	Structural change of layered perovskite La <sub>2</sub> Ti <sub>2</sub> O <sub>7</sub> at high pressures. <b>2007</b> , 180, 571-576	34

803	First-principles prediction of coexistence of magnetism and ferroelectricity in rhombohedral Bi <sub>2</sub> FeTiO <sub>6</sub> . <b>2008</b> , 372, 1904-1909	19
802	First-principle study of extrinsic defects in CuScO <sub>2</sub> and CuYO <sub>2</sub> . <b>2008</b> , 372, 3759-3762	11
801	Structural and dynamical properties of Ru(0001) surface. <b>2008</b> , 602, 3654-3659	7
800	The electronic band structure of InN, InAs and InSb compounds. <b>2008</b> , 43, 2935-2946	10
799	Improved wood-kirkwood detonation chemical kinetics. <b>2008</b> , 120, 37-43	3
798	Effect of Ternary Additions on the Stability of Ordered Phases in Ni-Mo Alloys—Transmission Electron Microscopy Results and First Principles Calculations. <b>2008</b> , 39, 1623-1629	9
797	Hydrostatic Compression Curve for Triamino-Trinitrobenzene Determined to 13.0 GPa with Powder X-Ray Diffraction. <b>2008</b> , 33, 286-295	77
796	First principles study of structural and electronic properties of Bex Zn <sub>1-x</sub> S and Bex Zn <sub>1-x</sub> Te alloys. <b>2008</b> , 245, 106-113	24
795	Structural, electronic and optical properties of IIIV <sub>2</sub> compounds (II = Be, Zn; IV = Si, Ge). <b>2008</b> , 245, 142-148	26
794	Structural, electronic and optical properties of lead zirconate. <b>2008</b> , 245, 2572-2580	8
793	Structural, electronic and optical properties of spinel MgAl <sub>2</sub> O <sub>4</sub> oxide. <b>2008</b> , 245, 2800-2807	73
792	Error propagation in multiscale approaches to the elasticity of polycrystals. <b>2008</b> , 245, 2636-2641	14
791	HP-Ca <sub>2</sub> Si <sub>5</sub> N <sub>8</sub> —a new high-pressure nitridosilicate: synthesis, structure, luminescence, and DFT calculations. <b>2008</b> , 14, 7892-902	31
790	Ab initio studies on Li <sub>4+x</sub> Ti <sub>5</sub> O <sub>12</sub> compounds as anode materials for lithium-ion batteries. <b>2008</b> , 9, 2104-8	95
789	First-principles lattice dynamics calculations of the phase boundary between beta-Si <sub>3</sub> N <sub>4</sub> and gamma-Si <sub>3</sub> N <sub>4</sub> at elevated temperatures and pressures. <b>2008</b> , 29, 2255-9	27
788	A 3D network of four-bonded germanium: a link between open and dense. <b>2008</b> , 47, 6790-3	30
787	Ein 3D-Netzwerk des vierbindigen Germaniums als Bindeglied zwischen offenen und dichten Elementstrukturen. <b>2008</b> , 120, 6895-6898	2
786	Ab initio investigation of phase separation in Ca <sub>1-x</sub> Zn <sub>x</sub> O alloys. <b>2008</b> , 372, 1910-1914	29

785	p-type doping of GaInNAs quaternary alloys. <b>2008</b> , 373, 165-168	6
784	Influence of Zr concentration on crystalline structure and its electronic properties in the new $Zr_xAl_{1-x}N$ compound in wurtzite phase: An ab initio study. <b>2008</b> , 39, 579-581	2
783	: New material. A DFT study. <b>2008</b> , 39, 563-565	1
782	Pressure-induced metal-insulator transition in. <b>2008</b> , 403, 1639-1641	9
781	Ab initio calculation of elastic properties of rock-salt and zinc-blend MgS under pressure. <b>2008</b> , 403, 1996-1999	27
780	Theoretical study of melting curves on Ta, Mo, and W at high pressures. <b>2008</b> , 403, 2065-2070	13
779	An ab initio study of possible pathways in the thermal decomposition of $NaAlH_4$ . <b>2008</b> , 181, 3037-3043	9
778	Structural and magnetic properties of double-perovskite $Ba_2MnMoO_6$ by density functional theory. <b>2008</b> , 320, e85-e87	15
777	Ab initio study of cubic complex $Bi_2CrCuO_6$ perovskite. <b>2008</b> , 320, e111-e113	3
776	Electronic and magnetic properties and their response to pressure in $Ni_2MnB$ . <b>2008</b> , 320, 2083-2088	10
775	Structural and electronic properties of rock salt phase of ZnO under compression. <b>2008</b> , 69, 1676-1683	13
774	Electronic and optical properties of the antifluorite semiconductors $Be_2C$ and $Mg_2X$ (, Si, Ge) under hydrostatic pressure. <b>2008</b> , 69, 1775-1781	36
773	Theoretical study of ground state and high-pressure phase of platinum carbide. <b>2008</b> , 69, 2907-2910	16
772	First principles study of barium chalcogenides. <b>2008</b> , 69, 2924-2927	36
771	$MgB_2$ under pressure and plane strain: a DFT study. <b>2008</b> , 179, 385-390	2
770	First-principles calculations of the palladium(II) acetylacetonate crystal structure. <b>2008</b> , 465, 63-66	5
769	Electron energy-loss spectroscopy and first-principles calculation studies on a $NiTi$ shape memory alloy. <b>2008</b> , 56, 395-404	22
768	Phase stabilities and thermal decomposition in the $Zr_{1-x}Al_xN$ system studied by ab initio calculation and thermodynamic modeling. <b>2008</b> , 56, 968-976	69

- 767 The effect of platinum on defect formation energies in  $\beta$ -NiAl. **2008**, 56, 3502-3510 30
- 766 Stability of TiBN solid solutions and the formation of nc-TiN/a-BN nanocomposites studied by combined ab initio and thermodynamic calculations. **2008**, 56, 4440-4449 38
- 765 Lattice stability, elastic constants and macroscopic moduli of NiTi martensites from first principles. **2008**, 56, 6232-6245 174
- 764 First-principles study of the pressure-induced rutile  $\rightarrow$   $\alpha$ -Cl<sub>2</sub> phase transition in MgF<sub>2</sub>. **2008**, 145, 283-287 20
- 763 Electronic structures, lattice dynamics, and electron-phonon coupling of simple cubic Ca under pressure. **2008**, 146, 181-185 35
- 762 First principles study of the elastic properties in X<sub>2</sub>S (X=Li, Na, K and Rb) compounds under pressure effect. **2008**, 147, 178-182 22
- 761 Elasticity properties of the low-compressible material ReB<sub>2</sub>. **2008**, 147, 301-304 29
- 760 Equation of state of hexagonal boron nitride. **2008**, 148, 390-394 23
- 759 Pressure induced, electronic and optical properties of zincblende InP. **2008**, 52, 749-755 7
- 758 Phase stabilities of self-organized nc-TiN/a-Si<sub>3</sub>N<sub>4</sub> nanocomposites and of Ti<sub>1-x</sub>Si<sub>x</sub>Ny solid solutions studied by ab initio calculation and thermodynamic modeling. **2008**, 516, 2264-2275 65
- 757 Thermal stability, microstructure and mechanical properties of Ti<sub>1-x</sub>Zr<sub>x</sub>N thin films. **2008**, 516, 6421-6431 71
- 756 Defects in Cu<sub>2</sub>O, CuAlO<sub>2</sub> and SrCu<sub>2</sub>O<sub>2</sub> transparent conducting oxides. **2008**, 516, 8130-8135 49
- 755 Phase stability in substitutionally Mn-doped GaAs: Role of lattice constraint. **2008**, 254, 7855-7857 1
- 754 Optical properties of the alkaline-earth fluorohalides matlockite-type structure SrFX (X=Cl, Br, I) compounds. **2008**, 403, 711-716 11
- 753 First-principles study of the structural and electronic properties of III-phosphides. **2008**, 403, 1876-1881 86
- 752 Ab initio calculations of elastic modulus and electronic structures of cubic. **2008**, 403, 2624-2628 26
- 751 Calculated structural, electronic and optical properties of Ga-based semiconductors under pressure. **2008**, 403, 3077-3088 15
- 750 First-principles study of pressure-induced phase transition in silicon carbide. **2008**, 403, 3543-3546 36

- 749 An ab initio study of the adsorption and dissociation of molecular oxygen on the (0 0 0 1) surface of double hexagonal close-packed americium. **2008**, 403, 4269-4280 7
- 748 Deriving linear isotherms for solids. **2008**, 271, 94-102 11
- 747 First principle calculation for structural properties and bowing parameter in Ga<sub>1-x</sub>Mn<sub>x</sub>N materials. **2008**, 11, 37-43 2
- 746 Impact of nanostructuring on the enthalpy of formation of metal hydrides. **2008**, 33, 4122-4131 97
- 745 Temperature dependence of the enthalpy of formation of metal hydrides characterized by an excess volume. **2008**, 33, 5617-5628 16
- 744 Phase stability of TiH<sub>2</sub> under high pressure and temperatures. **2008**, 33, 6667-6671 11
- 743 Structural, electronic and optical properties of SrCl<sub>2</sub> under hydrostatic stress. **2008**, 61, 165-171 6
- 742 Density functional theory study on transparent conductive oxide CuScO<sub>2</sub>. **2012**, 61, 227401 2
- 741 Research on softening of longitudinal mode under high pressure and equation of state of -Ce. **2012**, 61, 116401
- 740 A Ground State Study of Structural and Magnetic Properties of Co<sub>2</sub>CrGe: A GGA Method. **2012**, 9, 155-158 1
- 739 First-principles study of structure and stability in Si<sub>100</sub>-based materials. **2014**, 197-201
- 738 Estudio AB-Initio de las propiedades estructurales y electrónicas de la doble Perovskita Ba<sub>2</sub>InTaO<sub>6</sub>. **2013**, 18, 5-8
- 737 First-Principles Simulations of the Initial Corrosion-Process of Iron Surface. **2013**, 2809-2814
- 736 Structural and Electronic Properties of  $\epsilon$ -NbN Single Crystal: First Principles Calculations. 267-274
- 735 First-principles studies of the structural and thermodynamic properties of TiAl<sub>3</sub> under high pressure. **2013**, 62, 068105 4
- 734 Role of electronic structure on solubility of magnetic Mn impurity in GaInAs semiconductor alloys. **2013**, 37, 227-230
- 733 Spin-orbit Coupling Effect on the Structural Optimization: Bismuth Telluride in First-principles. **2013**, 23, 1-6 1
- 732 The Nuts and Bolts. 193-211

- 731 First principles calculations of solid phase transition of nitromethane. **2014**, 63, 098105 3
- 730 Theoretical Assessment of the Mechanical, Electronic, and Vibrational Properties of the Paramagnetic Insulating Cerium Dioxide and Investigation of Intrinsic Defects. **2014**, 431-446
- 729 The Importance of the Transition Metal Volume in A15 Superconductors. **1974**, 457-460
- 728 Third-Order Elastic Constants and Thermal Expansion of Scandium. **1978**, 57-68
- 727 Lattice Thermal Expansion of Praseodymium and Neodymium. **1984**, 49-57
- 726 Equations of State and Geophysical Equations of State. **1984**, 3-65
- 725 Application of Vectorization on Ab-initio Calculations of Silicon Carbide and Boron Nitride. **1989**, 167-176
- 724 Large Scale Computations in Solid State Physics. **1990**, 83-97
- 723 First-Principles Electronic Theory on a Possible High-Pressure Phase of Silica. **1990**, 23-35
- 722 Application of GGA to a Study of Structural and Magnetic Properties of 3d Transition Metals. **1993**, 201-210
- 721 LMTO/CVM Calculations of BCC Based Phase Ordering in The System Fe-Be. **1994**, 557-560
- 720 High Pressure Phase Diagram of Silicon: A Model System in Condensed Matter Physics. **1996**, 335-348
- 719 Total Energy Calculation of Solids Using Pseudopotentials. **1996**, 53-65
- 718 An Improved Technique for Determining the Equation of State of Concrete and Geological Materials. **1997**, 1767-1774
- 717 First Principles Calculations of Binary Alloy Phase Diagrams. **1998**, 39-52
- 716 Pressure-Induced Phase Transitions In Alkali Halides: Hf and Dft Study. **1999**, 499-507
- 715 REFERENCES. **1999**, 377-396
- 714 How Accurate are High-Pressure Experiments?. **1999**, 103-108 1

713 Investigations of Semiconductor Band Structure Using High Pressure.. **1999**, 109-120

712 Electronic Structure and Magnetism of Itinerant 5f Ferromagnets URhSi and URhGe. **1999**, 487-498

711 Wide and reversible tuning of an individual nanowire laser using hydrostatic pressure. **2015**,

710 Band Gap Characterization of Ternary BBi<sub>1-x</sub>NxAlloys: A First-Principles Study. **2015**, 128, B-46-B-49

709 Influence of Lanthanoid Dopant and N/O Substitution on The Electronic Structure and Luminescent Properties of Lanthanum Silicon Oxynitride Phosphors. 55-63

708 First-principles investigations on structure and thermodynamic properties of CaS under high pressures. **2016**, 65, 027101

707 Structural and electronic properties of TiX (X=N, As) in rock salt and zinc blende phase: A DFT study. **2016**,

706 Effect of K-Point Convergence on Derived Properties for Pure Crystals. **2016**, 275-282

705 Elastic Moduli of Tellurite Glasses. **2016**, 101-172

704 Crystal Structure and Bonding. **2017**, 347-401

703 Precipitation Reactions in Nickel-Hydrogen System: ab initio Study. **2016**, 38, 737-750

1

702 10 Thermal and Mechanical Properties of Graphene and SWCNTs. **2016**, 173-204

701 Effects of the doping of Al and O interstitial atoms on thermodynamic properties of -Al<sub>2</sub>O<sub>3</sub>:first-principles calculations. **2017**, 66, 016103

700 First principles study of mechanical properties of FeMnP<sub>1-x</sub>T<sub>x</sub> (T=Si, Ga, Ge) compounds. **2017**, 66, 126301

699 Modelling of Phase Transitions in Calcium-Strontium Superstructures at Low Pressures.. **2017**, 39, 113-125

698 Efectos de intercambio y correlaci3n en las propiedades estructurales y electr3ficas del TiO<sub>2</sub> en la fase rutilo. **2017**, 8,

2

697 Transiciones de Fase Inducidas por Presi3n en los Compuestos GaN, InN y AlN. **2017**, 8,

696 L12 yapıdaki Co<sub>3</sub>Al ve Co<sub>3</sub>Ta alaşımlarının mekanik ve dinamik özellikleri. **2017**, 32,

1

- 695 First-Principles Study of the Structural, Electronic, Magnetic and Thermal Properties of the Cr Doped  $\text{Ge}_6\text{Mn}_2\text{Te}_8$  and  $\text{Ge}_6\text{Fe}_2\text{Te}_8$  Systems. **2017**, 132, 1242-1250 1
- 694 Rh3Sc Bileşimin Dinamik, Mekanik ve Termal Özelliklerinin ab-initio İncelenmesi
- 693 Ru2FeGa Heusler alaşım yapısı, elektronik, elastik ve fonon özelliklerinin ilk prensip ile incelenmesi
- 692 CARBON ATOMS IN INTERSTITIAL SITES OF THE CEMENTITE CRYSTAL LATTICE: AB INITIO MODELLING. **2018**, 18, 34-45 0
- 691 From Electrons to Atoms: Designing an Interatomic Potential for Fe Alloys. 21-48
- 690 Effect of Co Substitution on Ni2MnGe Heusler Alloy: ab initio Study. **2018**, 133, 495-497
- 689 Güneş pilleri için ZnO'nun yapısal ve elektronik özelliklerinin incelenmesi: Ab-initio ile incelenmesi
- 688 Electro-chemo-mechanical effects of lithium incorporation in zirconium oxide. **2018**, 2,
- 687 The first-principle study on the formation energies of Be, Mg and Mn doped  $\text{CuInO}_2$ . **2019**, 68, 106102 0
- 686 B2 Kristal Yapısındaki OsAl Bileşimin Yapısal, Elektronik, Elastik, Termodinamik ve Fonon Özelliklerinin İncelenmesi B2 Kristal Yapısındaki OsAl Bileşimin Yapısal, Elektronik, Elastik, Termodinamik ve Fonon Özelliklerinin İncelenmesi.
- 685 BaRu2As2 Malzemesinin Fiziksel Özelliklerinin Yoğunluk Fonksiyonel Teorisi Kullanılarak İncelenmesi.
- 684 Mechanical Spectroscopy Studies of Hydrogen Mobility in Titanium Doped Iron Alloy. **2019**, 41, 1291-1301
- 683 Yoğunluk Fonksiyoneli Teorisi ile LiAlSi4ün Başlangıçta Elektronik ve Titreşim Özellikleri. 1340-1346
- 682 Theoretical Insights About the Chemical Dependent Role of Exchange-Correlation Functionals: A Case Study. **2020**, 341-357 0
- 681 The Effect of Spin-Orbit Interaction On Structural and Electronic Properties of  $\text{ScIr}_2$ . 406-411
- 680 Monoclinic semimetal IrSi synthesized under high pressure above 25 GPa: Crystal structure, electronic, and magnetic properties. **2020**, 4,
- 679 Investigation on Structural and Electronic Properties of  $\text{Zn}_{1-x}\text{Mg}_x\text{O}$  in Wurtzite Phase Using First Principal calculations. **2020**,
- 678 Effect of spin orbit coupling on opto-electronic and magnetic properties of full Heusler alloy,  $\text{Ru}_2\text{CrAl}$  for spintronic and optical devices: Theoretical investigations using DFT. **2021**, 249, 168250 0



