Igor R Shein

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7253963/publications.pdf

Version: 2024-02-01

233 papers	4,756 citations	156536 32 h-index	169272 56 g-index
235 all docs	235 docs citations	235 times ranked	4846 citing authors

#	Article	IF	Citations
1	Effect of Li and Li-RE co-doping on structure, stability, optical and electrical properties of bismuth magnesium niobate pyrochlore. Materials Research Bulletin, 2022, 145, 111520.	2.7	6
2	Photocatalytic Properties of Bi_{2â€“x}Ti₂O_{7â€“1.5x} (x = 0, 0.5) Pyrochlores: Hybrid DFT Calculations and Experimental Study. Inorganic Chemistry, 2020, 59, 12385-12396.	1.9	18
3	Ab Initio and Experimental Insights on Structural, Electronic, Optical, and Magnetic Properties of Cr-Doped Bi₂Ti₂O₇. Inorganic Chemistry, 2019, 58, 9904-9915.	1.9	18
4	Thermodynamic properties and lattice dynamics investigation of LuB2C: experiment and ab initio calculations. Physical Chemistry Chemical Physics, 2019, 21, 24684-24694.	1.3	2
5	Structural and Electronic Properties and Chemical Bonding in Layered 1111-Oxyarsenides LaRhAsO and LaIrAsO: AB Initio Simulation. Journal of Structural Chemistry, 2019, 60, 1859-1867.	0.3	0
6	Bismuth titanate pyrochlores doped by alkaline earth elements: First-principles calculations and experimental study. Solid State Ionics, 2018, 317, 183-189.	1.3	17
7	Electronic Structure, Mechanical and Dynamical Stability of Hexagonal Subcarbides M2C (M = Tc, Ru,) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	0.2	18
8	Ab initio thermodynamic characteristics of the formation of oxygen vacancies, and boron, carbon, and nitrogen impurity centers in anatase. Physics of the Solid State, 2018, 60, 37-48.	0.2	14
9	Electronic Properties and Fermi Surface for New Layered High-Temperature Superconductors CaAFe4As4 (A = K, Rb, and Cs): FLAPW-GGA Calculations. Journal of Superconductivity and Novel Magnetism, 2018, 31, 1683-1692.	0.8	11
10	Mechanical and Dynamic Stability of Complete and Nonstoichiometric 3C-SixCy from Ab Initio Calculations. Physics of the Solid State, 2018, 60, 2012-2018.	0.2	0
11	On the effect of non-stoichiometry on electronic and magnetic properties of BiOCuS layered oxysulfide: A preliminary consideration based on ab initio band structure simulations. Computational Condensed Matter, 2018, 16, e00306.	0.9	0
12	Impurity centers and electronic band structure of lithium-doped cadmium oxide. Ceramics International, 2018, 44, 17313-17318.	2.3	6
13	Structure and Thermodynamic Characteristics of Impurity Centers in Lithium-Doped Cadmium Oxide: an Ab Initio Paw-Study. Journal of Structural Chemistry, 2018, 59, 253-260.	0.3	2
14	Metal-metal bond excitation in colloidal solution of NbS 3. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 179, 46-50.	2.0	4
15	Experimental investigation and ab initio calculation of the properties of Sc-, in-doped bismuth titanates with the pyrochlore type structure. Physics of the Solid State, 2017, 59, 495-503.	0.2	10
16	Fe and C doped TiO2 with different aggregate architecture: Synthesis, optical, spectral and photocatalytic properties, first-principle calculation. Journal of Physics and Chemistry of Solids, 2017, 111, 473-486.	1.9	8
17	Electronic and mechanical properties, phase stability, and formation energies of point defects of niobium boronitride Nb2BN. Physics of the Solid State, 2017, 59, 1481-1491.	0.2	4
18	Structural, elastic and electronic properties of Ir-based carbides-antiperovskites Ir 3 M C (M Â=ÂTi, Zr,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 60-68.	0.9	7

#	Article	IF	Citations
19	Pressure-induced zircon to monazite phase transition in Y1â€“Ñ… La Ñ… PO4: First-principles calculations. Journal of Structural Chemistry, 2016, 57, 1513-1518.	0.3	5
20	Electronic structure and formation energies of nonstoichiometric dichalcogenides M x X2â€“y (Đœ = Nb,) Tj ETQq0 0 0 rgBT /Overlock 1	0.3	2
21	Molecular dynamics simulations of defect formation in thin graphite films using the density functional tight-binding method. Journal of Structural Chemistry, 2016, 57, 808-811.	0.3	2
22	Electronic structure of non-stoichiometric ZrCuSiAs-like layered LaZnAsO1â€“Î´ compositions: FLAPW-GGA modeling. Journal of Structural Chemistry, 2016, 57, 805-807.	0.3	0
23	Elastic and Electronic Properties of Superconducting CaPd 2 As 2 and SrPd 2 As 2 vs. Non-superconducting BaPd 2 As 2. Journal of Superconductivity and Novel Magnetism, 2014, 27, 155-161.	0.8	10
24	Synthesis, optical properties, and photocatalytic activity of lanthanide-doped anatase. Russian Journal of Inorganic Chemistry, 2014, 59, 29-33.	0.3	11
25	Electronic band structure, Fermi surface, structural and elastic properties of two polymorphs of MgFeSeO as possible new superconducting systems. JETP Letters, 2014, 98, 609-613.	0.4	0
26	Elastic, electronic properties and intra-atomic bonding in orthorhombic and tetragonal polymorphs of BaZn2As2 from first-principles calculations. Journal of Alloys and Compounds, 2014, 583, 100-105.	2.8	16
27	Synthesis and characterisation of new MO(OH)₂(M = Zr, Hf) oxyhydroxides and related Li₂MO₃salts. Dalton Transactions, 2014, 43, 2755-2763.	1.6	12
28	Structural, elastic and electronic properties of new layered superconductor HfCuGe2 in comparison with isostructural HfCuSi2, ZrCuGe2, and ZrCuSi2 from first-principles calculations. Intermetallics, 2013, 42, 130-136.	1.8	6
29	Effect of fluorine, nitrogen, and carbon impurities on the electronic and magnetic properties of WO3. Semiconductors, 2013, 47, 740-744.	0.2	3
30	Electronic band structure, optical absorption, and photocatalytic activity of iron-doped anatase. Physics of the Solid State, 2013, 55, 1903-1912.	0.2	15
31	Structural, electronic, mechanical, and magnetic properties and relative stability of polymorphic modifications of ReN2 from Ab initio calculation data. Physics of the Solid State, 2013, 55, 1821-1825.	0.2	4
32	Localization of vacancies and mobility of lithium ions in Li2ZrO3 as obtained by 6,7Li NMR. Journal of Solid State Chemistry, 2013, 208, 43-49.	1.4	30
33	Elastic Properties of New Pt-based Superconductors CaPt3P and SrPt3P as Evaluated from First-Principles Calculations. Journal of Superconductivity and Novel Magnetism, 2013, 26, 3167-3170.	0.8	3
34	Correlated band structure of superconducting NdFeAsO0.9F0.1: Dynamical mean-field study. JETP Letters, 2013, 98, 373-377.	0.4	1
35	Electronic band structure and optical absorption of nanotubular zinc oxide doped with Iron, Cobalt, or Copper. Physics of the Solid State, 2013, 55, 2450-2458.	0.2	4
36	Charge distribution and mobility of lithium ions in Li2TiO3 from 6,7Li NMR data. Journal of Structural Chemistry, 2013, 54, 111-118.	0.3	11

#	Article	IF	Citations
37	Electronic band structure, optical absorption and photocatalytic activity of anatase doped with bismuth or carbon. Journal of Alloys and Compounds, 2013, 548, 46-51.	2.8	9
38	Structural, elastic, and electronic properties of new 211 MAX phase Nb2GeC from first-principles calculations. Physica B: Condensed Matter, 2013, 410, 42-48.	1.3	28
39	Electronic band structure and Fermi surface of tetragonal low-temperature superconductor Bi2Pd as predicted from first principles. Journal of Superconductivity and Novel Magnetism, 2013, 26, 1-4.	0.8	23
40	The effect of arsenic vacancies on the electronic and magnetic properties of LaFeAs1â^'xO. Journal of Magnetism and Magnetic Materials, 2013, 335, 21-27.	1.0	2
41	First-principles calculations of elastic and electronic properties of tetragonal Th2NiC2 as a parent phase for new superconductors. Journal of Alloys and Compounds, 2013, 551, 338-342.	2.8	4
42	Ab initio Probing of Magnetic and Electronic Properties of Monoclinic Îµ-WO3 Doped with 3d Transition Metals Within GGA and GGA+U. Journal of Superconductivity and Novel Magnetism, 2013, 26, 2343-2346.	0.8	1
43	Electronic band structure and Fermi surface for new layered superconductor LaO0.5F0.5BiS2 in comparison with parent phase LaOBiS2 from first principles. JETP Letters, 2013, 96, 769-774.	0.4	29
44	Grapheneâ€like nanocarbides and nanonitrides of d metals (MXenes): synthesis, properties and simulation. Micro and Nano Letters, 2013, 8, 59-62.	0.6	84
45	Electronic, optical properties and chemical bonding in six novel 1111-like chalcogenide fluorides AMChF (A=Sr, Ba; M=Cu, Ag; and Ch=S, Se, Te) from first principles calculations. Journal of Solid State Chemistry, 2012, 196, 601-606.	1.4	12
46	Electronic band structure of pseudo-binary AlB2-like hexagonal silicides SrNixSi2â^'x as novel low-TC superconductors. Physica B: Condensed Matter, 2012, 407, 4592-4594.	1.3	1
47	Planar nano-block structures Tin+1Al0.5Cn and Tin+1Cn (n=1, and 2) from MAX phases: Structural, electronic properties and relative stability from first principles calculations. Superlattices and Microstructures, 2012, 52, 147-157.	1.4	59
48	Structural, electronic, elastic properties and chemical bonding in LaNi2P2 and LaNi2Ge2 from first principles. Intermetallics, 2012, 26, 1-7.	1.8	12
49	Structural, elastic, electronic properties and stability trends of 1111-like silicide arsenides and germanide arsenides MCuXAs (M=Ti, Zr, Hf; X=Si, Ge) from first principles. Journal of Alloys and Compounds, 2012, 533, 71-78.	2.8	13
50	Trends in structural, electronic properties and Fermi surface topology of 15 tetragonal ThCr2Si2-type phases AFe2Ch2, where A=Li, Na, K, Rb, and Cs; Ch=S, Se, and Te, as parent systems of new ternary ironâ€"chalcogenide superconductors. Computational Materials Science, 2012, 60, 1-6.	1.4	2
51	Electronic structure, Fermi surface, and chemical bonding in new layered oxyselenide: HgCuSeO. Journal of Structural Chemistry, 2012, 53, 634-638.	0.3	0
52	Graphene-like titanium carbides and nitrides Tin+1Cn, Tin+1Nn (n=1, 2, and 3) from de-intercalated MAX phases: First-principles probing of their structural, electronic properties and relative stability. Computational Materials Science, 2012, 65, 104-114.	1.4	286
53	Electronic, magnetic properties and correlation effects in the layered quaternary iron oxyselenide Na2Fe2Se2O from first principles. Solid State Communications, 2012, 152, 1969-1972.	0.9	2
54	Ab initio prediction of new 3D-like phases ThCuSiAs, ThCuGeAs and their structural, mechanical, and electronic properties. Journal of Materials Science, 2012, 47, 6741-6747.	1.7	4