677	DFT investigation on the electronic, optical and thermoelectric properties of novel half-Heusler compounds $\text{ScAuX}$ ( $X = \text{Si, Ge, Sn, Pb}$ ) for energy harvesting technologies. <b>2021</b> , 136, 1	0
676	Structural, Electronic and Optical Properties of $\text{Sc}_x\text{Ga}_{1-x}\text{P}$ Alloys An: Ab Initio Study. <b>2021</b> ,	
675	Comparative study by DFT method of structural, electronic and optical properties of monolayer, bilayer and bulk $\text{CdS}$ . <b>2021</b> , 127, 1	1
674	On the Origin of Zero Interface Resistance in the $\text{LiAlLaZrO Li}$ System: An Atomistic Investigation. <b>2021</b> ,	0
673	Anisotropic Interlayer Force Field for Transition Metal Dichalcogenides: The Case of Molybdenum Disulfide. <b>2021</b> , 17, 7237-7245	3
672	Influence of Oxygen Vacancies in Gas Sensors Based on Metal-Oxide Semiconductors: A First-Principles Study. <b>2020</b> , 309-314	1
671	Structural, electronic, magnetic and optical properties of polycrystalline $\text{FeAlB}$ and $\text{Fe}_2\text{AlB}_2$ : A first-principles study. <b>2020</b> ,	0
670	Synthesis, XRD analysis and electronic structure of $\text{InGaTe}_2$ chain semiconductor. <b>2021</b> , 35, 2150029	0
669	Structural and Physical Properties of $\text{DyCu}$ , $\text{NdAg}$ , $\text{LaCd}$ , $\text{YIn}$ , $\text{ErCu}$ , $\text{ErAg}$ , and $\text{ErAu}$ Rare-Earth Intermetallic Compounds: Ab initio Investigations Analyzed by Data Mining Technique. <b>2020</b> , 62, 2305-2317	1
668	Investigation of Electronic and Optical Properties of Novel Oxychalcogenides by Density Functional Theory. <b>2020</b> , 62, 120-129	
667	Optimizing Configurations for Determining the Electromagnetic Properties of $\text{CsFeF}_3$ , $\text{NaFeF}_3$ , and $\text{RbFeF}_3$ Fluorides: GGA vs GGA+U and TB-mBj Approaches. <b>2020</b> , 62, 71-94	
666	Structural Stability and Magnetic Ordering in $\text{BiFeO}_3$ Perovskite Oxide: A Comparative Study GGA+U vs L(S)DA+U. <b>2020</b> , 62, 52-70	1
665	Predicted double perovskite material $\text{Ca}_2\text{ZrTiO}_6$ with enhanced n-type thermoelectric performance. <b>2022</b> , 305, 122661	2
664	Structural, Electronic, Mechanical and Thermal Properties of $\text{CoVZ}$ ( $Z = \text{Si, Ge, Sn, Pb}$ ) half-Heusler Compounds. <b>2020</b> ,	
663	Layered Structures. <b>2020</b> , 415-445	
662	Structural phase transition, electronic and thermoelectric properties of osmium silicide. <b>2020</b> ,	
661	Comparing different water equations of state for aquarium tests. <b>2020</b> ,	
660	An investigation of bulk modulus and cohesive energy of $\text{GaP}$ in the local density approximation. <b>2020</b> ,	

- 659 Structural, Electronic, Optical and Magnetic Properties of  $\text{Co}_2\text{CrZ}$  (Z= Al, Bi, Ge, Si) Heusler Compounds. **2020**,
- 658 Automated fitting of a semi-empirical multiphase equation of state for carbon. **2020**, 5
- 657 Sized Crystals. **2020**, 447-468
- 656 BAND STRUCTURE, METALLIZATION AND STRUCTURAL PHASE TRANSITION OF NABR UNDER HIGHPRESSURE. **2018**, 5, 108-116
- 655 Intrinsic defects of GaSe. **2020**, 32, 285503 1
- 654 First-principle calculations to investigate structural, electronic, optical, thermodynamic, and thermoelectric properties of  $\text{ABO}_3$  (A=Cs, Rb and B= Ta, Nb) compounds. 1
- 653 The effect of substitutional doping of Ybn structural, electronic, and optical properties of  $\text{CsCa}(\text{Cl, Br, I})$  phosphors: a first-principles study. **2021**, 34, 0
- 652 Structural, Electronic, and Optical Properties of p-Type Semiconductors  $\text{Cu}_2\text{O}$  and  $\text{ZnRh}_2\text{O}_4$ : A Self-Consistent Hybrid Functional Investigation. **2021**, 2, 504-510 1
- 651 Analysis of NH -TPD Profiles for  $\text{CuSSZ-13}$  SCR Catalyst of Controlled Al Distribution - Complexity Resolved by First Principles Thermodynamics of NH Desorption, IR and EPR Insight into Cu Speciation\*. **2021**, 27, 17159-17180 2
- 650 Structural and Magnetic Behavior of  $\text{MoS}_2$  on Doping of Transition Metals: a DFT Study. **2021**, 34, 3441 0
- 649 Fundamental physical properties of non-toxic tin-based formamidinium  $\text{FASnX}_3$  (X = I, Br, Cl) hybrid halide perovskites: Future opportunities in photovoltaic applications. 4
- 648 Electronic Structure of the Face-Centred Cubic  $\text{MoO}_{1.9}$  Phase Obtained Due to Reduction of Hydrogen Bronze  $\text{H}_{1.63}\text{MoO}_3$ . **2008**, 651-658
- 647 Effect of local strain energy to predict accurate phase diagram of IIIIV pseudobinary systems: case of  $\text{Ga}(\text{As,Sb})$  and  $(\text{In,Ga})\text{As}$ . **2021**, 54, 045104 1
- 646 Electronic, phononic, and superconducting properties of trigonal  $\text{Li}_2\text{MSi}_2$  (M=Ir, Rh). **2020**, 0
- 645 Pressure-induced Pb-Pb bonding and phase transition in  $\text{PbSnO}$ . **2020**, 76, 979-991 4
- 644 Molecular Material Modeling of Cement Paste Composite in Shock Loading. **2020**, 117,
- 643 First-principle computations of ferromagnetic  $\text{HgCr}_2\text{Z}_4$  (Z = S, Se) spinels for spintronic and energy storage system applications. **2020**, 9, 16159-16166 3
- 642 The pressure effect on optoelectronic and mechanical properties of chalcopyrite  $\text{BeSiN}_2$ . **2020**, 24, 101263

641	DFT and Monte Carlo study of the structural, mechanical, electronic, magnetic and magnetocaloric properties of the Co <sub>2</sub> VGa Heusler alloy. <b>2022</b> , 787, 139261	2
640	First-principles calculations to investigate structural, mechanical, electronic, magnetic and thermoelectric properties of Ba <sub>2</sub> CaMO <sub>6</sub> (M=Re, Os) cubic double perovskites. <b>2022</b> , 626, 413554	0
639	Effect of pressure on structural and elastic properties of SnSe: First-principles calculations. <b>2022</b> , 342, 114596	
638	The effect of structural changes on half-metallic, elastic and magnetic properties of the FeWGa half-Heusler compound via first-principles studies. <b>2022</b> , 546, 168872	1
637	Thermal Elastohydrodynamic Lubrication of Axially Crowned Rollers. 1-21	0
636	Structural and electronic properties of ternary alloys of alkaline-earth oxides and chalcogenides. 1-21	
635	Investigating the magneto-electronic, structural, mechanical, and thermodynamic properties of filled skutterudite NdRu <sub>4</sub> Sb <sub>12</sub> and EuRu <sub>4</sub> Sb <sub>12</sub> : A first-principles perspective. <b>2022</b> , 122, e26834	
634	Study on graphene-like monolayer ZnS <sub>1-x</sub> O <sub>x</sub> : structural and optoelectronic properties. <b>2021</b> , 140, 1	
633	Effect of Ga excess concentration on the structural, electronic, magnetic, elastic and thermoelectric properties of Fe <sub>2-x</sub> NiGa <sub>1+x</sub> Heusler alloys: results of FP-LAPW calculations. <b>2021</b> , 136, 1	
632	Investigating the influence of pressure on SrFeO <sub>3</sub> and SrMnO <sub>3</sub> ferromagnets for high-pressure spintronic devices: a comparative DFT overview. <b>2021</b> , 127, 1	0
631	Ab initio calculations of Electronic, Magneto-Optical, and Transport Properties of the Ga <sub>1-2x</sub> Sm <sub>x</sub> Eu <sub>x</sub> N alloy (x = 0.0625) by GGA, GGA + U, and TB-mBj approximations. 1	
630	Theoretical investigations of structural, mechanical, electronic, and thermodynamic properties of BaNYO (Y = Mg, Ca, and Sr) alloys. 1	0
629	Computational investigation of structural, magnetic, elastic, and electronic properties of Half-Heusler ScVX (X = Si, Ge, Sn, and Pb) compounds. <b>2021</b> , 136, 1	1
628	Modeling structural, elastic, electronic and optical properties of ternary cubic barium based fluoroperovskites MBaF <sub>3</sub> (M = Ga and In) compounds based on DFT. <b>2021</b> , 139, 106345	1
627	Resistivity size effect due to surface steps on ruthenium thin films computed with a realistic tight-binding model. <b>2021</b> , 130, 195108	
626	Pressure induced structural, electronic and optical properties of wurtzite beryllium monoxide (w-BeO) from first-principle calculations. <b>2021</b> , 342, 114571	
625	Effect of cation exchange on structural, electronic, magnetic and transport properties of Ba <sub>2</sub> MReO <sub>6</sub> (M = In, Gd). <b>2021</b> , 546, 168816	2
624	Toward Durable Protonic Ceramic Cells: Hydration-Induced Chemical Expansion Correlates with Symmetry in the Y-Doped BaZrO <sub>3</sub> BaCeO <sub>3</sub> Solid Solution. <b>2021</b> , 125, 26216-26228	1

- 623 A reactive flow model for the 3,3'-diamino-4,4'-azoxyfuran based plastic bonded explosive (PBX 9701). **2021**, 130, 215903 2
- 622 First principles study of the structural, elastic, electronic and optical properties of the ternary alloys  $\text{Ca}_{0.75}\text{Zn}_{0.25}\text{S}$  and  $\text{Ca}_{0.75}\text{Zn}_{0.25}\text{Se}$ . **2021**, 29, e00609 0
- 621 Investigating effect of different Hubbard values on the electronic structure, magnetic and optical properties of Ru doped GaN. **2021**, 29, e00608
- 620 Skutterudite materials;  $\text{Al}_y\text{Fe}_x\text{Co}_{4-x-y}\text{Sb}_{12}$  ( $x = y = 1$ ;  $x = 2, y = 1$ ) for spintronics and optoelectronics applications. **2021**, 29, e00613
- 619 Monolayer Transition Metal Oxides (MTMOs): CoO, FeO and NiO: A First Principles Study. **2022**, 59-70
- 618 First-principle calculations of the electronic, structural, optical, thermoelectric and elastic properties of  $\text{CeXO}_3$  ( $X = \text{Ti, V and Cr}$ ) perovskites. **2021**, 15, 1078-1093 0
- 617 Structural, elastic, electronic and optical properties of the half-Heusler  $\text{ScPtSb}$  and  $\text{YPtSb}$  compounds under pressure. **2021**, 24, 43702 0
- 616 Structural, Elastic, and Electronic Properties of Holmium based Compounds  $\text{HoX}_3$  ( $X = \text{Pd, Pt}$ ). **2021**, 01, 29-33
- 615 Metamagnetism in Hexagonal  $\text{CrSn}$  : A First Principle Study. 1
- 614 Superexchange Ferromagnetic Coupling and Thermodynamic Features of the  $\text{La}_2\text{FeCoO}_6$  Semiconductor. 1
- 613 A robust three-parameter reference curve for condensed phase materials. **2022**, 131, 015902 1
- 612 Structural, Magnetic, Electronic, Thermoelectric, Optic And Elastic Properties Of  $\text{Co}_2\text{Mn}_{1-x}\text{Ti}_x\text{Ge}$  Heusler Alloys. **2022**, 790, 139328 1
- 611 Local orders, lattice distortions and electronic structure dominated mechanical properties of  $(\text{ZrHfTaM}_1\text{M}_2)\text{C}$  ( $M = \text{Nb, Ti, V}$ ). 0
- 610 First-principles investigation of the structural and dynamical stability, electronic and thermal properties of two-dimensional  $\text{Y}_{n+1}\text{C}_n$  ( $n = 1, 2, \text{ and } 3$ ) MXenes. **2022**, 31, 100328 0
- 609 First-principles study of structural, electronic, elastic, and optical properties of the tetragonal  $\text{AlnS}_2$  ( $A = \text{K, Rb, Cs}$ ) chalcogenides. **2022**, 30, e00644 0
- 608 First-principles calculations to investigate ultra-wide bandgap semiconductor behavior of  $\text{NaMgF}_3$  fluoro-perovskite with external static isotropic pressure and its impact on optical properties. **2022**, 252, 168532 2
- 607 Ab initio investigation of phase stability, thermo-physical and mechanical properties of  $(\text{Mo}_{0.2}\text{Cr}_{0.2}\text{Ta}_{0.2}\text{Nb}_{0.2}\text{X}_{0.2})\text{Si}_2$  ( $X = \text{W, V}$ ) high-entropy refractory metal silicides. **2022**, 203, 111116 0
- 606 Chemical bonding, magnetic and electronic properties, mechanical and dynamical stabilities of  $\text{DyOs}_4\text{P}_{12}$  filled-skutterudite: DFT and QAIM insight. **2022**, 278, 125684 1

605	Structure, mechanical stability, lattice dynamics and thermodynamic properties of C15-Laves phase Mg <sub>2</sub> Ce. <b>2022</b> , 342, 114641	0
604	Computational evaluation of optoelectronic, thermodynamic and electron transport properties of CuYZ <sub>2</sub> (Z= S, Se and Te) chalcogenides semiconductors. <b>2022</b> , 277, 125553	3
603	Hydrostatic compression and pressure phase transition of major Portland cement constituents □ Insights via molecular dynamics modeling. <b>2022</b> , 7, 100017	
602	First principles study on electronic properties and mechanical stability of HfRhZ (Z='As and Sb) half Heusler alloys. <b>2022</b> , 581, 126468	1
601	First-principles studies of electronic structure, magnetic and optical properties of rare-earth (RE= Sm, Eu, Gd, and Er) doped ZnS. <b>2022</b> , 30, e00632	0
600	A DFT study of mechanical properties of hcp rhenium. <b>2022</b> , 30, 103035	
599	Analysis of physical properties of the orthorhombic perovskite compound EuCrO <sub>3</sub> using DFT approach. <b>2022</b> , 307, 122808	0
598	Theoretical investigation of structural, electronic and optical properties of Sc-doped SnO <sub>2</sub> . <b>2022</b> , 30, e00642	1
597	Binary TiBe system. Part II: Modelling of pressure-dependent phase stabilities. <b>2022</b> , 76, 102383	2
596	The structural, electronic, optical, thermodynamical and thermoelectric properties of the Bi <sub>2</sub> Al <sub>4</sub> Se <sub>8</sub> compound for solar photovoltaic semiconductors. <b>2022</b> , 141, 106415	0
595	Signature of half-metallicity in BiFeO <sub>3</sub> : A DFT study. <b>2022</b> , 204, 111107	1
594	Computational insights into the structural, mechanical, optical, electronic and magnetic properties of EuTiO <sub>3</sub> semiconductor in cubic-perovskite using FP-LAPW method. <b>2022</b> , 142, 106455	0
593	New Half Metal Perovskite NbScO <sub>3</sub> for Spintronic Sensing Applications. <b>2021</b> , 5,	
592	Structural, Elastic and Electronic Properties of Transition Metal Hydrides TiH <sub>2</sub> and ZrH <sub>2</sub> from First Principles Calculations. <b>2021</b> ,	1
591	Structural, electronic, and thermodynamic properties of a rare earth dihydride TbH <sub>2</sub> . <b>2021</b> ,	
590	DFT study of structural, electronic, magnetic, elastic, vibrational, thermodynamic and thermoelectric properties of XCrP (X= Ni, Pd and Pt). <b>2022</b> , 31, e00645	
589	Electronic, Structural, Mechanical, and Thermodynamic Properties of CoYSb (Y = Cr, Mo, W) Half-Heusler Compounds as Potential Spintronic Materials. <b>2022</b> , 3, 22-33	0
588	Metal-insulator transition and local-moment collapse in negative charge transfer CaFeO <sub>3</sub> under pressure. <b>2022</b> , 105,	0

587	Phase Evolution, Polymorphism, and Catalytic Activity of Nickel Dichalcogenide Nanocrystals. <b>2022</b> , 34, 746-755	0
586	Oxynitride Perovskite: Computational Approach to Correlate Structural, Electronic, and Optical Properties of c-BiAlO <sub>3</sub> /N <sub>3</sub> . <b>2022</b> , 4, 375-385	3
585	First principles study of electronic, optical, and thermoelectric properties of K <sub>2</sub> Pd (Cl/Br) <sub>6</sub> for solar cells and renewable energy. <b>2022</b> , 97, 035803	1
584	Superconductivity in InTe under Compression Induced by Electronic and Structural Phase Transitions.. <b>2022</b> , 1226-1233	1
583	Temperature- and vacancy-concentration-dependence of heat transport in Li <sub>3</sub> ClO from multi-method numerical simulations. <b>2022</b> , 8,	1
582	Defect chemistry of LaGaO <sub>3</sub> doped with divalent cations. <b>2022</b> , 374, 115828	0
581	Theoretical Insight into the Stability, Magneto-electronic and Thermoelectric Properties of XCrSb (X: Fe, Ni) Half-Heusler Alloys and Their Superlattices. <b>2022</b> , 35, 875	1
580	Adsorption of H <sub>2</sub> S on AgO(001) surface: A density-functional theory investigation.	0
579	Cobalt based new quaternary Heusler alloys for Spintronic and thermoelectric applications: an Ab-initio study. 1-11	2
578	Stochastic many-body calculations of moiré states in twisted bilayer graphene at high pressures. <b>2022</b> , 8,	4
577	Experimental and theoretical study on structural and electronic properties of Zn <sub>1-x</sub> Mg <sub>x</sub> O from (x=0 to 0.375) in wurtzite phase. <b>2022</b> , 107155	
576	Speed of Sound, Density, and Related Thermophysical Properties of the Methyl Caprate + Methyl Oleate Binary System from 0.1 MPa to 70 MPa at 303.15 K. <b>2022</b> , 43, 1	1
575	Spin and spin-orbit coupling effects in nickel-based superalloys: A first-principles study on Ni <sub>3</sub> Al doped with Ta/W/Re. <b>2022</b> , 31, 016105	2
574	First-principles study of the structural, electronic, optical, and thermoelectric properties of the RhVZ (Z= Si, Ge, Sn). <b>2022</b> , 107162	0
573	Mg substitution in zinc selenide: Enhanced optoelectronic and thermoelectric performance.	1
572	Exploring the Synthesis of Alkali Metal Anti-perovskites. <b>2022</b> , 34, 947-958	2
571	Study on New High-Pressure Phases and Electronic Properties of Iodine Chloride Employing Ab Initio Calculations. <b>2022</b> , 51, 1632	0
570	Influence of Isostatic Pressure on the Elastic and Electronic Properties of KSiF:Mn.. <b>2022</b> , 15,	

- 569 Band engineering of modified rhombohedral  $\text{Cu}_4\text{Mn}_2\text{Te}_4$ : ab initio approach. 1-29
- 568 Structural, electronic and magnetic properties of the Half-Heusler alloy  $\text{CrZSi}$  ( $Z = \text{Sc, Ti}$ ). **2022**, 583, 126556 1
- 567 Hybrid density functional theory study on zinc blende GaN and diamond surfaces and interfaces: Effects of size, hydrogen passivation, and dipole corrections. **2022**, 30, e00653
- 566 Computational study of mechanical properties in  $\text{CuAlZn}$ . **2022**, 30, e00631
- 565 Study on quaternary diamond-like  $\text{Li}_2\text{CaGeO}_4$  properties for optoelectronic applications. **2022**, 30, e00646
- 564 Effects of temperature and pressure on the mechanical and thermodynamic properties of high-boride  $\text{WB}_4$  from first-principles predictions. **2022**, 30, 103187 2
- 563 Tuning of optoelectronic and transport properties of zinc-blend magnesium chalcogenides through doping of Hg atom(s): The mBJ-GGA+U based first-principle calculations. **2022**, 30, e00650 0
- 562 Narrow gap electronic structure and thermoelectric performance of p-type  $\text{ErMSb}$  ( $M = \text{Ni, Pd}$ ) half Heusler compounds. **2022**, 631, 413709 0
- 561 Electronic and magnetic properties of MAX phase  $\text{Cr}_2\text{SiC}$  with GGA+U approximation. **2022**, 308, 122870 1
- 560 Molecular dynamics study of phonon and thermoelectric properties of hydrogen-passivated silicon carbide nanotubes. **2022**, 198, 110899 0
- 559 Structural, electronic, magnetic, optical, thermoelectric and thermodynamic properties of  $\text{R}_2\text{Rh}_3\text{Ge}$  ( $R = \text{Gd and Er}$ ). **2022**, 163, 110581
- 558 Theoretical study of copper nitrides  $\text{Cu}_n\text{N}$  ( $n=1, 3$  and  $4$ ): insight first-principles calculations. 1-14
- 557 Theoretical investigation of nitrogen-vacancy defects in silicon. **2022**, 12, 025112 0
- 556 Theoretical Study of the Structural and Electronic Properties of the Tetragonal Chalcopyrite Compound  $\text{ZnTiS}_2$ . **2021**, 55, 491
- 555 Investigation of structural, mechanical and optoelectronic properties of cubic  $\text{Cd}_{1-x}\text{Zn}_x\text{Hg}_y\text{Se}$  quaternary alloys through first-principle calculations. **2022**, 45, 1
- 554 Synchrotron x-ray total scattering and modeling study of high-pressure-induced inhomogeneous atom reconfiguration in an equiatomic  $\text{Zr}_{50}\text{Cu}_{50}$  metallic glassy alloy. **2022**, 105, 0
- 553 Verification of a Specialized Hydrodynamic Simulation Code for Modeling Deflagration and Detonation of High Explosives. **2022**, 7, 1
- 552 Investigation of New 2D Half Metallic Ferromagnetic Materials. 0

- 551 DFT Investigation of the Structural and Optoelectronic Properties of Alkali Metal Hydrides MH (M=Li, Na). **2022**, 12, 8151-8156
- 550 Ab initio comparative study of B2MnX intermetallics with X = V, Nb, Ta. **2022**, 95, 1 0
- 549 Off-Centered Pb Interstitials in PbTe.. **2022**, 15,
- 548 Investigating the Magnetic, Mechanical, Electronic, Optical, and Anisotropic Properties of ZrCoFeX (X = Si, Ge) Quaternary Heusler Alloys via First Principles. 1
- 547 First principles study of monolayer Sb2S2Te and a mathematical model of a thin-film thermoelectric generator with maximum power point tracing. **2022**, 36, 117-130 2
- 546 First-principles quantum analysis on the role of V-doping on the tuning of electronic and optical properties of spinel oxides MnTi2O4. **2022**, 278, 115643 2
- 545 Methodological Approach to the High-Pressure Synthesis of Nonmagnetic Li2B4+B?6+O6 Oxides. **2022**, 34, 186-196 1
- 544 First-principal investigations of electronic, structural, elastic and optical properties of the fluoroperovskite TlLF (L = Ca, Cd) compounds for optoelectronic applications.. **2022**, 12, 7002-7008 0
- 543 Atomic Interactions. **2022**, 1-43
- 542 Insight into the exemplary structural, elastic, electronic and optical nature of GaBeCl and InBeCl: a DFT study.. **2022**, 12, 8172-8177 1
- 541 First principle investigation of Niobium (Nb) doped MgO. **2022**, 51, 2091-2095
- 540 Anharmonic Grüneisen theory based on self-consistent phonon theory: Impact of phonon-phonon interactions neglected in the quasiharmonic theory. **2022**, 105, 1
- 539 Theoretical investigation on the optoelectronic properties of ZrxSi1-xO2 tetragonal hypothetical alloys from zircon family. **2022**, 128, 1 0
- 538 The comparative study of structural, electronic, and optical properties of hydrogen peroxide and its dihydrate under pressures: first-principle calculations.. **2022**, 28, 72 1
- 537 Morphological, Structural and Hydrogen Storage Properties of LaCrO3 Perovskite-Type Oxides. **2022**, 15, 1463 0
- 536 Dependence of the Elastic Stiffness Tensors of PETN, RDX, RDX, ?-RDX, ?-CL-20, DAAF, FOX-7, and HMX on Hydrostatic Compression. **2022**, 47, 0
- 535 Correlation-Consistent Gaussian Basis Sets for Solids Made Simple.. **2022**, 18, 1595-1606 4
- 534 Pressure-induced phase transition and increase of oxygen-iodine coordination in magnesium iodate. **2022**, 105, 0



533	Structural, electronic, vibrational, thermoelectric and mechanical properties of Li based quaternary Heusler compound LiTiCoSn: A DFT approach. <b>2022,</b>	0
532	First principle study of band gap tuning in Cs <sub>2</sub> InSbX <sub>6</sub> (X = Cl, Br, I) for optoelectronic and thermoelectric applications. <b>2022, 97, 045801</b>	1
531	Investigation of structural, elastic, electronic, and magnetic properties for X <sub>2</sub> LuSb (X = Mn and Ir) full-Heusler alloys. 1	2
530	Electronic properties and stability of M <sub>2</sub> O <sub>3</sub> (M = Al, Ga, In) and alloy (M <sub>x</sub> Ga <sub>1-x</sub> ) <sub>2</sub> O <sub>3</sub> in $\bar{R}3m$ and $R\bar{3}m$ phases: A theoretical study. <b>2022, 105, 4554-4563</b>	0
529	Ab initio investigations of point and complex defect structures in B <sub>2</sub> -FeAl. <b>2022, 6,</b>	1
528	First-Principles Surface Characterization and Water Adsorption of Fe <sub>3</sub> P Schreibersite. <b>2022, 6, 512-520</b>	0
527	Pressure Inhomogeneities across Large Samples Using Gas Pressure Media at Low Temperatures.	
526	Hybridization-driven strong anharmonicity in Yb-filled skutterudites. <b>2022, 105,</b>	1
525	Predicting and Correlating Speed of Sound in Long-Chain Alkanes at High Pressure. <b>2022, 43, 1</b>	0
524	Minimizing pressure inhomogeneities across large samples under helium pressure media at low temperatures. <b>2022, 24, 15-22</b>	
523	Li <sub>3</sub> As and Li <sub>3</sub> P revisited: DFT modelling on phase stability and ion conductivity.	1
522	A First-Principles Investigation on Electronic Structure and Optical Properties of Tetragonal Iron Antimonide FeSb <sub>2</sub> . 1	
521	Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CL-20) Lattice: Part I, Infrared Spectra.	1
520	Pressure Dependence of Structural and Elastic Properties of Na <sub>2</sub> O: First-Principles Calculations. <b>2022, 224, 256-263</b>	0
519	First-Principles Calculations of Pressure Effects on the Structural, Electronic, Elastic, and Thermodynamic Properties of Rb <sub>2</sub> M <sub>2</sub> F <sub>6</sub> (M = Si, Ni, Pd) Crystals. 2100607	
518	Comparative Study of ZnO Nanomaterials Synthesized by Green and Electrospinning Methods. 72, 81-93	1
517	Combination of optical properties acquired by first principles calculations with the empirical Tauc method for determining the band gap energy of alkaline-earth metal oxides: MO (M = Be, Mg, Ca, Sr, Ba). <b>2022, 1-10</b>	
516	First-principles calculations to investigate transformation of optically inactive zinc-blend beryllium chalcogenides to optically active semiconductor alloys through doping of Hg atom(s). <b>2022, 413881</b>	0

- 515 Revisiting the Cu-Zn Disorder in Kesterite Type  $\text{Cu}_2\text{ZnSnSe}_4$  Employing a Novel Approach to Hybrid Functional Calculations. **2022**, 12, 2576 0
- 514 Molecular Inclusion of Small Aging Products into the Hexanitrohexaazaisowurtzitane (CL-20) Lattice: Part II, Polymorph Dependence.
- 513 Structural stability, electronic, mechanical, and thermodynamic properties of the new MAX phases  $\text{Mn}_2\text{SiC}_1$ ,  $\text{Mn}_3\text{SiC}_2$  and  $\text{Mn}_4\text{SiC}_3$ : ab-initio calculations. 1 0
- 512 Thermodynamic properties of phagraphene. 1-7
- 511 Pressure dependence of the electronic, optical, thermoelectric, thermodynamic properties of  $\text{CsVO}_3$ : first-principles study. 1-25
- 510 High Pressure and Temperature Dependence of the Structural, Electronic, Thermal and Transport Properties of  $\text{U}_3\text{Si}_2$  : Computational Insights. 2100630
- 509 Role of intrinsic defects in cubic  $\text{NaNbO}_3$ : A computational study based on hybrid density-functional theory. **2022**, 131, 124106 1
- 508 Exploring structural, electronic, optical, magnetic, and thermoelectric properties of Pt doped and Pt-Cu/Au co-doped GaN. **2022**, 97, 045809
- 507 Investigation of the Structural, Electronic, Elastic, Thermodynamic, and Thermoelectric Properties of  $\text{HfXPb}$  ( $X = \text{Ni, Pd, Pt}$ ): First-Principles Study. **2022**, 51, 1-14
- 506 Prediction of structural, electronic, mechanical, thermal, and thermoelectric properties in  $\text{PbMO}_3$  ( $M = \text{Sb, Bi}$ ) perovskite compounds: a DFT study. **2022**, 137, 1 0
- 505 Topological nodal line semimetal in an all-sp<sup>2</sup> monoclinic carbon. **2022**, 24, 043007 0
- 504 Opto-electronic, thermodynamic and charge carriers transport properties of  $\text{Ta}_2\text{FeNiSn}_2$  and  $\text{Nb}_2\text{FeNiSn}_2$  double half-Heusler alloys. **2022**, 37, 055013 1
- 503 Temperature and pressure driven spin transitions and piezochromism in a Mn-based hybrid perovskite. **2022**, 6, 0
- 502 Insight into the Exemplary Physical Properties of Zn-Based Fluoroperovskite Compounds  $\text{XZnF}$  ( $X = \text{Al, Cs, Ga, In}$ ) Employing Accurate GGA Approach: A First-Principles Study.. **2022**, 15, 1
- 501 Second nearest-neighbor modified embedded atom method interatomic potentials for  $\text{Na-M}_3\text{N}$  ( $M = \text{Cu, Mn, Ni}$ ) ternary systems. **2022**, 206, 111305
- 500 Pressure induced isostructural phase transition in biskyrmion host hexagonal  $\text{MnNiGa}$ . 1
- 499 Atomistic simulations of the deformation behavior of an Nb nanowire embedded in a NiTi shape memory alloy. **2022**, 228, 117764 0
- 498 Theoretical prediction of lanthanum composition effects on structural, electronic and thermal properties of  $\text{La}_x\text{Sc}_{1-x}\text{N}$  alloys. **2022**, 96,

- 497 A systematic DFT study of  $(\text{Ti}_3/2\text{RE}_{1/2})\text{AlC}$  alloys: A new database for adjustable mechanical and electronic properties. **2022**, e00681
- 496 Exploring structural, electronic, optical, and magnetic properties of Os doped and Os-Mn/Ru co-doped GaN. **2022**, 258, 168930 ○
- 495 Physical properties of  $\text{LiXH}$  ( $X = \text{B, Al}$ ) hydrogen storage materials: ab-initio study. **2022**, 347, 114731 1
- 494 Ferromagnetism in V and Cr doped ScN diluted magnetic semiconductor in B3 phase: A DFT study. **2022**, 347, 114724
- 493 First-principles calculations of electronic and optical properties of  $\text{AgGa}_{1-x}\text{Tl}_x\text{S}_2$  alloys: Analyses and design for solar cell applications. **2022**, 309, 122996 1
- 492 Ab initio investigations of electronic structure, mechanical properties, phonon stability, and thermodynamics of the MgBr system. **2022**, 199, 110968 ○
- 491 First-principles study of half-metallic properties in  $\text{X}_2\text{CrAl}$  ( $X = \text{Co and Mn}$ ) FullHeusler and their quaternary  $\text{MnCoCrAl}$  and  $\text{CoMnCrAl}$  compounds. **2022**, 139, 109408 ○
- 490 New insights into the piezoelectric, thermodynamic and thermoelectric properties of lead-free ferroelectric perovskite  $\text{Na}_{0.5}\text{Bi}_{0.5}\text{TiO}_3$  from Ab initio calculations. **2022**, 31, 103371 1
- 489 A comparative study in rocksalt and zincblende structured binary and doped alkaline earth pnictides SrP and SrAs by first-principles perspective. **2022**, 31, e00674 ○
- 488 First-principles quantum-computational analysis on the interplay between intermagnetic and intermetallic properties of lead-doped cerium-bismuthides  $\text{CePb}_x\text{Bi}_{1-x}$ : A new example of heavy-fermionic magnetic conductors. **2022**, 31, e00668 1
- 487 New half-metallic ferromagnetic oxides  $\text{XBe}_3\text{O}_4$  ( $X = \text{Li and Na}$ ). **2022**, 31, e00665 ○
- 486 A DFT study of electronic, optical and thermoelectric properties of Ge-halide perovskites  $\text{CsGeX}_3$  ( $X = \text{F, Cl and Br}$ ). **2022**, 31, e00663 1
- 485 Atomistic prediction on the composition- and configuration-dependent bandgap of  $\text{Ga}(\text{As,Sb})$  using cluster expansion and ab initio thermodynamics. **2022**, 280, 115713 ○
- 484  $d_{0\bar{1}1}$  half-Heusler compounds as a potential class of three-dimensional Chern insulators. **2022**, 280, 115710 ○
- 483 Taming the optical response via (Ca:Zr) co-doped impurity in c-BaTiO<sub>3</sub>: A comprehensive computational insight. **2022**, 144, 106573 1
- 482 Magneto-electronic, mechanical and thermoelectric properties of high-temperature phase of  $\text{Sr}_2\text{CrSbO}_6$  double perovskite oxide. **2022**, 31, 103393
- 481 Zirconium aluminides studied with first principles calculations: Hyperfine interactions and site preference of dopants. **2022**, 310, 123042
- 480 First-principles study of optoelectronic and thermoelectric properties of  $\text{LiCaX}$  ( $X = \text{N, P and As}$ ) half-Heusler semiconductors. **2022**, 310, 123020 ○