#	Article	IF	Citations
55	Ab Initio Probing of the Magnetic and Electronic Properties of ThCr2Si2-Like Charge-Balanced KFeAgTe2. Journal of Superconductivity and Novel Magnetism, 2012, 25, 151-154.	0.8	3
56	Impurity-Induced Magnetization of Layered Semiconductor LaCuSeO as Predicted from First-Principles Calculations. Journal of Superconductivity and Novel Magnetism, 2012, 25, 1509-1513.	0.8	5
57	Structural, electronic properties and inter-atomic bonding in layered chalcogenide oxides LaMChO (where MÂ=ÂCu, Ag, and ChÂ=ÂS, Se) from FLAPW-GGA calculations. Solid State Sciences, 2012, 14, 89-93.	1.5	27
58	Structural, electronic, magnetic and elastic properties of tetragonal layered diselenide KCo2Se2 from first principles calculations. Physica B: Condensed Matter, 2012, 407, 271-275.	1.3	22
59	Ab initio probing of the electronic band structure and Fermi surface of fluorine-doped WO3 as a novel low-T C superconductor. JETP Letters, 2012, 95, 66-69.	0.4	6
60	Mechanical properties and electronic structure of zircon: Ab inito FLAPW-GGA calculations. Inorganic Materials: Applied Research, 2012, 3, 7-10.	0.1	3
61	The influence of oxygen deficiency on structural and electronic properties of layered superconductor (Fe2As2)(Sr4V2O6â˜x). Journal of Materials Science, 2012, 47, 3663-3668.	1.7	2
62	Nanotubes of layered iron-based superconductors: Simulations of atomic structure and electronic properties. Computational Materials Science, 2011, 50, 824-827.	1.4	3
63	Electronic band structure and inter-atomic bonding in layered 1111-like Th-based pnictide oxides ThCuPO, ThCuAsO, ThAgPO, and ThAgAsO from first principles calculations. Computational Materials Science, 2011, 50, 2736-2740.	1.4	7
64	Structure-induced semiconductor â† metal transition in lead monosulfide PbS: Ab initio calculations. Doklady Physical Chemistry, 2011, 437, 50-53.	0.2	0
65	Magnetization of zircon induced by 3d impurities: Ab initio calculations. Doklady Physical Chemistry, 2011, 438, 90-93.	0.2	2
66	Structural, electronic, and magnetic properties of layered cobalt pnictide oxides (Co2As2)(Sr4Sc2O6) and (Co2P2)(Sr4Sc2O6) from first principles. Solid State Sciences, 2011, 13, 837-842.	1.5	1
67	Electronic bands, Fermi surface, and elastic properties of new 4.2K superconductor SrPtAs with a honeycomb structure from first principles calculations. Physica C: Superconductivity and Its Applications, 2011, 471, 594-596.	0.6	11
68	Structural, electronic properties and chemical bonding in protonated lithium metallates Li2â˜x H x MO3 (M = Ti, Zr, Sn). Journal of Structural Chemistry, 2011, 52, 1043-1050.	0.3	13
69	Ab initio study of the nature of the chemical bond and electronic structure of the layered phase Ca10(Pt4As8)(Fe2As2)5 as a parent system in the search for new superconducting iron-containing materials. Theoretical and Experimental Chemistry, 2011, 47, 292-295.	0.2	7
70	23Na NMR in binary lithium-sodium cobaltite. Bulletin of the Russian Academy of Sciences: Physics, 2011, 75, 1157-1159.	0.1	1
71	Magnetic and Electronic Properties of Nitrogen-Doped Lanthanum Sesquioxide La2O3 as Predicted from First Principles. Journal of Superconductivity and Novel Magnetism, 2011, 24, 1693-1696.	0.8	5
72	Structural, Electronic Properties and Fermi Surface of ThCr2Si2-Type Tetragonal KFe2S2, KFe2Se2, and KFe2Te2 Phases as Parent Systems of New Ternary Iron-Chalcogenide Superconductors. Journal of Superconductivity and Novel Magnetism, 2011, 24, 2215-2221.	0.8	14