- 479 Probing the physical properties of Boron Nitride with randomly distributed vacancies: A promising semiconductor for optoelectronics. **2022**, 348-349, 114744 1
- 478 About the gold properties and the approximations used to calculate high-pressure high-temperature properties. **2022**, 31, e00673 0
- 477 First principles calculations of structural, electronic, elastic and thermodynamic properties of ZnNi<sub>3</sub>X (X = N and C). **2022**, 31, e00676 0
- 476 Investigating a novel magnetic MAX phase nitride and its (001)-surfaces. **2022**, 31, 103456
- 475 Electronic, magnetic, elastic, thermal and thermoelectric proprieties of CoMnZ (Z=Al, Ge, Sn).. **2022**, 114, 108165 0
- 474 Manipulation of the ferromagnetic ordering in magnetic semiconductor (La,Ca)(Zn,Mn)AsO by chemical pressure. **2022**, 554, 169276
- 473 Elucidating the influence of high pressure on magnetic attributes of NdFeO<sub>3</sub>. **2022**, 220, 115796 0
- 472 Proposition of new stable rare-earth ternary semiconductor sulfides of type LaTlS<sub>2</sub> (La= Er, Eu, Tb): Ab-initio study and prospects for optoelectronic, spintronic and thermoelectric applications. **2022**, 146, 106662 0
- 471 Dynamical and mechanical stability, electronic properties, bonding and weak interactions analysis of new compounds MgS<sub>2</sub> and MgSe<sub>2</sub> in Pa<sub>3</sub>? space group structure: Ab initio study. **2022**, 146, 106659 1
- 470 First-Principles Study of Electronic Structure And Physical Properties of IIIIN Semiconductors. **2021**, 15, 949-953
- 469 First-Principles Calculations of Structural, Thermodynamic, and Elastic Properties of Lead Chalcogenides PbX (X = S, Se, and Te) in NaCl (B1) Phase. **2021**, 66, 2084-2090 1
- 468 A comprehensive computational investigations on the physical properties of TiXSb (X: Ru, Pt) half-Heusler alloys and Ti<sub>2</sub>RuPtSb<sub>2</sub> double half-Heusler. **2022**, 122, 1 1
- 467 Molecular Dynamics Simulation of the Soret Effect on Two Binary Liquid Solutions with Equimolar -Alkane Mixtures.. **2022**, 7, 518-527 1
- 466 Prediction study of magnetic stability, structural and electronic properties of Heusler compounds Mn<sub>2</sub>ZPtZ (Z = V, Co): DFT+U+TB-mBJ calculation. **2022**, 96, 1
- 465 Pentagraphite C8 : An all- sp<sup>2</sup> topological nodal-line semimetal. **2021**, 104, 2
- 464 On the possibility that PbZrO<sub>3</sub> not be antiferroelectric. **2021**, 7, 2
- 463 Theoretical prediction of anisotropic in elasticity, density of states and thermodynamic properties of TiX (X = Fe, Co, Zn). **2021**, 94, 1
- 462 Thermodynamic Calculation of Fe<sub>3</sub> and Fe<sub>2</sub> Melting Diagrams at Pressures from 0.1 MPa to 7 GPa. **2021**, 22, 531-538 1

461	Structural, elastic, electronic and optical investigations of fluoride-perovskite NaBeF <sub>3</sub> : first-principles calculations. <b>2022</b> , 102, 634-649	2
460	Pressure induced structural phase transitions of technologically significant mercurous chloride at room temperature: An account from first-principle DFT and Born-Oppenheimer molecular dynamics studies. <b>2021</b> , 130, 225103	0
459	The effect of uniaxial stress on magneto-electronic properties and band Jahn-Teller distortion of Ni <sub>2</sub> MnGa Heusler alloy: an ab initio study. 1-16	0
458	Theoretical investigations of physical properties of Pt-based half-Heusler alloys PtMnZ (Z = Se, Sn, Te) for spintronic applications. 1-21	
457	Structural, Electronic and Magnetic Properties of CaSe Doped with 3d (V, Cr and Mn). <b>2021</b> , 11,	
456	Effect of Ti incorporation on the electronic structure and optical properties of MoS <sub>2</sub> (a first principle study). <b>2021</b> , 96, 125878	0
455	Electron structure and thermodynamics of solid solutions in Ni <sub>3</sub> Al system. <b>2018</b> , 2, 101-109	3
454	First Principles Calculations of Structural, Electronic and Optical Properties of Sn-Doped ZnS.	
453	Enhancing efficiency and scope of first-principles quasiharmonic approximation methods through the calculation of third-order elastic constants. <b>2022</b> , 6,	0
452	The elastic, mechanical, and thermodynamic properties of NaXH (X = B, Al) intended for the storage of hydrogen: An ab-initio study. <b>2022</b> , 413851	0
451	Impact of 3d-transition metal [T = Sc, Ti, V, Cr, Mn, Fe, Co] on praseodymium perovskites PrTO <sub>3</sub> : standard spin-polarized GGA and GGA+U investigations. <b>2022</b> , 45, 1	0
450	Abnormal Evolution of a Layered Structure and Band Gap in AgInP <sub>2</sub> S <sub>6</sub> under Compression.	
449	Temperature- and Pressure-Dependent Phonon Dynamics Properties of Gallium Selenide Telluride.	0
448	First-principles calculations for fundamental and spectroscopic screening of hybrid perovskite (HC(NH <sub>2</sub> ) <sub>2</sub> PbI <sub>3</sub> ) formamidinium lead iodide. <b>2022</b> , 126149	1
447	Uncertainty quantification for a multi-phase carbon equation of state model. <b>2022</b> , 131, 155104	1
446	Data_Sheet_1.doc. <b>2020</b> ,	
445	First-Principles Insights into Complex Interplays Among Nano-Phases in an Al-Cu-Li-Zr Alloy.	
444	Pressure-Induced Structural Phase Transitions on Multiferroic Ca <sub>m</sub> N <sub>7</sub> O <sub>12</sub> .	

- 443 Assessment of the Heat Capacity by Thermodynamic Approach Based on Density Functional Theory Calculations.
- 442 Effect of doping titanium ions on semi-conducting behavior, photovoltaic, and thermoelectric perovskite-type oxides  $VSc_{1-x}Ti_xO_3$ : Ab-initio study. 1
- 441 Atomistic simulations of magnetoelastic effects on sound velocity. **2022**, 105, 0
- 440 The Effect of Pressure on Band Parameters and Optical Characteristics in Indium Nitride. 0
- 439 Machine-learning correction to density-functional crystal structure optimization. 1 1
- 438 Structural, electronic and optical properties of  $Be_2X$  ( $X=C, Si, Ge$ ,. **2022**, e00693
- 437 Valence fluctuation driven superconductivity in orthorhombic lead telluride. **2022**, 105,
- 436 Investigation of the Structural, Elastic, Electronic, and Optical Properties of Half-Heusler  $CaMgZ$  ( $Z = C, Si, Ge, Sn, Pb$ ) Compounds. 1 2
- 435 Equation of state for generalized pressure. **2022**, 105, 1
- 434 Structural, electronic, mechanical, and thermodynamic properties of  $Cu_{1-x}Ti_x$  intermetallic compounds: First-principles calculations. **2022**, 114814 0
- 433 Exploring the exemplary structural, electronic, optical and elastic nature of inorganic ternary cubic fluoroperovskites  $XBaF_3$  ( $X= Al$  and  $Tl$ ) employing the accurate TB-mBJ approach. 0
- 432 Green synthesis of AgCl nanoparticles using *Calotropis gigantea*: Characterization and their enhanced antibacterial activities. **2022**, 139699 0
- 431 Thermodynamics and Magnetism of  $SmFe_{12}$  Compound Doped with Co and Ni: An Ab Initio Study. **2022**, 12, 4860 2
- 430 Structural and electronic properties of the random alloy  $Zn_{1-x}S_x$ . **2022**, 105,
- 429 First-principles calculations to investigate structural, electronic and phonon properties of sodium bromide (NaBr) and sodium iodide (NaI) crystals. **2022**, 31, e00682 0
- 428 Cyclic and tensile deformations of Gold/Silver core shell systems using newly parameterized MEAM potential. **2022**, 169, 104304 0
- 427 Density functional study of electronic, elastic and optical properties of  $GaAs_{1-x}N_x$  ( $x=0, 0.25$ . **2022**, 31, e00689
- 426 Influence of hydrostatic pressure and concentration of Ge on the topological band order of  $SnSi_{1-x}Ge_x$  alloys. **2022**, 281, 115742 0

- 425 Pursuit of stability, electronic and thermoelectric properties of novel PdVGa half heusler compound. **2022**, 351, 114796 ○
- 424 Spin polarized study of alkaline earth-cubic lead perovskites (PbXO<sub>3</sub>, X = Mg, Ca & Sr) for emerging spintronic technology. **2022**, 590, 126699 ○
- 423 Enhanced thermoelectric performance from bulk to monolayer BiSbS<sub>3</sub> from first principle study. **2022**, 211, 111497
- 422 Antiperovskite materials as promising candidates for efficient tandem photovoltaics: First-principles investigation. **2022**, 147, 106727 ○
- 421 Exciton properties, optical phonon modes, polaron characteristics and plasma frequency of GaSb upon compression. **2022**, 147, 106694 ○
- 420 An efficient and stable lead-free organic-inorganic tin iodide perovskite for photovoltaic device: Progress and challenges. **2022**, 8, 5753-5763 1
- 419 Study of phase transitions and lattice dynamics, elastic and electronic properties, bonding and weak interactions analysis of YCuS<sub>2</sub> in P212121, I4<sub>1</sub>2d and P. **2022**, 167, 110756
- 418 Electronic and magnetic properties of iridium-based novel Heusler alloys. **2022**, 555, 169405
- 417 Thermodynamic description of high-pressure phase equilibria in the Fe-N system. **2022**, 914, 165304
- 416 Delving into guest-free and He-filled sI and sII clathrate hydrates: a first-principles computational study. **2022**, ○
- 415 Verification of stability and unraveling the electronic and physical properties of bulk and (001)-surfaces of newly synthesized Ti<sub>2</sub>ZnX (X = C, N) MAX phases. **2022**, 102032 1
- 414 Chemical pressure enlarged camouflage color zone in Mn(IV)-activated yellow-green pigments. **2022**, 25, 100902
- 413 Physical characteristics of ferromagnetic Cr-based LiCr<sub>2</sub>X<sub>4</sub> (X = S, Se) spinels for spintronic and solar energy devices applications. **2022**, 137, ○
- 412 A comprehensive analysis on elastic, mechanical, thermodynamic and thermoelectric properties of PbSnO<sub>3</sub>: A density functional theory study. ○
- 411 Deep potential development of transition-metal-rich carbides.
- 410 Pressure-induced electronic transitions in samarium monochalcogenides. **2022**, 105, ○
- 409 Density functional study of structural and optoelectronic properties of wurtzite Mg<sub>1-x</sub>Zn<sub>x</sub> ternary alloys. **2022**,
- 408 Investigation of novel quaternary Heusler alloys XRuCrZ (X = Co, Ni, Rh, and Pd; Z = Si and Ge) via first-principles calculation for spintronics and thermoelectric applications. **2022**, 12, 055223 1

- 407 The effect of N-incorporation on the structural and optoelectronic properties of GaP and GaAs for optical telecommunication applications: First-principles study. **2022**, 262, 169282
- 406 The stability analysis and efficiency of the new MAX-phase compounds  $M_3\text{GaC}_2$  (M: Ti or Zr): A first-principles assessment. **2022**, 38, 105621 1
- 405 Electronic structure, optical and elastic properties of  $\text{AgAlS}_2$  crystal under hydrostatic pressure. **2022**, 148, 106814 0
- 404 Physical properties of  $\text{KTaO}_3$  compound for optoelectronic and thermoelectric applications: A DFT study. **2022**, 148, 106811 0
- 403 Bismides ternary alloys  $\text{GaSb}_1-x\text{Bi}_x$ : Structural, optoelectronic, and thermodynamic properties under pressure.
- 402 Pressure-Induced Enhanced Optical Absorption in Sulfanite Compound  $\text{Cu}_3\text{TaX}_4$  (X = S, Se, and Te): An ab Initio Study. 1
- 401 Effects of Electron Correlations on the Magnetic Stability of  $\text{Rh}_2\text{TMSn}$  Full Heusler Alloys (TM=Cr, Mn, and Fe).
- 400 Revisiting Activity Tuning Using Lattice Strain: CO Decomposition in Terrace  $\text{Ru}(0001)$  and Stepped  $\text{Ru}(1015)$  Surfaces.
- 399 A comparative investigation of different exchange-correlation functionals oriented prediction of structural, electronic, optical, and transport properties of the novel quaternary  $\text{LiTiCoSn}$ .
- 398 Unraveling the  $\text{MnMoO}_4$  polymorphism: a comprehensive DFT investigation of  $\beta$  and  $\gamma$  phases. 0
- 397 Structural, electronic and elastic properties of  $\text{FeCrAs}$  Half-metallic ferromagnetic Half-Heusler Alloy: A First-Principles study. **2022**,
- 396 Investigating the potential of lead-free double perovskite  $\text{Cs}_2\text{AgBiBr}_6$  material for solar cell applications: A theoretical study. 1
- 395 Investigations of martensitic, thermodynamics, elastic, electronic, magnetic, thermal and thermoelectric properties of  $\text{Co}_2\text{FeZ}$  Heusler alloys (Z=Si; Ge; Al; Ga): a first principle study. 1
- 394 The study of optical and thermoelectric behaviour of thalium based flouropervoskite ( $\text{TlSiF}_3$ ) for photovoltaic and renewable energy applications by DFT. **2022**, 123266 0
- 393 Evaporation of dark matter from celestial bodies. **2022**, 2022, 042 0
- 392 Magneto-Electronic and Optical Properties of Full Heusler Alloy,  $\text{Y}_2\text{FeSi}$ : a First Principle Calculation With and Without Spin-Orbit Coupling Effect. 0
- 391 First-principles calculations to investigate the structural, mechanical, electronic, magnetic and thermodynamic characteristics of the full-Heusler alloys  $\text{Pd}_2\text{MnSb}$ ,  $\text{Pd}_2\text{MnIn}$ , and  $\text{Pd}_2\text{MnSb}_{1-x}\text{In}_x$  ( $x = 0.25, 0.5, 0.75$ ). **2022**, e00697
- 390 Theoretical insights on structural, mechanical and thermodynamic properties of  $\text{MCoB}$  (M=Nb, Mo, and W) ternary borides under high pressure. **2022**, 106931 0



- 389 Classical Force-Field Parameters for CsPbBr<sub>3</sub> Perovskite Nanocrystals. 1
- 388 Physical properties and superconductivity in the cubic A15-type Ta<sub>3</sub>Ge compound: A first principles study. **2022**, 114838
- 387 First-principles prediction of anomalously strong phase dependence of transport and mechanical properties of lithium fluoride. **2022**, 235, 118077 0
- 386 Combined Deep Learning and Classical Potential Approach for Modeling Diffusion in UiO-66. 1
- 385 Ab initio Study of New Fe<sup>n+1</sup>CdC<sub>n</sub> (n = 1B) MAX Material in Its Stable Magnetic Configuration. 0
- 384 Ultra-high efficiency, stability and low-cost perovskite solar cell materials Cs<sub>2</sub>Zr<sub>1-x</sub>Ti<sub>x</sub>I<sub>6</sub>. **2022**, 282, 115794 1
- 383 Comparative study of the fundamental properties of Ga<sub>2</sub>O<sub>3</sub> polymorphs. **2022**, 312, 123272
- 382 An Analytic Overview of Equations of Substantial State in Plasmonic Perspective. **2022**, 41-119
- 381 Thermodynamic Calculations of the Fe-Ta Melting Diagram in the Context of Gallium Nitride Crystallization under High Temperatures and Pressures. **2022**, 44, 73-78
- 380 Structural, electronic, magnetic, optical and thermoelectric properties of Co<sub>2</sub>Fe<sub>1-x</sub>Ti<sub>x</sub>Al alloys: GGA and GGA+U approaches. 1
- 379 Piezochromic luminescence of dicoronylene: Key for revealing hidden Raman modes at high pressure. **2022**,
- 378 First-principles insights into thermoelectric properties of topological nontrivial semimetal LiAuTe material. **2022**, 97, 075703
- 377 First-principles prediction of the half-metallicity in quaternary Heusler CoRhCrAl thin films. **2022**, 97, 075812
- 376 Nonlinear Arrhenius behavior of self-diffusion in Ti and Mo. **2022**, 6,
- 375 First-principle study of structural, dynamical, elastic, electronic, optical and thermodynamic properties of Na<sub>2</sub>ZnSn<sub>4</sub> compound.
- 374 Thermodynamic behavior of Na-majorite and knorringite-majorite garnet systems. **2022**, 1-8
- 373 Phosphide in gallium bismuth: structural, electronic, elastic, and optical properties of GaP<sub>x</sub>Bi<sub>1-x</sub> alloys. **2022**, 28,
- 372 Computational delving into conceivable thermoelectric and spintronic applications of NH<sub>4</sub>AF<sub>3</sub> (A = Fe and Co) ferromagnets.

- 371 The electronic, magnetic and half-metallic predictions of  $M_x$  ( $M = \text{Ag, Cd, Y, Zr, Nb}$ , and  $x = 0, 0.125, 0.25, 1$ ) $W_{1-x}\text{Sn}$  alloys. 1-24 0
- 370 Insight into the spin-polarized structural, electronic, and magnetic properties of  $\text{Nd}_2\text{GaO}_4$  and  $\text{Nd}_2\text{InO}_4$  compounds. **2022**, 137, 0
- 369 Heavy thallium based fluoroperovskite  $\text{TlAF}_3$  ( $A = \text{Ge, Sn and Pb}$ ) compounds: a computational investigation. **2022**, 54, 0
- 368 Solid-state performance of a meta-GGA screened hybrid density functional constructed from Pauli kinetic enhancement factor dependent semilocal exchange hole. 1
- 367 Elastic Anisotropy of 1,3,5-Triamino-2,4,6-Trinitrobenzene as a Function of Temperature and Pressure: A Molecular Dynamics Study. 0
- 366 The Structural, Mechanical, Lattice Dynamical, and Thermal Properties of 3D Dirac Semimetals  $\text{BaXBi}$  ( $X = \text{Cu, Ag, Au}$ ) from First-Principles Calculations. 2200132
- 365 Thermoelectric properties and thermal stability of ferromagnetic half metallic  $\text{CoVTe}$  alloy, first principles study. 1-20
- 364 Density functional theory study on the magneto-electronic, mechanical, thermal, and transport properties of a novel  $\text{Co}_2\text{VGa}_{0.5}\text{Al}_{0.5}$  quaternary Heusler alloy. 0
- 363 Characterization of quaternary Heusler alloys  $\text{CoFeYGe}$  ( $Y = \text{Ti, Cr}$ ) with respect to structural, electronic, magnetic, mechanical, and thermoelectric features. 0
- 362 Effect of Strain on the Electronic Structure and Phonon Stability of  $\text{SrBaSn}$  Half Heusler Alloy. **2022**, 27, 3785 1
- 361 First-principles calculations to investigate structural, electronic, thermoelectric, and optical properties of heavy thallium perovskite  $\text{TlPbX}_3$  ( $X = \text{Cl, Br, I}$ ). **2022**, 283, 115781 0
- 360 Probing the chemical reactivity of the  $\text{B}_2\text{O}_3$  -I (1 0 1) Surface: Interaction with  $\text{H}_2\text{O}$  and  $\text{H}_2\text{S}$ . **2022**, 599, 153999
- 359 Experimental methods, apparatuses and results of experimental measurements of the thermodynamic properties. **2022**, 13-249
- 358 Influence of High Pressure on  $\text{Ce}^{3+}$  Luminescence in  $\text{LuAlO}_3$  and  $\text{YAlO}_3$  Single Crystals and Single Crystalline Layers.
- 357 Conceptual Density Functional Theory under Pressure: Part I. XP-PCM Method Applied to Atoms. 0
- 356 Orthorhombic  $\text{C}_32$ : A Topological Semimetal with Nodal Ring.
- 355 First-Principal Study of Structural, Elastic, Electronic and Magnetic Properties for the Ternary and Quaternary Heusler Compounds  $(\text{CoFe}_{1-x})_2\text{CrSn}$ .
- 354 Thermal and mechanical properties of the clathrate-II  $\text{Na}_{24}\text{Si}_{136}$ . **2022**, 105, 0

- 353 DFT insights into half metallic ferromagnetism of new cubic Perovskite  $\text{VYO}_3$  for spintronics application. **2022**,
- 352 Phase evolution and thermal stability of novel high-entropy  $(\text{Mo}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2}\text{V}_{0.2}\text{W}_{0.2})\text{Si}_2$  ceramics. **2022**, 0
- 351 Electronic-structural, thermo-electric, and thermo-mechanical properties of  $\text{M}_2\text{AC}$  and  $\text{M}_2\text{AB}$  ( $\text{M} = \text{Nb}$  or  $\text{Mo}$ ,  $\text{A} = \text{Al}$  or  $\text{Ga}$ ) compounds.
- 350 First-principles calculations to investigate new ferromagnetic quaternary Heusler alloys  $\text{FeZrTiZ}$  ( $\text{Z} = \text{Si}, \text{Sn}, \text{Pb}$ ): Compatible for spin polarized device and waste heat recovery applications. **2022**, 106964 1
- 349 The Stability and Electronic and Thermal Transport Properties of New Tl-Based MAX-Phase Compound  $\text{Ta}_2\text{TiX}$  ( $\text{X}: \text{C}$  or  $\text{N}$ ). 2200195 0
- 348 Emerging study on lead-free hybrid double perovskite  $(\text{CH}_3\text{NH}_3)_2\text{AgInBr}_6$ : Potential material for energy conversion between heat and electricity. 2
- 347 Exploration of glassy state in Prussian blue analogues. **2022**, 13, 1
- 346 On the structure of  $\text{SbTe}$ . **2022**, 132, 015106 1
- 345 A first-principles investigation of electronic structure and ferromagnetic properties in alkali metal-doped  $\text{ZnS}/\text{Se}$  semiconductors.
- 344 First-principles calculations on the electronic structure and thermoelectric properties of quaternary Heusler compounds:  $\text{LiScPtSi}$  and  $\text{LiScPdGe}$ . **2022**, 103961
- 343 Theoretical study of electronic, magnetic, optical and thermoelectric properties of  $\text{XMnO}_2$  ( $\text{X} = \text{Au}, \text{Ag}, \text{Cu}$ ) oxides by DFT. **2022**, 123432 1
- 342 Predicting Speed of Sound in Fatty Acid Alkyl Esters and Biodiesels at High Pressure. 1
- 341 Investigating the Structural Symmetrization of  $\text{CsI}_3$  at High Pressures through Combined X-ray Diffraction Experiments and Theoretical Analysis. **2022**, 61, 10977-10985 0
- 340 Ground-state properties of p-type delafossite transparent conducting oxides  $2\text{H-CuMO}_2$  ( $\text{M} = \text{Al}, \text{Sc}$  and  $\text{Y}$ ): DFT calculations. **2022**, 32, 103995
- 339 Equation of state, thermoelastic properties and melting curves of some intermetallic compounds  $\text{LiBC}$ ,  $\text{MgB}_2$  and  $\text{TiB}_2$ . **2022**, 32, e00710
- 338 Exchange-correlation and spin-orbit coupling effects in 18-electrons transparent conductors half-Heusler: Ab-initio study. **2022**, 32, e00690 1
- 337 DFT calculations of solute-vacancy binding in Zirconium-based  $\text{ZrNbSn}$  alloy. **2022**, 32, 101221
- 336 Structural, electronic, and optical properties of rare-earth-doped  $\text{SrTiO}_3$  perovskite: A first-principles study. **2022**, 643, 414160 0

- 335 First principles study of the structural stability, lattice dynamics, optical and thermoelectric properties of NaSrX(X = As, Sb and Bi). **2022**, 149, 106840 1
- 334 First-principles investigations of Na<sub>2</sub>CuMCl<sub>6</sub> (M = Bi, Sb) double perovskite semiconductors: Materials for green technology. **2022**, 150, 106947 1
- 333 Analysis of structural, elastic and optoelectronic properties of indium-based halide perovskites InACl<sub>3</sub> (A = Ge, Sn, Pb) using density functional theory. **2022**, 150, 106973 0
- 332 Effects of transition metal doping on CsGeBr<sub>3</sub> perovskite: First-principles study. **2022**, 12, 075122
- 331 First-principal study of structural, elastic, electronic and magnetic properties for the ternary and quaternary Heusler Compounds (Co<sub>x</sub>Fe<sub>1-x</sub>). **2022**, e00720
- 330 Temperature-dependent bandgap of (In,Ga)As via : A ython ackage for roperty rediction of pseudobinary systems using canonical ensemble. **2022**, 804, 139887
- 329 Investigations of Lead Free Halides in Sodium Based Double Perovskites Cs<sub>2</sub>NaBiX<sub>6</sub>(X=Cl, Br, I): an Ab Initio Study. **2021**, 74-80 0
- 328 Ab-Initio Study of Structural, Mechanical, and Dynamical Stability, Electronic, Thermal, and Optical Properties of Silver Halide Ag<sub>x</sub> (X = F, Cl, Br, and I) Semiconductors.
- 327 Rhodium-based half-Heusler alloys as thermoelectric materials. **2022**, 24, 19844-19852 1
- 326 Compositional Glass: A State with Inherent Chemical Disorder, Exemplified by Ti-rich Ni<sub>3</sub>(Al,Ti)<sub>1</sub>D<sub>024</sub> Phase. **2022**, 12, 1049
- 325 Uniting Nonempirical and Empirical Density Functional Approximation Strategies Using Constraint-Based Regularization. **2022**, 13, 6896-6904 0
- 324 Low electronic conductivity of Li<sub>7</sub>La<sub>3</sub>Zr<sub>2</sub>O<sub>12</sub> solid electrolytes from first principles. **2022**, 6, 1
- 323 Computational Study of Elastic, Structural, Electronic, and Optical Properties of GaMF<sub>3</sub> (M = Be and Ge) Fluoroperovskites, Based on Density Functional Theory. **2022**, 27, 5264
- 322 First-Principles Study of the 30° and 90° Partial Dislocations in HgTe, CdTe, and Hg<sub>0.7</sub>Cd<sub>0.3</sub>Te. 2200180 0
- 321 Density Functional Theory assessment of the lithiation thermodynamics and phase evolution in Si-based amorphous binary alloys. **2022**,
- 320 First-principles study the structural phase transition, elastic and thermodynamic properties of HfCr<sub>2</sub>.
- 319 Phase transitions and compressibility of alkali-bearing double carbonates at high pressures: a first-principles calculations study. **2022**, 49,
- 318 Structural, Elastic, Electronic, Magnetic, and Thermoelectric Characteristics of MgEu<sub>2</sub>X<sub>4</sub> (X = S, Se) Spinel Compounds: Ab-Initio Calculations. 2200191

- 317 Structural, elastic, electronic, optic and thermodynamic properties of  $\text{Li}_2\text{BaSnX}_4$  (X= S and Se) alloys: A first-principle study. **2022**, e00718 ○
- 316 Role of exact exchange in the structural and electronic properties of the  $\text{Fm}\bar{3}\text{m}$  and  $\text{I}4\text{mm}$  phases of Cerium: a density functional theory study.
- 315 Computational study of  $\text{Cs}_2\text{ScXBr}_6$  (X=Ag, Tl) for renewable energy devices. **2022**, 414277
- 314 Thermodynamic phase diagrams, thermoelectric, and half-metallic properties of  $\text{KCaX}_2$  (X=N, O) and their [001] films.
- 313 Theoretical Study of Half-Heusler  $\text{CsXAs}$  (X = Ca, Sr, and Ba) from First Principle Calculations. ○
- 312 Stability, magnetic, electronic, elastic, thermodynamic, optical, and thermoelectric properties of  $\text{Co}_2\text{TiSn}$ ,  $\text{Co}_2\text{ZrSn}$  and  $\text{Co}_2\text{HfSn}$  Heusler alloys from calculations using generalized gradient approximation techniques. 1
- 311 First-Principle Study of the Thermodynamic Properties of  $\text{VSb}_2$  Compound as a Function of Pressure and Temperature. 418, 3-9
- 310 First-Principles Investigation of Structural, Elastic, Thermoelectric, Electronic, and Optical Properties of Ordered Double Perovskite  $\text{Ba}_2\text{MWO}_6$  (M = Mg, Zn, and Cd). ○
- 309 Broad Elastic Softening of (Mg,Fe)O Ferropericlase Across the Iron Spin Crossover and a Mixed-Spin Lower Mantle. **2022**, 127,
- 308 Short-Range Crystalline Order-Tuned Conductivity in  $\text{Cr}_2\text{Si}_2\text{Te}_6$  van der Waals Magnetic Crystals. **2022**, 16, 13134-13143 1
- 307 Thermoelectric and optoelectronic properties of novel lead-free halide perovskites  $\text{CsRbTiX}_6$  (X= I, Br and Cl) for photovoltaic applications. **2022**, e00733 ○
- 306 The half-metallic predictions of M (M = Y, Zr, Nb) $\text{BcBn}$  diluted ternary alloys via GGA and GGA + mBJ. **2022**, 95, ○
- 305 Ab initio investigation of the magnetic and ferroelectric properties of  $\text{BaCuF}_4$  under hydrostatic pressure. **2022**, 106,
- 304 Consequences of Tuning Rare-Earth RE3+-Site and Exchange-Correlation Energy U on the Optoelectronic, Mechanical, and Thermoelectronic Properties of Cubic Manganite Perovskites  $\text{REMnO}_3$  for Spintronics and Optoelectronics Applications. **2022**, 7, 27903-27917 ○
- 303 Novel semiconductor compounds  $\text{XZrZ}$  (X =Ni, Cu and Z=C, B) suitable for clean energy in optoelectronic and thermoelectric devices. **2022**, 32, e00730 ○
- 302 First-principles investigation on narrow bandgap  $\text{InSb}_{1-x}\text{Bi}_x$  dilute bismide alloys for highly efficient long-wavelength infrared optoelectronics. **2022**, 125, 104319 ○
- 301 Pressure induced modulations in the optoelectronic properties of  $\text{Hg}_2\text{Cl}_2$  compound: Insights from the first-principle calculations. **2022**, 284, 115903
- 300 Cobalt-based full Heusler compounds  $\text{Co}_2\text{FeZ}$  (Z = Al, Si, and Ga): A comprehensive study of competition between XA and L21 atomic ordering with ab initio calculation. **2022**, 284, 115906 ○

- 299 Computational insights into the relation between elements physical properties and mechanical properties of 3d, 4d, and 5d transition metal carbides via machine learning. **2022**, 354, 114896
- 298 Structural modeling of ZnFe<sub>2</sub>O<sub>4</sub> systems using Buckingham potentials with static molecular dynamics. **2022**, 354, 114914
- 297 First-principles prediction of thermodynamic properties and mechanical properties of Ti<sub>2</sub>AX (A=Al, Ga; X=C, N) M<sub>2</sub>AX phase at different pressures and temperatures. **2022**, 204, 111380
- 296 First-principles WC-GGA and mBJ calculations for structural, electronic, optical and elastic properties of M<sub>x</sub>Ga<sub>1-x</sub>Sb (M=Al, In, B) ternary alloys. **2022**, 151, 107033
- 295 Electronic structure and magnetic properties of bulk and (001) surfaces of  $\eta$ -Fe<sub>4</sub>C from first principles. **2022**, 562, 169741
- 294 Mechanical, thermal, electronic, and magnetic properties of Ca<sub>0.75</sub>Er<sub>0.25</sub>S alloy from a DFT approach: A promising material for spintronic applications. **2022**, 33, 104237
- 293 Effect of 5d state-based full-Heusler alloys on the structural, electronic and magnetic properties of new half metallic ferromagnetism. **2022**, 33, 104277 ○
- 292 Synchrotron radiation X-ray diffraction and Raman spectroscopy study of l-asparagine monohydrate doped with Fe(III) at high pressure. **2022**, 283, 121716
- 291 Validation of lattice Boltzmann based software for blood flow simulations in complex patient-specific arteries against traditional CFD methods. **2023**, 203, 957-976 1
- 290 Investigation of the structural properties and the magneto-electronic performances in new Ba<sub>1-x</sub>Cr<sub>x</sub>S materials. **2022**, 54, ○
- 289 Theoretical investigations on electronic and optical properties of half heusler alloy, FeNbSb for opto-electronic applications. **2022**, 54, ○
- 288 Pressure induced band gap shifting from ultra-violet to visible region of RbSrCl<sub>3</sub> perovskite. **2022**, 9, 095902 ○
- 287 First-principles insights into complex interplays among nano-phases in an Al-Cu-Li-Zr alloy. **2022**, 239, 118304 ○
- 286 First-principles calculations to investigate electronic, structural, optical, and thermoelectric properties of semiconducting double perovskite Ba<sub>2</sub>YBiO<sub>6</sub>. **2022**, 170, 207397 1
- 285 Orthorhombic C32: A topological semimetal with nodal ring. **2022**, 451, 128397 ○
- 284 Analysis of structural stability and optoelectronic properties of new direct band gap halide double perovskites Cs<sub>2</sub>XRhCl<sub>6</sub>. **2022**, 355, 114928 ○
- 283 Effect of L21 and XA ordering on structural, martensitic, electronic, magnetic, elastic, thermal and thermoelectric properties of Co<sub>2</sub>FeGe Heusler alloys. **2022**, 355, 114932 1
- 282 Effects of atomic displacements on band gaps of Na<sub>2</sub>MgXO<sub>6</sub> (X= Co, Fe) double perovskite oxides: GGA and GGA+U approaches. **2022**, 152, 107078 ○