#	Article	IF	Citations
73	Composition of beryllium oxide ceramics. Refractories and Industrial Ceramics, 2011, 51, 377-381.	0.2	12
74	Electronic structure and Fermi surface of new K intercalated iron selenide superconductor KxFe2Se2. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 1028-1031.	0.9	59
75	Elastic properties of superconducting MAX phases from firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 228-232.	0.7	68
76	Elastic and electronic properties of hexagonal rhenium subâ€nitrides Re₃N and Re₂N in comparison with<i>hcp</i>â€Re and wurtziteâ€like rhenium mononitride ReN. Physica Status Solidi (B): Basic Research, 2011, 248, 1369-1374.	0.7	41
77	Elastic properties and interâ€atomic bonding in layered Feâ€“Cu arsenide oxide Sr₂Fe₂CuAs₂O₂. Physica Status Solidi (B): Basic Research, 2011, 248, 2165-2169.	0.7	0
78	Structural, electronic, and magnetic properties of tungsten oxycarbides WC_{1â€“<i>x</i>}O_{<i>x</i>} and WO_{3â€“<i>x</i>}C_{<i>x</i>} from first principles calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 2884-2892.	0.7	6
79	Electronic band structure and Fermi surface of new low-temperature Ni-based superconductors: 3.3K (Ni2P2)(Sr4Sc2O6) and 2.7K (Ni2As2)(Sr4Sc2O6) from first principles. Physica B: Condensed Matter, 2011, 406, 676-682.	1.3	3
80	Stability, structural, elastic, and electronic properties of polymorphs of the superconducting disilicide YIr2Si2. Physica B: Condensed Matter, 2011, 406, 3525-3530.	1.3	21
81	Electronic band structure and Fermi surface of new 3.7K superconductor LiCu2P2 from first-principles calculations. Physica C: Superconductivity and Its Applications, 2011, 471, 226-228.	0.6	6
82	Structural, electronic properties and inter-atomic bonding in layered ironâ€“pnictide oxides (Fe2As2)(Sr4O6), where M are Mg and Ti. Physics Letters, Section A: General, Atomic and Solid State Physics, 2011, 375, 2075-2078.	0.9	2
83	Elastic properties and inter-atomic bonding in new superconductor from first principles calculations. Solid State Communications, 2011, 151, 671-673.	0.9	11
84	Structural, elastic, electronic and magnetic properties of ThCr2Si2 from first-principles calculations. Solid State Communications, 2011, 151, 1165-1168.	0.9	10
85	Electronic band structure, Fermi surface, and elastic properties of polymorphs of the 5.2 K iron-free superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Sr</mml:mi><mml:msub><mml:mi mathvariant="normal">Pt</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">As</mml:mi><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>from first-principles calculations. Physical Review B, 2011, [illegible]	1.1	40
86	Fermi surface, structural and electronic properties of ThCr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>Si<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>-type charge-balanced KFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	2
87	Band structure of new layered arsenides SrRu2As2 and BaRu2As2. Physics of the Solid State, 2010, 52, 6-11.	0.2	5
88	Effect of spin-orbit coupling on structural, electronic, and mechanical properties of cubic thorium monocarbide ThC. Physics of the Solid State, 2010, 52, 2039-2043.	0.2	11
89	Effect of 4d metal impurities on the structure, electronic properties, and stability of hexagonal WC from data of FLAPW-GGA calculations. Physics of the Solid State, 2010, 52, 2450-2457.	0.2	2
90	Electronic structure of Ti-doped Sr4Sc2Fe2As2O6 as a possible parent phase for the new FeAs superconductors. Open Physics, 2010, 8, .	0.8	6

#	Article	IF	Citations
91	Tungsten carbides and nitrides and ternary systems based on them: the electronic structure, chemical bonding and properties. Russian Chemical Reviews, 2010, 79, 611-634.	2.5	14
92	Trends in stability, elastic and electronic properties of cubic Rh, Ir, Pd and Pt carbides depending on carbon content: MC versus M4C from first-principles calculations. Journal of Physics and Chemistry of Solids, 2010, 71, 803-809.	1.9	18
93	Structural, electronic, and magnetic properties of CaCNi3, SrCNi3, and BaCNi3 antiperovskites in comparison to superconducting MgCNi3. Journal of Structural Chemistry, 2010, 51, 170-172.	0.3	6
94	Electronic structure of cubic tungsten subnitride W2N in comparison to hexagonal and cubic tungsten mononitrides WN. Journal of Structural Chemistry, 2010, 51, 199-203.	0.3	15
95	Electronic structure and magnetic properties of RhH x (x = 0.25, 1.00, 1.33) rhodium hydrides according to the FLAPW-GGA band calculation data. Journal of Structural Chemistry, 2010, 51, 956-959.	0.3	3
96	Effect of Li and Na impurities on the electronic and magnetic properties of beryllium oxide. Journal of Structural Chemistry, 2010, 51, 960-963.	0.3	1
97	Single crystals and light-transmitting BeO-ceramic for electronic technology. Refractories and Industrial Ceramics, 2010, 51, 167-171.	0.2	5
98	Structural, elastic, electronic and magnetic properties of perovskite-like Co3WC, Rh3WC and Ir3WC from first principles calculations. Solid State Sciences, 2010, 12, 814-817.	1.5	26
99	The influence of carbon non-stoichiometry on the electronic properties of thorium monocarbide ThC. Solid State Sciences, 2010, 12, 1580-1584.	1.5	7
100	Ab initio study of elastic and electronic properties of cubic thorium pnictides ThPnÂand Th3Pn4 (PnÂ=ÂP,) Tj ETQq0 0 0 rgBT /Overlock	1.5	14
101	Electronic band structure of new â€œ122â€•pnictogen-free superconductor SrPd2Ge2 as compared with SrNi2Ge2 and SrNi2As2 from first principles calculations. Physica B: Condensed Matter, 2010, 405, 3213-3216.	1.3	28
102	Elastic properties of antiperovskite-type Ni-rich nitrides MNNi3 (M=Zn, Cd, Mg, Al, Ga, In, Sn, Sb, Pd, Cu,) Tj ETQq0 0 0 rgBT /Overlock 10 4615-4619.	1.3	61
103	Structural, elastic, electronic properties and Fermi surface for superconducting Mo2GaC in comparison with V2GaC and Nb2GaC from first principles. Physica C: Superconductivity and Its Applications, 2010, 470, 533-537.	0.6	43
104	Electronic properties of novel 6 K superconductor LiFeP in comparison with LiFeAs from first principles calculations. Solid State Communications, 2010, 150, 152-156.	0.9	24
105	Electronic band structure and inter-atomic bonding in tetragonal BiOCuS as a parent phase for novel layered superconductors. Solid State Communications, 2010, 150, 640-643.	0.9	19
106	Stability, structural, elastic and electronic properties of RuN polymorphs from first-principles calculations. Solid State Communications, 2010, 150, 953-956.	0.9	6
107	Origin of incompressibility and hardness from electronic and mechanical properties of hard material ruthenium diboride. Solid State Communications, 2010, 150, 1095-1098.	0.9	11
108	Design of novel magnetic materials based on ZrCuSiAs-like semiconducting pnictide-oxides from first-principles calculations. Solid State Communications, 2010, 150, 2069-2071.	0.9	18