- 281 Sonohydrothermal-assisted ZnS nanocrystals for improved structural, electronic, and optical properties: Experimental and ab initio methods. **2022**, 286, 115983 ○
- 280 Influence of high pressure on Ce<sup>3+</sup> luminescence in LuAlO<sub>3</sub> and YAlO<sub>3</sub> single crystals and single crystalline layers. **2022**, 252, 119276 ○
- 279 Structural, elastic, electronic, optical and thermoelectric response of lead-free double perovskite Rb<sub>2</sub>TlInX<sub>6</sub> (X=Cl, I) for energy storage devices: DFT+SOC investigations. **2022**, 152, 107081 ○
- 278 Structural stability, mechanical, and optoelectronic properties of new stable phases for the ternary alloy Mg<sub>1-x</sub>Al<sub>x</sub>O. **2022**, 33, e00739 ○
- 277 First principles study of adsorption and simulation of desorption properties of Pd<sub>1-x</sub>Ag<sub>x</sub>. **2022**, 33, e00741 ○
- 276 First-principles calculations to investigate physical properties of single-cubic (Ba<sub>0.82</sub>K<sub>0.18</sub>)(Bi<sub>0.53</sub>Pb<sub>0.47</sub>)O<sub>3</sub> novel perovskite superconductor. **2022**, 33, 104302 4
- 275 Site-dependent mechanical properties of 3d transition metal-doped MnV intrinsic ductile intermetallic: First-principles and data mining study. **2022**, 215, 111801 ○
- 274 The mechanical, dynamical, thermodynamical properties and elastic anisotropies of cubic YbAu compound under pressure. **2022**, 33, 104456 ○
- 273 First principles calculations of structural, electronic and optical properties of Sn-doped ZnS. **2022**, 646, 414335 ○
- 272 B2-disorder effects on the structural, electronic and magnetic properties of Co<sub>2</sub>MnAl Heusler alloy. **2022**, 563, 169871 ○
- 271 Modulation of the optoelectronic properties of CdSe<sub>2</sub>. **2022**, 33, e00745 ○
- 270 First-principles molecular dynamics simulations of UCl<sub>n</sub>MgCl<sub>2</sub> (n = 3, 4) molten salts. ○
- 269 Dft Investigation of Half-Metallic Ferromagnetic Mg<sub>2</sub>X<sub>4</sub> (X = S, Se) Spinel for Spintronic Applications. ○
- 268 An ab initio investigation of the temperature-dependent energetic barriers towards CrAlB and (Mo,Cr)AlB formation in a metastable synthesis scenario. **2022**, 14, 12866-12874 ○
- 267 Structural, electronic, magnetic and elastic properties of xenon-based fluoroperovskites XeMF<sub>3</sub> (M = Ti, V, Zr, Nb) via DFT studies. **2022**, 12, 27508-27516 ○
- 266 Ab initio study of lithium intercalation into a graphite nanoparticle. ○
- 265 A theoretical study of the Pnma and R3 m phases of Sb<sub>2</sub>S<sub>3</sub>, Bi<sub>2</sub>S<sub>3</sub>, and Sb<sub>2</sub>Se<sub>3</sub>. 1
- 264 Understanding the structure-band gap relationship in SrZrS<sub>3</sub> at elevated temperatures: a detailed NPT MD study. **2022**, 10, 12032-12042 ○

- 263 Spintronic Properties in Complex Perovskites: A Concordance Between Experiments and Ab-Initio Calculations. **2022**, 183-207 ○
- 262 Electronic, magnetic, optical and thermoelectric properties of co-doped  $\text{Sn}_{1-x}\text{Mn}_x\text{As}_2\text{O}_7$  (A = Mo, Tc): a first principles insight. **2022**, 12, 28451-28462 ○
- 261 Study of Structural, Elastic, Thermal and Transport Properties of Ternary  $\text{X}(\text{X}=\text{Co}, \text{Rh} \text{ and } \text{Ir})\text{MnAs}$  Obtained by DFT. **2022**, 47-57 ○
- 260 Structural, Thermal, and Electronic Investigation of  $\text{ZrCo}_{1-x}\text{Ni}_x\text{Bi}$  ( $x=0, 0.25, 0.75, \text{ and } 1$ ) Half-Heusler Alloys. **2022**, 103-111 ○
- 259 Structural, thermodynamics, optical, electronic, magnetic and thermoelectric properties of Heusler  $\text{Ni}_2\text{MnGa}$ : An ab initio calculations. **2022**, 54, ○
- 258 Theoretical Investigations into the Different Properties of Al-Based Fluoroperovskite  $\text{AlMF}_3$  (M = Cr, B) Compounds by the TB-MBJ Potential Method. **2022**, 15, 5942 ○
- 257 High Formability Bromide Solid Electrolyte with Improved Ionic Conductivity for Bulk-Type All-Solid-State Lithium Metal Batteries. **2022**, 5, 10604-10610 ○
- 256 Investigating structural, electronic, magnetic, and optical properties of Co-doped and Co-X (X = Fe, Mn) co-doped  $\text{MoS}_2$  for optoelectronic applications. **2022**, 28, ○
- 255 Structural, electronic and magnetic properties of the double perovskite  $\text{Ba}_2\text{GdNbO}_6$  with octahedral tilting effect: first-principles calculations. 1-20 ○
- 254 Novel Class of Rhenium Borides Based on Hexagonal Boron Networks Interconnected by Short B<sub>2</sub> Dumbbells. **2022**, 34, 8138-8152 ○
- 253 Theoretical investigation of magnesium compositional variation of structural and optoelectronic properties of wurtzite  $\text{Mg}_x\text{Zn}_{1-x}\text{Se}$  ternary alloys through first-principle calculations. **2022**, 96, ○
- 252 Pressure Effect on the Speed of Sound of Waste Cooking Oil Biodiesel. ○
- 251 Structural, magnetic, and optoelectronic properties of new ferromagnetic semiconductors  $\text{Cd}_{0.75}\text{Os}_{0.25}\text{S}$  and  $\text{Cd}_{0.75}\text{Ir}_{0.25}\text{S}$ : Insight from DFT computations. **2022**, 54, ○
- 250 Optoelectronic Study of  $\text{CuAlX}_2$  (X = S, Se, Te) Chalcopyrite Semiconductor. **2022**, 96, 1986-1994 ○
- 249 Elastic Properties of Confined Fluids in Nanopores: An Acoustic-Propagation Model. ○
- 248 Theoretical predictions of melting behaviors of hcp iron up to 4000 GPa. **2022**, 106, 1
- 247 Theoretical Investigation of Structural, Electronic, and Optical Properties of  $\text{ZnSnP}_2$  Semiconductor. **2022**, ○
- 246 Structural, elastic, electronic, magnetic, and half-metallic properties of a novel rare earth-based quaternary Heusler Alloys  $\text{LaXTiSi}$  (X = Co, Rh, Ir). ○



- 245 Study of ferromagnetism and thermoelectric behaviour of thiospinels  $\text{MgFe}_2(\text{S/Se})_4$  for spintronics and energy harvesting. ○
- 244 Polymer lubrication: Pressure-viscosity-temperature dependence of film thickness for highly loaded compliant contacts in EHL regime. 1-47 ○
- 243 First-principles study of water incorporation in Fe-containing wadsleyite. **2022**, 106940 ○
- 242 Thermodynamic Dynamic Interrelations in Glass-Forming Polymer Fluids. ○
- 241 Role of doping and defect quenching in antiferroelectric  $\text{NaNbO}_3$  from first principles. **2022**, 106, ○
- 240 Computational study of structural, electronic, elastic and vibrational properties of  $\text{LiAlSi}$ ,  $\text{NaAlSi}$ , and  $\text{KAlSi}$  Half-Heusler alloys. ○
- 239 Phase stability of  $(\text{Al}_x\text{Ga}_{1-x})_2\text{O}_3$  polymorphs: A first-principle. **2022**, 6, ○
- 238 Structural, Elastic Stability, Electronic, and Magnetic Properties of the Quaternary Heusler Alloy  $\text{CoMnVSi}$ : An Ab Initio Study. **2022**, 96, 2166-2172 ○
- 237 Electronic and Magnetic Properties of  $\text{Mn}_2\text{YSn}$  ( $\text{Y} = \text{Ru, Rh, and Pd}$ ) Heusler Alloys Under Hydrostatic Pressure. ○
- 236 Density, Speed of Sound, Compressibility, and Excess Properties in a Carbon Dioxide + n-Docosane Binary Mixture from 10 to 70 MPa. ○
- 235 Structural, electronic, elastic, vibrational and thermodynamic properties of antiperovskites  $\text{Mg}_3\text{NX}$  ( $\text{X} = \text{Ge, Sn}$ ): A DFT study. **2022**, 453, 128478 2
- 234 Impact of a dopant vis-a-vis site and concentration on the photovoltaic effect of  $\text{BiFeO}_3$ . **2022**, 647, 414366 ○
- 233 Stabilities and half-metallic ferromagnets features of new quaternary Heusler alloys  $\text{RhCoVX}$  ( $\text{X} = \text{Si, Ge and Sn}$ ). Ab-initio study. **2022**, 33, e00753 ○
- 232 First principles investigations of optoelectronic and magnetic properties of co-doped zinc sulphide by 3d and 4f elements. **2022**, 33, e00746 ○
- 231 Structural, magnetic, electric and electronic aspects of the  $\text{Ba}_2\text{YbSbO}_6$  perovskite material. 161-171 ○
- 230 FIRST-PRINCIPLES CALCULATIONS OF THE STRUCTURAL, ELECTRONIC AND ELASTIC PROPERTIES OF  $\text{SrGeO}_3$  AND  $\text{SrZrO}_3$  CUBIC PEROVSKITES.. **2021**, 6, 7-18 ○
- 229 Tight Binding and Density Functional Theory of Tailoring Electronic Properties in  $\text{Al}_{1-x}\text{In}_x\text{N}/\text{AlN}/\text{GaN}$  High Electron Mobility Transistors (HEMTs). **2022**, 669-707 ○
- 228 Combined description of pressure-volume-temperature and dielectric relaxation of several polymeric and low-molecular-weight organic glass-formers using SL-TS2 approach. 1

- 227 Structural, and electronic properties of ZnX (X = S, Se, Te) by first-principles calculation. **2022**, 0
- 226 Spin-Polarized Study of the Structural, Optoelectronic, and Thermoelectric Properties of the Melilite-Type Gd<sub>2</sub>Be<sub>2</sub>GeO<sub>7</sub> Compound. **2022**, 12, 1397 0
- 225 Quasiplastic deformation in shocked nanocrystalline boron carbide: Grain boundary sliding and local amorphization. **2022**, 0
- 224 The stability, mechanical, electronic, and thermal features of the new superhard double transition-metal mono-nitrides and mono-carbides compounds. 1
- 223 Band structure engineering in Fe<sup>3d</sup> based lanthanide filled p-type skutterudites RFe<sub>4</sub>Sb<sub>12</sub> (R = Nd, Sm) to enhance the Seebeck coefficient and thermoelectric figure of merit. **2022**, 132, 155103 0
- 222 First principles study of structural, elastic, electronic, magnetic and thermoelectric properties of ZrRhYZ (Y = Hf, La; Z = Al, Ga, In) quaternary Heusler alloys. **2022**, 137, 0
- 221 Multifield driven bond relaxation on the dielectric constant of GaN, InN, and ZnO. **2022**, 132, 165107 0
- 220 Silver impurities effects on CeO<sub>2</sub> structural, electronic, magnetic, and optical properties: ab initio study. **2022**, 95, 0
- 219 GGA and GGA + U Study of ThMn<sub>2</sub>Si<sub>2</sub> and ThMn<sub>2</sub>Ge<sub>2</sub> Compounds in a Body-Centered Tetragonal Ferromagnetic Phase. **2022**, 27, 7070 0
- 218 Electronic Structure-, Phonon Spectrum-, and Effective Mass- Related Thermoelectric Properties of PdXSn (X = Zr, Hf) Half Heuslers. **2022**, 27, 6567 0
- 217 Half-metallic ferromagnetism in non-magnetic double perovskite oxides Sr<sub>2</sub>MSbO<sub>6</sub> (M=Al, Ga) doped with C and N. 1-16 0
- 216 Electron Beam as Straightener to De-Wrinkle Large 2D Black Phosphorus Flake: An In Situ TEM Monitoring. 2201320 0
- 215 A Critical Study of Structural and Electronic Properties of Co<sub>2</sub>TiN Full-Heusler Alloy. **2023**, 203-209 0
- 214 Reassigning the Pressure-Induced Phase Transitions of Methylammonium Lead Bromide Perovskite. **2022**, 144, 20099-20108 1
- 213 Electronic and optical properties of quaternary selenides for optoelectronic applications: Insights from DFT+U-computations. 0
- 212 Comparisons of the Magnetic and Half-Metallic Properties of Sb-V-Te Compounds in Low and Rich Vanadium Region. 0
- 211 Intercalation of Sr in AA stacked bilayer graphene : DFT study of the electronic structure and optical properties. **2022**, 104714 0
- 210 Understanding the Difference in Bulk Modulus between Y-doped SrCeO<sub>3</sub> and Y-doped SrZrO<sub>3</sub> by Ultrasonic Transmission Method and Density Functional Theory. **2022**, 101616 0

- 209 Investigating the effect of alkali metals on the structural & optoelectronic properties of hexafluorozirconate red phosphors  $A_2ZrF_6$  (A= Cs, K, Na) using first-principles calculations: A prospect for warm-white LEDs (w-LEDs) applications. **2022**, 123689 ○
- 208 Investigation of mechanical properties of  $KCaH_3$  and  $KSrH_3$  orthorhombic perovskite hydrides under high pressure for hydrogen storage applications. **2022**, 95, ○
- 207 Valence Transitions in  $Yb_{1+x}In_{1-x}Cu_4$  Studied by High-resolution X-ray Absorption Spectroscopy, X-ray Diffraction, and Photoelectron Spectroscopy. **2022**, 91, ○
- 206 Comparative study of the structural, electronic, optical and thermoelectric properties of  $LaNiZ$  (Z= Sb, Bi) compounds. **2022**, 33, e00755 ○
- 205 First principles calculations of the inorganic halide perovskite  $RbSnBr_3$ : Optical and thermoelectric properties of its three phases. **2022**, 33, e00761 ○
- 204 First-principles calculations on structural, electronic, elastic, optical and thermoelectric properties of thallium based chloroperovskites  $TlMCl_3$  (M = Zn and Cd). **2022**, 33, e00756 ○
- 203 First principle studies on electronic and thermoelectric properties of  $Fe_2TiSn$  based multinary Heusler alloys. **2023**, 216, 111856 ○
- 202 A unified DFT exploration on transport and thermodynamic properties of L21 structure of  $Rh_2XZn$  ( $X' = Mn, Fe$ ) ferromagnets. **2023**, 287, 116099 ○
- 201 Theoretical study of the structural, electronic and optical properties of the  $t-Se_{1-x}Te_x$  system for  $x = 0.03, 0.04$  and  $0.08$  and for these systems containing a defect in the dihedral angle. **2023**, 648, 414349 ○
- 200 Structural, elastic, electronic and optical properties of double perovskites  $Ba_2NaXO_6$  (X = Cl, Br, I): First-principles study. **2023**, 153, 107165 ○
- 199 Theoretical studies of optoelectronic properties of  $AlP_{1-x}Bi_x$  ternaries: Promising light sources for fiber optic communications. **2023**, 202, 110591 ○
- 198 Impact of substitutional doping of  $Tl^+$  on optoelectronic and thermoelectric properties of NaF phosphor material. **2023**, 172, 111023 ○
- 197 Defects study in zinc blende  $ZnS$  utilizing optimized hybrid functional. **2023**, 216, 111827 ○
- 196 Examining computationally the structural, elastic, optical, and electronic properties of  $CaQCl_3$  (Q = Li and K) chloroperovskites using DFT framework. **2022**, 12, 32338-32349 ○
- 195 Fathoming the anisotropic magnetoelasticity and magnetocaloric effect in  $GdNi$ . **2022**, 106, ○
- 194 Thermophysical properties of  $FLiBe$  using moment tensor potentials. **2022**, 120803 ○
- 193 Scrutinized the inherent spin half-metallicity and thermoelectric response of f-electron-based  $RbMO_3$  (M = Np, Pu) perovskites: a computational assessment. **2022**, 12, ○
- 192 The Structural, Electronic, Magnetic, Mechanical, and Lattice Dynamical Properties of the Novel Full-Heusler Alloys  $Mn_2HfX$  (X = Si and Ge): Ab Initio Study. ○