#	Article	IF	Citations
109	Elastic and electronic properties of the new perovskite-like superconductor ZnNNi₃ in comparison with MgCNi₃. Physica Status Solidi (B): Basic Research, 2010, 247, 72-76.	0.7	25
110	Ab initio calculation of the electronic structure, Fermi surface, and elastic properties of the new 7.5-K superconductor Nb2InC. JETP Letters, 2010, 91, 410-414.	0.4	13
111	Structural and electronic properties and the fermi surface of the new non-centrosymmetric superconductors: 3.6 K CaIrSi3 and 2.3 K CaPtSi3. JETP Letters, 2010, 92, 343-347.	0.4	16
112	Structural, elastic and electronic properties of new antiperovskite-like ternary nitrides AlNNi3, GaNNi3 and InNNi3 as predicted from first principles. Computational Materials Science, 2010, 49, 457-461.	1.4	20
113	10.1007/s11451-008-1026-z. , 2010, 50, 146.		0
114	Electronic and structural properties of low-temperature superconductors and ternary pnictides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

#	Article	IF	Citations
127	Band structure of a new layered La3Ni4P4O2 superconductor. JETP Letters, 2009, 89, 285-289.	0.4	4
128	Band structure of new layered superconductors BaRh2P2 and BaIr2P2. JETP Letters, 2009, 89, 357-361.	0.4	7
129	Electronic properties of hexagonal tungsten monocarbide (h-WC) with 3d impurities from first-principles calculations. Physica B: Condensed Matter, 2009, 404, 1887-1891.	1.3	27
130	Structural, electronic and magnetic properties of Î· carbides (Fe3W3C, Fe6W6C, Co3W3C and Co6W6C) from first principles calculations. Physica B: Condensed Matter, 2009, 404, 3544-3549.	1.3	96
131	Structural, electronic properties and intra-atomic bonding in new ThCr2Si2-like arsenides SrRu2As2, BaRu2As2, SrRh2As2 and BaRh2As2 from first principles calculations. Solid State Communications, 2009, 149, 1860-1865.	0.9	18
132	Influence of carbon, nitrogen and oxygen impurities on the ductility and electronic properties of fcc iridium: First-principles study. Solid State Communications, 2009, 149, 1807-1809.	0.9	11
133	Elastic properties and chemical bonding in ternary arsenide SrFe2As2 and quaternary oxyarsenide LaFeAsO â€“ Basic phases for new 38â€“55K superconductors from first principles. Physica C: Superconductivity and Its Applications, 2009, 469, 15-19.	0.6	35
134	The influence of nitrogen vacancies on the magnetic and electronic properties of ruthenium mononitride: First-principles study. Journal of Magnetism and Magnetic Materials, 2009, 321, 3624-3629.	1.0	12
135	First-principles study of structural, elastic and electronic properties of thorium dicarbide (ThC2) polymorphs. Journal of Nuclear Materials, 2009, 393, 192-196.	1.3	13
136	Ab initio predictions of stability and electronic properties of cubic rhodium carbides RhC_x as dependent on carbon content. Physica Status Solidi - Rapid Research Letters, 2009, 3, 218-220.	1.2	9
137	Elastic properties of single- and polycrystalline LaFeAsO, SrFe2As2, and LiFeAs basic phases for new FeAs superconductors. Technical Physics Letters, 2009, 35, 961-963.	0.2	24
138	Electronic structure of tungsten aluminum carbides W2AlC and WAlC2. Russian Journal of Inorganic Chemistry, 2009, 54, 1433-1439.	0.3	8
139	Electronic and elastic properties of the superconducting nanolaminate Ti2InC. Physics of the Solid State, 2009, 51, 1608-1612.	0.2	16
140	Thorium compounds with non-metals: Electronic structure, chemical bond, and physicochemical properties. Journal of Structural Chemistry, 2008, 49, 348-370.	0.3	25
141	Electronic structure and magnetic properties of double perovskites Sr2FeMO6 (M = Sc, Ti, ..., Ni, Cu) according to the data of FLAPW-GGA band structure calculations. Journal of Structural Chemistry, 2008, 49, 781-787.	0.3	24
142	Elastic and electronic properties of hexagonal and cubic polymorphs of tungsten monocarbide WC and mononitride WN from firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2008, 245, 1590-1597.	0.7	73
143	Structural, elastic and electronic properties of superconducting anti-perovskites MgCNi3, ZnCNi3 and CdCNi3 from first principles. Physica C: Superconductivity and Its Applications, 2008, 468, 1-6.	0.6	50
144	Atomic models of non-stoichiometric layered diborides M1â^'xB2 (M=Mg, Al, Zr and Nb) from first principles. Physica C: Superconductivity and Its Applications, 2008, 468, 2224-2228.	0.6	9