191	Ab initio study on fcc Pr with correlation matrix renormalization theory. <b>2022</b> , 106,	0
190	The Structural, Electronic, Magnetic and Elastic Properties of Full-Heusler Co <sub>2</sub> CrAl and Cr <sub>2</sub> MnSb: An Ab Initio Study. <b>2022</b> , 12, 1580	1
189	High pressure structural stability of UO <sub>2</sub> by evolutionary algorithm. <b>2022</b> , 45,	0
188	Metastable $\text{Li}_2\text{TiTeO}_6$ : Negative Chemical Pressure Interception and Polymorph Tuning of SHG.	0
187	First-principle investigation of LiSrX (X=P and As) half-Heusler semiconductor compounds.	0
186	Dynamic Response of Single Crystal Al, Cu & Ni Upon Impact : MD and Ab-Initio Calculations.	1
185	Study of Structural, Elastic and Thermodynamic Properties of Metal Carbides MC (M = Ir, Rh and Ru) Using First-Principles Calculations.	0
184	Pressure Induced Reduction in SrUO <sub>4</sub> $\rightarrow$ Topotactic Pathway to Accessing Extreme Incompressibility. <b>2022</b> , 118508	0
183	Atomic composition/configuration dependent bulk moduli of Al <sub>2</sub> O <sub>3</sub> composites. <b>2022</b> , 12, 115008	0
182	First-principles calculations to investigate structural, electronic, optical, and magnetic properties of a scintillating double perovskite halide (Cs <sub>2</sub> LiCeCl <sub>6</sub> ). <b>2022</b> ,	0
181	Structural, elastic, thermodynamic, electronic, magnetic, thermoelectric and optical investigation of chromate spinels TCr <sub>2</sub> O <sub>4</sub> [T = V <sup>2+</sup> , Mn <sup>2+</sup> , Fe <sup>2+</sup> ] for optoelectronic applications. <b>2022</b> , 127041	0
180	Investigation of the Optoelectronic and Photovoltaic Properties of YxIn <sub>1-x</sub> P Alloys Using First Principles Calculations. <b>2022</b> ,	0
179	aflow++: A C++ framework for autonomous materials design. <b>2023</b> , 217, 111889	1
178	Meta-magnetism and exchange interaction in binary alloy Fe <sub>2</sub> Ge. <b>2023</b> , 565, 170230	0
177	An insight into the structural, electronic, magnetic and optical properties of Cs doped and Cs-X (X=Mn, Fe) co-doped CdS for optoelectronic applications. <b>2023</b> , 135, 107079	0
176	High-pressure equation of state of cesium fluoride to 120 GPa. <b>2017</b> , 6, 011101-011101	0
175	First-principles study of structural, electronic, elastic and optical properties of alkali lead iodides MPbI <sub>3</sub> (M = Li, Na, K). <b>2023</b> , 24, 1-21	0
174	A DFT insight into structural, mechanical, elasto-acoustic, and anisotropic properties of AePdH <sub>3</sub> (Ae = Ca, Sr, Ba) perovskites under pressure. <b>2023</b> , 34, e00774	0

173	Electronic structure, magnetic and thermodynamic properties of yttrium based half Heusler alloys YXZ (X = Fe, Co, Cr; Z = As, Sb): A first principles study. <b>2023</b> , 34, e00776	0
172	Ab initio methods for the computation of physical properties and performance parameters of electrochemical energy storage devices.	0
171	Effect of Pressure on the Electronic Band Structure and Circular Photocurrent in Tellurium. <b>2022</b> , 135, 575-587	0
170	Advancing descriptor search in materials science: feature engineering and selection strategies. <b>2022</b> , 24, 113049	0
169	DFT insights into the origin of d0 ferromagnetism, mechanical stability, elastic, and acoustic anisotropy in AZrO3 (A= K, rb, Cs) cubic perovskites. <b>2022</b> , 414521	0
168	Electronic structures and strengthening mechanisms of superhard high-entropy diborides.	0
167	Analysis of phase stability, elastic, electronic, thermal, and optical properties of Sc <sub>1-x</sub> Y <sub>x</sub> N via ab initio methods. <b>2023</b> , 29,	0
166	First-principles structural, elastic and optoelectronics study of sodium niobate and tantalate perovskites. <b>2022</b> , 12,	1
165	First-Principles Calculations of the Phonon, Mechanical and Thermoelectric Properties of Half-Heusler Alloy V <sub>1-x</sub> Si <sub>x</sub> Alloys. <b>2022</b> , 12, 1838	0
164	Modeling the structural, electronic, optoelectronic, thermodynamic, and core-level spectroscopy of X <sub>B</sub> nO <sub>3</sub> (X = Ag, Cs, Hf) perovskites. <b>2022</b> , 114003	0
163	Pressure-dependent bandgap study of MBE grown {CdO/MgO} short period SLs using diamond anvil cell. <b>2022</b> , 121, 242103	0
162	Full-potential KKR within the removed-sphere method: A practical and accurate solution to the Poisson equation. <b>2022</b> , 106,	0
161	Ab initio structural optimization at finite temperatures based on anharmonic phonon theory: Application to the structural phase transitions of BaTiO <sub>3</sub> . <b>2022</b> , 106,	0
160	A density model for high-pressure carbonate-rich melts applied to carbonatitic magmatism in the upper mantle. <b>2022</b> , 121275	0
159	Hindered Trench Migration Due To Slab Steepening Controls the Formation of the Central Andes. <b>2022</b> , 127,	1
158	First-principles calculations to investigate structural, elastic, electronic and thermodynamic properties of NbCoSn and VRhSn Half-Heusler compounds. <b>2022</b> , 43, 106132	0
157	Diluted effect on the structural, magnetic, electronic, thermodynamic, optical and thermoelectric properties of the Heusler alloys Co <sub>2</sub> Fe <sub>1-x</sub> Ti <sub>x</sub> Ga: GGA and GGA + U approaches. <b>2023</b> , 55,	1
156	First principle calculation of structural, electronic, optical, elastic and thermodynamic properties of group IIA metal iodides: Structure-property correlation. <b>2022</b> , 111195	0

- 155 Crystal Chemistry and Physical Properties of A Quaternary Intermetallic Compound,  $[Al_{0.8718}Cu_{0.0256}Si_{0.1026}]_{13}Fe_4$ . **2022**, 12, 2112 ○
- 154 Structural, elastic, mechanical, and thermodynamic characteristic of  $NaReO_3$  and  $KReO_3$  perovskite oxides from first principles study. **2022**, 137, 1
- 153 Structural, electronic, mechanical and phonon properties of half-Heusler  $GaNiSb$ ,  $InNiSb$  and  $InPdSb$  alloys via first-principles calculations. **2022**, e00779 ○
- 152 Ab initio study of magnetic structure transitions of  $FePS_3$  under high pressure. **2022**, 106, ○
- 151 Evidence of Pressure-induced Multiple Electronic Topological Transitions in  $BiSe$ . **2022**, 100956 ○
- 150 The analysis of structural, elastic, and electronic properties of  $Na_3N$  compound under high hydrostatic pressure with the first principles method. ○
- 149 Theoretical investigations of structural, electronic, optical and elastic properties of wurtzite  $ZnO_{1-x}Se_x$  ternary alloys using first principle method. ○
- 148 Half-metallic ferromagnetism in new quaternary Heusler alloys  $CoXP$  ( $X = Cr$  and  $Fe$ ). 1-15 ○
- 147 First-principles computational study on structural, elastic, magnetic, electronic, and thermoelectric properties of  $Co_2MnGe$ : a potential Heusler ternary compound. **2022**, 95, ○
- 146 Investigating structural, electronic, magnetic, and optical properties of Zr doped and Ti-Zr co-doped GaN for optoelectronic applications. **2023**, 98, 015821 ○
- 145 Structural, Electronic, Magnetic, Elastic, Thermoelectric, and Thermal Properties of  $Co_2FeGa_{1-x}Six$  Heusler Alloys: First-Principles Calculations. 1
- 144 First principal study of structural, electronic, magnetic, thermodynamic, optical and thermoelectric properties of  $Nd(Co_{1-x}Fex)_2$  ( $x=0$  to 1). **2022**, 111194 ○
- 143 Structural, Electronic and Optical Properties of Titanium Based Fluoro-Perovskites  $MTiF_3$  ( $M = Rb$  and  $Cs$ ) via Density Functional Theory Computation. **2022**, 7, 47662-47670 ○
- 142 Insight into the Structural, Mechanical and Optoelectronic Properties of Ternary Cubic Barium-Based  $BaMCl_3$  ( $M = Ag, Cu$ ) Chloroperovskites Compounds. **2023**, 13, 140 1
- 141 Structural, electronic, magnetic, and optical investigations of sodium chalcogenides: First-principles calculations. **2023**, 13, 015110 ○
- 140 Insight into the Physical Properties of Fluoro-Perovskites Compounds of TI-Based  $TiMF_3$  ( $M = Au, Ga$ ) Compounds Studied for Energy Generation Utilizing the TB-MBJ Potential Approximation Approach. **2023**, 16, 686 ○
- 139 Electronic, magnetic, and pressure-induced elastic investigations of  $MnY_2O_4$  oxide spinel. **2023**, 138, ○
- 138 Analysis of flow field in a blast simulator combined-driven by explosive charge and compressed gas. 10, ○

- 137 Pressure-induced reentrant Dirac semimetallic phases in twisted bilayer graphene. **2023**, 107, ○
- 136 Modeling thermophysical properties of glasses. **2023**, 13, ○
- 135 Study on density and lattice compression of Al, Cu and AlCu in high temperature and pressure from statistical moment method. ○
- 134 Evolution of austenite lattice parameter during isothermal transformation in a 0.4 C low alloyed steel. **2023**, 101685 ○
- 133 First-principles based computational framework for the thermal conductivity of complex intermetallics: The case study of MgZn<sub>2</sub> and Mg<sub>4</sub>Zn<sub>7</sub>. **2023**, 133, 015101 ○
- 132 First-principles calculations for comparative band structure study of SrTiO<sub>3</sub> perovskite on bulk and layered phases for efficient optoelectronic conversion. **2023**, 1220, 114006 ○
- 131 Band gap tuning of non-toxic Sr-based perovskites CsSrX<sub>3</sub> (X = Cl, Br) under pressure for improved optoelectronic applications. **2023**, 34, 105188 ○
- 130 Enhanced photocatalysis activity of doped magnetic semiconductor (Rh/Ir):CdS by improving charge-carrier transfer mechanism. **2023**, 652, 414643 ○
- 129 Electronic, mechanical, and optical properties of BP nanotubes: A first-principles study. **2023**, 34, e00785 ○
- 128 First-Principles Calculations to Investigate Effect of X<sup>+</sup>Cations Variation on Structural, Mechanical, Electronic and Optical Properties of the XCdCl<sub>3</sub> Chloroperovskites. **2023**, 289, 116228 ○
- 127 Electronic and phonon contributions to the Thermoelectric properties of newly discovered half-Heusler alloys XHfPb (X = Ni, Pd, and Pt). **2023**, 174, 111196 ○
- 126 Structural, phonon, thermodynamic, and electronic properties of MgFeH<sub>3</sub> at different pressures: DFT study. **2023**, 1221, 114030 ○
- 125 Pressure effect on the structural, electronic, and magnetic properties of the battery cathode material LiMn<sub>2</sub>O<sub>4</sub>: An ab-initio study. **2023**, 175, 111198 ○
- 124 Comparison of Electronic and Magnetic Properties of 4d Transition Metals Based NbAl<sub>2</sub>F<sub>4</sub> and TcAl<sub>2</sub>F<sub>4</sub> Spinel. **2022**, 9, 452-460 ○
- 123 Structural stability, electronic, magnetic, elastic, thermal, thermoelectric and optical properties of L21 and xa phases of Ti<sub>2</sub>FeGe heusler compound: GGA and GGA+U methods. 1-24 ○
- 122 Optoelectronic properties and lattice thermal conductivity of Cs<sub>2</sub>CuBiX<sub>6</sub> (X = F, Cl, Br, I) double perovskites: Thermodynamic and ab initio approaches. **2023**, e00791 ○
- 121 The dynamic-loading response of carbon-fibre-filled polymer composites. **2023**, 195-244 ○
- 120 Structural, electronic and thermoelectric properties of LiAlX<sub>2</sub> (X=S and Se) chalcopyrites: promising for thermoelectric power generators. **2023**, 20, 73-83 ○

- 119 Pressure-Induced Structural Phase Transitions in the Chromium Spinel  $\text{LiInCr}_4\text{O}_8$  with Breathing Pyrochlore Lattice. **2023**, 13, 170 ○
- 118 DFT study of cobalt based quaternary full-Heusler compound for spintronics and thermoelectric technologies. ○
- 117 Molecular Dynamics Approach to the Physical Mixture of  $\text{In}_2\text{O}_3$  and  $\text{ZrO}_2$ : Defect Formation and Ionic Diffusion. **2023**, 24, 2426 ○
- 116 Solids that are also liquids: elastic tensors of superionic materials. **2023**, 9, ○
- 115  $\text{MgTi}$  System up to 20 GPa: Its Phase Diagram and Stable Magnesium Carbides. **2023**, 127, 1965-1972 ○
- 114 Structural Stability and Electronic Transport Properties of Nb 2 C-MXenes under High Pressure. 2201071 ○
- 113 Ab-initio simulation of the structural, electronic and optical properties for the vacancy-ordered double perovskites  $\text{ATiI}$  ( $\text{A} = \text{Cs}$  or  $\text{NH}$ ); a time-dependent density functional theory study. **2023**, 176, 111262 ○
- 112 Elastic, electronic, thermal and magnetic investigations of  $\text{PrX}$  ( $\text{X} = \text{Fe, Ru}$ ) superconductors materials. **2023**, 35, 105545 ○
- 111 Theoretical investigation of the physical properties of cubic perovskite oxides  $\text{SrXO}_3$  ( $\text{X} =$ . **2023**, 158, 107340 ○
- 110 Effect of hydrostatic pressure on structural, mechanical, and electronic properties of energetic molecular perovskite  $(\text{C}_6\text{H}_{14}\text{N}_2)(\text{NH}_2\text{NH}_3)(\text{ClO}_4)_3$ : A DFT-D insight. ○
- 109 Structural, half-metallic, electronic, magnetic and pressure-induced elastic changes of  $\text{PdVSi}$ ,  $\text{PdVGe}$ ,  $\text{PdVSn}$ , and  $\text{PdVSb}$  alloys. **2023**, 58, 5349-5361 ○
- 108 A general framework for dislocation models. **2023**, 222, 112107 ○
- 107 Spin and current transport in the robust half-metallic magnet  $\text{CoFeGe}$ . ○
- 106 Synthesis, Characterization, and Magnetocaloric Properties of Double Perovskite  $\text{BaSrNiMoO}_6$  for Magnetic Refrigeration Applications. ○
- 105 Investigation of Structural, Mechanical, Dynamic Stability and Electronic Properties of Anti-perovskite Nitrides  $\text{ANLa}_3$  ( $\text{A} = \text{Al, Ga}$ ): A DFT and DFPT Studies. ○
- 104 Cluster structure of doped atoms and elastic properties in  $\text{ENi}$  by first-principles calculations. **2023**, 224, 112183 ○
- 103 Prediction of mechanical properties of  $\text{AlTiCrVNb}$  high entropy alloys with B2 ordered structure. **2023**, 24, 440-448 ○
- 102 First-principles theory-based design of highly reflective metals for radiative cooling. **2023**, 49, 1-5 ○