#	Article	IF	Citations
145	Electronic structure and magnetism in BeO nanotubes induced by boron, carbon and nitrogen doping, and beryllium and oxygen vacancies inside tube walls. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 41, 164-168.	1.3	53
146	Electronic and magnetic properties of new quaternary oxybismuthides LaOMBi (where M=V, Cr, â€¦, Ni,) Tj ETQq0 0 0 rgBT /Overlock 10 5838-5840.	0.9	10
147	Magnetism without magnetic ions in non-magnetic perovskites SrTiO3, SrZrO3 and SrSnO3. Journal of Magnetism and Magnetic Materials, 2008, 320, 936-942.	1.0	55
148	Structural, elastic and electronic properties and formation energies for hexagonal (W0.5Al0.5)C in comparison with binary carbides WC and Al4C3 from first-principles calculations. Physica B: Condensed Matter, 2008, 403, 2654-2661.	1.3	26
149	Elastic properties of carbide, nitride, and boride ceramics with WC-type structures. Technical Physics Letters, 2008, 34, 841-844.	0.2	9
150	Effect of chromium on the electronic structure and magnetic properties of cementite. Physics of Metals and Metallography, 2008, 105, 568-573.	0.3	12
151	Specific features of steady-state implantation of crystalline silicon with a molecular oxygen-nitrogen beam: Si L 2, 3 x-ray emission spectra. Physics of the Solid State, 2008, 50, 146-151.	0.2	0
152	Energy band structure and X-ray spectra of phenakite Be2SiO4. Physics of the Solid State, 2008, 50, 615-620.	0.2	5
153	Band structure and properties of polymorphic modifications of lower tungsten carbide W2C. Physics of the Solid State, 2008, 50, 1420-1426.	0.2	21
154	Magnetic properties and electronic structure of the LaGaO3 perovskite doped with nickel. Physics of the Solid State, 2008, 50, 2121-2126.	0.2	12
155	First principles calculations of structural states of nonstoichiometric (B/Mg > 2) magnesium diboride. Doklady Physical Chemistry, 2008, 420, 140-143.	0.2	0
156	New superconductor with a layered crystal structure: Nickel oxybismuthide LaO1â^'Î´NiBi. JETP Letters, 2008, 87, 649-651.	0.4	25
157	Electronic structure of new oxygen-free 38-K superconductor Ba1â^'x K x Fe2As2 in comparison with BaFe2As2 from the first principles. JETP Letters, 2008, 88, 107-110.	0.4	44
158	Band structure of a new (16â€“18 K) superconductor LiFeAs compared to Li0.5FeAs and LiCoAs. JETP Letters, 2008, 88, 329-333.	0.4	7
159	Band structure of SrFeAsF and CaFeAsFâ€”the base phases of a new group of oxygen-free FeAs superconductors. JETP Letters, 2008, 88, 683-687.	0.4	14
160	Elastic properties of quaternary oxypnictides LaOFeAs and LaOFeP as basic phases for new 26â€“52K superconducting materials from first principles. Scripta Materialia, 2008, 59, 1099-1102.	2.6	87
161	First-principles calculations of the elastic and electronic properties of the cubic perovskites SrMO3 (M=Ti, V, Zr and Nb) in comparison with SrSnO3. Solid State Sciences, 2008, 10, 217-225.	1.5	83
162	Electronic structure and Fermi surface of the superconductors LaNiBiO and LaCuBiO from first principles. Physical Review B, 2008, 78, .	1.1	21

#	Article	IF	Citations
163	Elastic properties of mono- and polycrystalline hexagonal AlB₂-like diborides of s, p and d metals from first-principles calculations. Journal of Physics Condensed Matter, 2008, 20, 415218.	0.7	234
164	Structural, vibrational, electronic, and luminescence properties of the cyclotetravanadatesA2M(VO3)4(A=Na,Ag;M=Ca,Sr). Physical Review B, 2008, 77, .	1.1	21
165	MAGNETIZATION OF BERYLLIUM MONOXIDE (BeO) WITHOUT MAGNETIC IMPURITIES: A FIRST-PRINCIPLES STUDY. International Journal of Modern Physics B, 2008, 22, 4987-4992.	1.0	14
166	Non-stoichiometric s-, p- and d-metal diborides: synthesis, properties and simulation. Russian Chemical Reviews, 2008, 77, 467-486.	2.5	24
167	Electronic and elastic properties of non-oxide anti-perovskites from first principles: Superconducting<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Cd</mml:mi><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">Ni</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>in comparison with magnetic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inli	1.1	26
168	Bending of MgO tubes: Mechanically induced hexagonal phase of magnesium oxide. Physical Review B, 2007, 75, .	1.1	14
169	Structural, elastic and electronic properties of metastable diamond-like Ti, Fe and Zn monocarbides: Density functional-based tight binding calculations. Diamond and Related Materials, 2007, 16, 243-247.	1.8	3
170	Magnetization of carbon-doped MgO nanotubes. Physical Review B, 2007, 75, .	1.1	34
171	First-principles study on the structural, cohesive and electronic properties of rhombohedral Mo2B5 as compared with hexagonal MoB2. Physica B: Condensed Matter, 2007, 387, 184-189.	1.3	18
172	Electronic and magnetic properties of beryllium oxide with 3d impurities from first-principles calculations. Physica B: Condensed Matter, 2007, 400, 47-52.	1.3	13
173	First principle prediction of vacancy-induced magnetism in non-magnetic perovskite SrTiO3. Physics Letters, Section A: General, Atomic and Solid State Physics, 2007, 371, 155-159.	0.9	59
174	Elastic and electronic properties and stability of SrThO3, SrZrO3 and ThO2 from first principles. Journal of Nuclear Materials, 2007, 361, 69-77.	1.3	56
175	Electronic structure and magnetic properties of Fe3C with 3d and 4d impurities. Physica Status Solidi (B): Basic Research, 2007, 244, 1971-1981.	0.7	23
176	Electronic structure and stability of thorium carbonitrides. Physica Status Solidi (B): Basic Research, 2007, 244, 3198-3205.	0.7	13
177	Synthesis, crystal structure, and electronic properties of double orthovanadate Sr2Bi2/3 (VO4)2. Doklady Physical Chemistry, 2007, 415, 186-189.	0.2	3
178	Ultrasound velocity and absorption in BeO, Al2O3, ZrO2, and SiO2 ceramics. Inorganic Materials, 2007, 43, 1361-1364.	0.2	6
179	Magnetization of beryllium oxide in the presence of nonmagnetic impurities: Boron, carbon, and nitrogen. JETP Letters, 2007, 85, 246-250.	0.4	16
180	Electronic structure, chemical bonding and elastic properties of the first thorium-containing nitride perovskite TaThN3. Physica Status Solidi - Rapid Research Letters, 2007, 1, 89-91.	1.2	218