- 101 Dependence of predicted bulk properties of hexagonal hydroxyapatite on exchange correlation functional. **2023**, 224, 112153 ○
- 100 Theoretical study of structural, electronic, elastic and optical properties of  $Mg_{1-x}Cr_xS$  in ferromagnetic rock-salt structure. **2023**, 657, 414778 ○
- 99 Automated calculations of exchange magnetostriction. **2023**, 224, 112158 ○
- 98 Electronic properties of half-Heusler compounds  $XCrSb$  ( $X = Fe, Ru, Os$ ): Potential applications as spintronics and high-performance thermoelectric materials. **2023**, 49, 70-77 ○
- 97 Half metallic Heusler alloys  $XMnGe$  ( $X = Ti, Zr, Hf$ ) for spin flip and thermoelectric device application [Material computations]. **2023**, 159, 107367 ○
- 96 First-principles calculations to investigate structural, electronic, magnetic, optical, mechanical and thermoelectric properties of rare-earth aluminate perovskite  $XAlO_3$  ( $X = Ce, Nd, Gd$ ) compounds. **2023**, 301, 127691 ○
- 95 First principles insight into physical properties of  $CaX_2O_4$  ( $X = In, Gd$ ) spinels for optical and spintronic applications. **2023**, 322, 123999 ○
- 94 Anisotropic excitonic absorption in  $SbI_3$  films: Theory and experiment. **2023**, 343, 134359 ○
- 93 Which crystal structure is present on the surface of  $Ti_2CrAl$  compound - a deduction from electronic structure measurements and calculations. **2023**, 733, 122288 ○
- 92 Structural, Elastic, Electronic, and Magnetic Properties of Full-Heusler Alloys  $Sc_2TiAl$  and  $Sc_2TiSi$  Using the FP-LAPW Method. **2023**, 9, 108 ○
- 91 Structural parameters, electronic structure and linear optical functions of  $LuXCo_2Sb_2$  ( $X = V, Nb$  and  $Ta$ ) double half Heusler alloys. **2023**, 657, 414809 ○
- 90 Investigation of structural, opto-electronic, mechanical and thermoelectric properties of Rb-based fluoro-perovskites  $RbXF_3$  ( $X = Rh, Os, Ir$ ) via first-principles calculations. **2023**, 27, 101627 ○
- 89 Insights into structural, elastic, mechanical, opto-electronic, and thermoelectric properties of rubidium-based fluoroperovskites  $RbXF_3$  ( $X = Zn, Cd, Hg$ ). **2023**, 178, 111357 ○
- 88 A review on the advancements in the characterization of the high-pressure properties of iodates. **2023**, 136, 101092 ○
- 87 Electronic structure and magnetic properties of  $YX_2CrZ$  ( $X = Fe, Co, Ni$ ;  $Z = Al, Ga, In$ ) quaternary Heusler alloys. **2023**, 97, 733-749 ○
- 86 Ab-initio Calculations of the Half-metallic Ferromagnetic New Variant Perovskites  $Li_2CrO_6$  and  $Li_2CuO_6$ . 1-1 ○
- 85 The structural, magnetic, and pressure-induced elastic predictions of  $ZrPd_2O_4$  oxide spinel via GGA, GGA+mBJ, and GGA+U approximations. **2023**, 568, 170417 ○
- 84 Optoelectronic and transport properties of new perovskites  $CsInTiX_6$  ( $X = Br, I$  and  $Cl$ ) for thermoelectric and photovoltaic applications. **2023**, 233, 116316 ○

- 83 Ab-initio investigation of the structural stability, electronic and optical properties of the LiBO<sub>2</sub> compound by using the GOW0+BSE approach. **2023**, 34, e00789 ○
- 82 An insight on the origin of half-metallicity of new equiatomic quaternary Heusler alloys PtRuTiZ (Z = Al/Si): GGA and GGA+U approaches. **2023**, 220, 112039 ○
- 81 Enhancement of thermoelectric performances in n-type RbCrZ (Z = S, Se, Te) half-metallic ferromagnetic alloys via charge carrier concentration or chemical potential. **2023**, 653, 414678 ○
- 80 Improving thermodynamic properties and desorption temperature in MgH<sub>2</sub> by doping Be: DFT study. **2023**, 49, 497-508 ○
- 79 First-principles study of SrTe and BaTe: Promising wide-band-gap semiconductors with ambipolar doping. **2023**, 48, 90-96 ○
- 78 Electronic, magnetic and optical properties of Cr and Fe doped ZnS and CdS diluted magnetic semiconductors: revised study within TB-mBJ potential. **2023**, 55, ○
- 77 DFT investigation of half-metallic ferromagnetic rare earth based spinels MgHo<sub>2</sub>Z<sub>4</sub> (Z = S, se). **2023**, ○
- 76 Theoretical study of thermal and magneto-electronic properties of YbX<sub>2</sub> (X = Co and Fe) intermetallic compounds. ○
- 75 Electronic, mechanical, optical and thermodynamic properties of the quaternary semiconductors Sr<sub>3</sub>GeMgN<sub>4</sub> and Ba<sub>3</sub>GeMgN<sub>4</sub>. **2023**, 290, 116292 ○
- 74 Influence of baric and thermobaric effects on dielectric properties of complex oxide ceramics La<sub>1.8</sub>Sr<sub>0.2</sub>Ni<sub>0.8</sub>Co<sub>0.2</sub>O<sub>4+δ</sub>. **2023**, 49, 16879-16890 ○
- 73 Effective band gap engineering in multi-principal oxides (CeGdLa-Zr/Hf)O<sub>x</sub> by temperature-induced oxygen vacancies. **2023**, 13, ○
- 72 First-principles study of the strain effect with half-metallic ferromagnetism in Cd<sub>1-x</sub>V<sub>x</sub>Te alloys: supercell approaches. **2023**, 98, 035828 ○
- 71 First-principles calculations to investigate structural, electronic, elastic and optical properties of radium based cubic fluoro-perovskite materials. **2023**, 9, e13687 ○
- 70 Structural, mechanical, electronic, and thermoelectric properties of TiZrCo<sub>2</sub>Bi<sub>2</sub>, TiHfCo<sub>2</sub>Bi<sub>2</sub>, and ZrHfCo<sub>2</sub>Bi<sub>2</sub> double half Heusler semiconductors. ○
- 69 First-principles study on structural, electronic, and elastic properties of SrFCl. ○
- 68 DFT insights of mechanical, optoelectronic and thermoelectric properties for Cs<sub>2</sub>ScTiX<sub>6</sub> (X = Cl, Br, I) double perovskites. **2023**, 55, ○
- 67 First principles approach for promising oxide ion conducting ABGa<sub>3</sub>O<sub>7</sub> melilite structures. **2023**, 25, 7028-7031 ○
- 66 Properties of the double half-heusler alloy ScNbNi<sub>2</sub>Sn<sub>2</sub> with respect to structural, electronic, optical, and thermoelectric aspects. **2023**, 363, 115103 ○

65	Investigation of structural, opto-electronic and thermoelectric properties of titanium based chloro-perovskites $\text{XTiCl}_3$ ( $X = \text{Rb}, \text{Cs}$ ): a first-principles calculations. <b>2023</b> , 13, 6199-6209	1
64	Phase stability and physical properties of lanthanum dicarbide under pressure. 1-18	0
63	Cooperative Pseudo Jahn Teller distortion derives phase transitions in bismuth oxide. <b>2023</b> , 299, 127534	0
62	The effect of temperature on electronic, elastic and thermodynamic properties of $\text{Co}_2\text{MnX}$ (. <b>2023</b> , 655, 414751	0
61	Thermoelectric Performance of n-type Filled Skutterudites $\text{RECo}_4\text{Sb}_{12}$ Using Rare Earths as Filler Atoms ( $\text{RE}=\text{Nd}, \text{Sm}, \text{Eu}, \text{Yb}$ ). <b>2023</b> , 12, 033006	0
60	The First-Principles Investigation of Structural Stability, Mechanical, Vibrational, Thermodynamic, and Optical Properties of $\text{CaHfS}_3$ for Optoelectronic Application. <b>2023</b> , 2023, 1-13	0
59	A DFT+U Based Study of Full-Heusler Alloy $\text{Ru}_2\text{VSi}$ . <b>2023</b> , 407,	0
58	The study of new double perovskites $\text{K}_2\text{AgAsX}_6$ ( $X = \text{Cl}, \text{Br}$ ) for energy-based applications. <b>2023</b> , 17,	0
57	Anomalous hydrogen diffusion in VCr alloys: Trapping hydrogen via shallow potential well domains. <b>2023</b> , 465, 128701	0
56	Electronic properties of single-crystalline $\text{Fe}_4\text{O}_5$ .	0
55	First-principles calculations to investigate electronic, magnetic and half-metallic ferromagnetic properties of full-Heusler $\text{Mn}_2\text{OsSn}$ . 1-25	0
54	A Comprehensive First-Principles Investigation of $\text{SnTiO}_3$ Perovskite for Optoelectronic and Thermoelectric Applications. <b>2023</b> , 13, 408	1
53	Tantalum half-Heusler alloys $\text{RbTaSi}$ and $\text{RbTaGe}$ : potential candidates for desirable thermoelectric and spintronic applications. <b>2023</b> , 13, 7087-7101	0
52	Ti-6Al-4V to over 1.2 TPa: Shock Hugoniot experiments, ab initio calculations, and a broad-range multiphase equation of state. <b>2023</b> , 107,	0
51	Physics-separating artificial neural networks for predicting sputtering and thin film deposition of AlN in Ar/ $\text{N}_2$ discharges on experimental timescales. <b>2023</b> , 56, 194001	0
50	Large-strain Elastic and Elasto-Plastic Formulations for Host-Inclusion Systems and Their Applications in Thermobarometry and Geodynamics. 323,	0
49	DFT computational study for investigating structural, electronic, magnetic, elastic and thermodynamic properties of the full-Heusler alloys $\text{Rh}_2\text{MnTi}$ for industrial applications.	0
48	Toward better understanding of the high-pressure structural transformation in beryllium by the statistical moment method. <b>2023</b> , 25, 9073-9082	0

- 47 Phase Transition of Zeolite X under High Pressure and Temperature. **2023**, 56, 13-21 ○
- 46 Effect of hydrostatic strain on the mechanical properties and topological phase transition of bi-alkali pnictogen NaLi<sub>2</sub>Bi. **2023**, 98, 045905 ○
- 45 Crystallographic structural variations in nano-crystalline Sc<sub>2</sub>O<sub>3</sub> under pressure. **2023**, 98, 045707 ○
- 44 Ultralow lattice thermal conductivity, negative thermal expansion, elastic and thermoelectric properties of Lanthanum Nitride: Insights from first-principle calculations. **2023**, 98, 045920 ○
- 43 Optical properties of ZnSe using linear response theory. **2023**, 35, 215901 ○
- 42 Strongly Correlated Electronic Properties of FeO Studied by the SCAN+U Functional. **2023**, 127, 5513-5518 ○
- 41 Thermoelectric Performance of an n-Doped CaSbK Half-Heusler Compound. **2023**, 52, 3499-3507 ○
- 40 Advances in the generalized entropy theory of polymer glass formation. **2023**, 53, 616-627 ○
- 39 Theoretical Study of Pressure-Induced Phase Transitions in Sb<sub>2</sub>S<sub>3</sub>, Bi<sub>2</sub>S<sub>3</sub>, and Sb<sub>2</sub>Se<sub>3</sub>. **2023**, 13, 498 ○
- 38 Study of electronic, magneto-optical and transport properties of double perovskite Ca<sub>2</sub>XMnO<sub>6</sub> (X = Ti, Cr) under uniaxial compressive strain by using a DFT method. **2023**, 37, ○
- 37 A study of the structural, thermodynamic, magnetic, and optoelectronic properties of the Dy<sub>2</sub>Be<sub>2</sub>GeO<sub>7</sub> complex oxide via ab initio methods. **2023**, 138, ○
- 36 p<sub>III</sub> Phase Diagram of Phosphorus Revisited. **2023**, 127, 6088-6092 ○
- 35 Tailoring high-energy storage NaNbO<sub>3</sub>-based materials from antiferroelectric to relaxor states. **2023**, 14, ○
- 34 Phase stability, electronic and local structures of Li-doped (K,Na)NbO<sub>3</sub> under hydrostatic pressure from first principles calculation. **2023**, 129, ○
- 33 A first-principles study of electronic, optical and thermoelectric properties of TlXF<sub>3</sub> (X: Zn, Sr) perovskite crystal structure. **2023**, 98, 055907 ○
- 32 First principle study on transition metal ammine borohydrides with amphoteric hydrogen for hydrogen storage applications. **2023**, ○
- 31 DFT-Based Investigation of the Structural Stability, Elastic, Electronic, and Magnetic in Pd<sub>2</sub>CrGe Heusler Alloy. ○
- 30 Calculation of the mechanical and magnetic stability of the full Heusler alloys Ru<sub>2</sub>MnX (X = Ta, V): using ab initio approach. ○

- 29 First-Principles Study of the Structural, Phase-Stability, Electronic, Magnetic, and Elastic Properties of Heusler Alloys VXRh<sub>2</sub> (X=Si, Ge, and Sn). ○
- 28 A study of the physical properties of GaN, GaP and their mixed ternary alloys for the applications in optoelectronics devices. **2023**, 46, ○
- 27 First-principles calculations to investigate optical and electrical properties of the half-Heusler materials TiXSn (X = Ni, Pt). **2023**, 49, 778-791 ○
- 26 A DFT study of electronic structure and optical properties of the pure, doped and co-doped CaZrO<sub>3</sub> perovskite for photovoltaic applications. ○
- 25 DFT assessment on stabilities, electronic and thermal transport properties of CoZrSb<sub>1-x</sub>Bix half-Heusler alloys and their superlattices. **2023**, 138, ○
- 24 Elastic Properties of Binary d-Metal Oxides Studied by Hybrid Density Functional Methods. ○
- 23 Effects of the antiferrodistortive instability on the structural behavior of BaZrO<sub>3</sub> by atomistic simulations. **2023**, 107, ○
- 22 First-principle investigations of structural, electronic, thermal, and mechanical properties of AlP<sub>1-x</sub>Bix alloys. **2023**, 29, ○
- 21 First-principles study on novel Fe-based quaternary Heusler alloys, with robust half-metallic, thermoelectric and optical properties. **2023**, 13, 10847-10860 ○
- 20 Compressional behavior of the aragonite-structure carbonates to 6 GPa. **2023**, 50, ○
- 19 Density functional theory (DFT) simulation and approach to property-driven investigations in ceramic and composites materials. **2023**, 461-490 ○
- 18 The optoelectronic application of CsSnI<sub>3</sub> upon substitution with Pb: A DFT approach. ○
- 17 Half-metallicity, mechanical, optical, thermodynamic, and thermoelectric properties of full Heusler alloys Co<sub>2</sub>TiZ (Z = Si; Ge; Sn). **2023**, 55, ○
- 16 Insight into the structural, electronic, optical, and elastic properties of niobium carbide. 1-13 ○
- 15 Classical Force Field Parameters for InP and InAs Quantum Dots with Various Surface Passivations. **2023**, 127, 3427-3436 ○
- 14 Modelling of the structural, electronic, magnetic properties and magnetocaloric effect of Cr<sub>2</sub>Ge<sub>2</sub>Te<sub>6</sub> and Cr<sub>2</sub>Si<sub>2</sub>Te<sub>6</sub> compounds: DFT combined with the Monte Carlo method. ○
- 13 Lattice constants and magnetism of L1<sub>0</sub>-ordered FePt under high pressure. **2023**, 122, 152406 ○
- 12 First-principles calculations of structural, electronic, elastic, and thermal properties of phase M<sub>2</sub>CdC (M = Sc, V, and Nb). ○

- 11 New investigated lead free double perovskite materials  $\text{Rb}_2\text{LiBiX}_6$  (X= Cl, F, Br, I) for optoelectronics and solar cell applications via first principle calculations. **2023**, 366-367, 115162 ○
- 10 Study of structural, magnetic and electronic properties of a new off-stoichiometric series of full-Heusler alloy  $\text{Co}_2\text{Nb}_{1+Z}\text{Ti}$  (Z = Sn, In, Ga): Ab initio approach. **2023**, 170117 ○
- 9 Development of a Ni-Al reactive force field for Ni-based superalloy: Revealing electrostatic effects on mechanical deformation. **2023**, ○
- 8 Density functional theory investigation on the structural, mechanical, lattice dynamical and thermal properties of nodal-line semimetals  $\text{CaAgX}$  (X: P, As). **2023**, 46, ○
- 7 First-principles investigations of physical properties of  $\text{CdXP}_2$  (X = Si, Ge, and Sn) ternary chalcopyrite. ○
- 6 Insight into physical properties of carbon-doped  $\text{BeSiP}_2$  and  $\text{BeGeP}_2$  chalcopyrite: An ab initio study. **2023**, 124054 ○
- 5 Full optimization of quasiharmonic free energy with an anharmonic lattice model: Application to thermal expansion and pyroelectricity of wurtzite GaN and ZnO. **2023**, 107, ○
- 4 Machine learning for shock compression of solids using scarce data. **2023**, 133, ○
- 3 Inverse-perovskites  $\text{Sc}_3\text{GaX}$  (X = B, C, N): A comprehensive theoretical investigation at ambient and elevated pressures. **2023**, 35, e00808 ○
- 2 Theoretical insight of stabilities and optoelectronic properties of double perovskite  $\text{Cs}_2\text{CuIrF}_6$ : Ab-initio calculations. **2023**, 29, ○
- 1 ANALYSIS OF TiFe INTERMETALLIC COMPOUND BY DFT. ○