#	Article	IF	Citations
181	Short-range atomic order in Fe2B powders. Physics of Metals and Metallography, 2007, 103, 470-480.	0.3	11
182	Effect of metal vacancies on the energy parameters of s-, p-, and d-metal diborides. Russian Journal of Inorganic Chemistry, 2007, 52, 238-241.	0.3	5
183	Cesium adsorption on the Î²2-GaAs(001) surface. Journal of Experimental and Theoretical Physics, 2007, 104, 590-601.	0.2	9
184	Effect of high doses on the Si L 2,3 x-ray emission spectra of silicon implanted with iron ions under steady-state conditions. Physics of the Solid State, 2007, 49, 75-81.	0.2	4
185	Elastic parameters of single-crystal and polycrystalline wurtzite-like oxides BeO and ZnO: Ab initio calculations. Physics of the Solid State, 2007, 49, 1067-1073.	0.2	49
186	Ab initio calculations of the stability and structural defects of the B2 CuxFe1â^'x Al phases. Physics of the Solid State, 2007, 49, 1253-1258.	0.2	12
187	Band structure, elastic and magnetic properties, and stability of antiperovskites MCNi3(M = Y â^' Ag) according to FLAPW-GGA calculations. Physics of the Solid State, 2007, 49, 1704-1714.	0.2	22
188	Simulation of the structural, electronic, and magnetic properties of Fe3C1â^'x Bx borocementites. Physics of the Solid State, 2007, 49, 2298-2302.	0.2	5
189	Elastic properties of thorium ceramics ThX (X = C, N, O, P, As, Sb, S, Se). Technical Physics Letters, 2007, 33, 128-131.	0.2	13
190	Novel magnetic half-metallic materials based on ionic insulators doped with nonmagnetic impurities: MgO + B, C, N Systems. Technical Physics Letters, 2007, 33, 541-544.	0.2	25
191	Estimate of the solubility of titanium in beryllium oxide based on quantum-chemical calculations. Glass and Ceramics (English Translation of Steklo I Keramika), 2007, 64, 439-441.	0.2	0
192	Vacancy-induced magnetism of beryllium monoxide. Journal of Structural Chemistry, 2007, 48, 1145-1147.	0.3	4
193	Electronic band structure of thorium hydrides: ThH2 and Th4H15. Physica B: Condensed Matter, 2007, 389, 296-301.	1.3	22
194	Influence of lattice vacancies on the structural, electronic, and cohesive properties of niobium and molybdenum borides from first-principles calculations. Physical Review B, 2006, 73, .	1.1	47
195	Electronic properties of superconducting ternary alloys (Ca,Sr,Ba)(Ga1â^'xSix)2 with AlB2-like structure. Computational Materials Science, 2006, 36, 203-206.	1.4	5
196	Electronic properties of ThSiO4 polymorphs (thorite and huttonite) from first principles calculations. Physica Status Solidi (B): Basic Research, 2006, 243, R44-R46.	0.7	4
197	Electronic structure of cubic thorium monocarbide and hexaboride. Doklady Physical Chemistry, 2006, 407, 106-109.	0.2	7
198	Electronic structure of tetragonal thorium silicate in comparison with thorium dioxide. Doklady Physical Chemistry, 2006, 409, 198-201.	0.2	3

#	Article	IF	Citations
199	Ab initio calculations of the electronic properties of new superconducting nanolaminates: Nb2SnC and Nb2SC1â^'x. Doklady Physical Chemistry, 2006, 411, 317-321.	0.2	21
200	Electronic band structure and stability of fluorite-like phases in the Mg-Sn-B system. Inorganic Materials, 2006, 42, 7-13.	0.2	1
201	First-principle study of B1-like thorium carbide, nitride and oxide. Journal of Nuclear Materials, 2006, 353, 19-26.	1.3	53
202	The influence of oxygen vacancies on the electronic and magnetic properties of perovskite-like SrFeO3-x. Journal of Physics and Chemistry of Solids, 2006, 67, 1436-1439.	1.9	23
203	Electronic and structural properties of cementite-type M3X (M=Fe, Co, Ni; X=C or B) by first principles calculations. Physica B: Condensed Matter, 2006, 371, 126-132.	1.3	130
204	Effects of atomic relaxation and the electronic structure of niobium (100) and (110) surfaces. Physics of Metals and Metallography, 2006, 102, 604-610.	0.3	14
205	Energy-band structure of the A(Sn1â^'x Mx)O3 (A = Ca, Sr, Ba; M = Mn, Fe, Co) perovskite-type phases: A search for new magnetic semimetals. Semiconductors, 2006, 40, 1261-1265.	0.2	17
206	First-principle quantum-chemical calculations of several thermomechanical parameters of beryllium ceramics. Refractories and Industrial Ceramics, 2006, 47, 310-313.	0.2	7
207	Velocity and absorption of ultrasound in beryllium oxide ceramic. Glass and Ceramics (English) Tj ETQq1 1 0.784314 rgBT /Overlock 1	0.2	1
208	Thorite versus huttonite: stability, electronic properties and X-ray emission spectra from first-principle calculations. Physics and Chemistry of Minerals, 2006, 33, 545-552.	0.3	15
209	Effect of Lattice Vacancies on the Band Structure of the Ag[sub 5]Pb[sub 2]O[sub 6] Ternary Oxide. Physics of the Solid State, 2005, 47, 599.	0.2	6
210	New half-metallic ferromagnets: Double perovskites SR(FeM)O3 (M = Sn, Ti, Zr). JETP Letters, 2005, 82, 220-223.	0.4	8
211	Band Structure and the Magnetic and Elastic Properties of SrFeO[sub 3] and LaFeO[sub 3] Perovskites. Physics of the Solid State, 2005, 47, 2082.	0.2	74
212	Elastic properties and chemical bonding in fluoritelike Be2B, AlBeB, MgBeB, and NaBeB. Journal of Structural Chemistry, 2005, 46, 535-537.	0.3	7
213	Electronic structure of Î±-Al2O3 in the bulk and on the surface. Russian Physics Journal, 2005, 48, 1127-1133.	0.2	4
214	Structural, luminescence, and electronic properties of the alkaline metal-strontium cyclotetravanadatesM2Sr(VO3)4, (M=Na, K, Rb, Cs). Physical Review B, 2005, 72, .	1.1	28
215	Interatomic interactions and electronic structure of NbSe2 and Nb1.25Se2 nanotubes. Journal of Structural Chemistry, 2004, 45, 547-556.	0.3	3
216	Electronic band structure and chemical bonding in the new antiperovskites AsNMg3 and SbNMg3. Journal of Solid State Chemistry, 2004, 177, 61-64.	1.4	29

#	Article	IF	Citations
217	Electronic properties of the novel 18-K superconducting Y2C3 as compared with 4-K YC2 from first principles calculations. Solid State Communications, 2004, 131, 223-227.	0.9	26
218	Electronic structure and thermoelectric properties of skutterudite compounds. Journal of Physics Condensed Matter, 2004, 16, 979-987.	0.7	26
219	Electronic properties of the novel 18-K superconducting Y2C3 as compared with 4-K YC2 from first principles calculations. Solid State Communications, 2004, 131, 223-223.	0.9	3
220	Electronic Band Structure of the Fluorite-like Borides AlBeB, MgBeB, and NaBeB. Inorganic Materials, 2003, 39, 694-695.	0.2	6
221	Electronic Structure and Chemical Bonding in Crystalline and Nanosized Forms of Magnesium Diboride. Doklady Physical Chemistry, 2003, 388, 43-47.	0.2	6
222	Band structure of superconducting dodecaborides YB12 and ZrB12. Physics of the Solid State, 2003, 45, 1429-1434.	0.2	35
223	Effect of metal vacancies on the band structure of Nb, Zr, and Y diborides. Physics of the Solid State, 2003, 45, 1617-1621.	0.2	18
224	Band structure of new superconducting AlB2-like ternary silicides M(Al0.5Si0.5)2and M(Ga0.5Si0.5)2(where M Â Ca, Sr and Ba). Journal of Physics Condensed Matter, 2003, 15, L541-L545.	0.7	32
225	Effect of Co doping on the electronic structure ofMgCNi3. Physical Review B, 2002, 66, .	1.1	32
226	Electronic properties of new Ca(AlxSi1â^'x)2 and Sr(GaxSi1â^'x)2 superconductors in crystalline and nanotubular states. JETP Letters, 2002, 76, 189-193.	0.4	24
227	Band structure of ZrB2, VB2, NbB2, and TaB2 hexagonal diborides: Comparison with superconducting MgB2. Physics of the Solid State, 2002, 44, 1833-1839.	0.2	68
228	Energy Bands and Chemical Binding in MgCNi3 Superconductor. Journal of Structural Chemistry, 2002, 43, 168-171.	0.3	4
229	Electronic structure of the new MgCNi3 superconductor and related intermetallic compounds. JETP Letters, 2001, 74, 122-127.	0.4	19
230	The band structures of superconducting MgB2 and the isostructural compounds CaGa2, AgB2, AuB2, ZrBe2, and HfBe2. Physics of the Solid State, 2001, 43, 2213-2218.	0.2	22
231	Quinate:NAP(P)+-oxidoreductase from Larix sibirica: purification, characterization and function. Trees - Structure and Function, 1995, 10, 46.	0.9	11
232	Electronic Structure of Fluoriteâ€Like TiF₂. Physica Status Solidi (B): Basic Research, 1990, 157, K29.	0.7	0
233	Lattice vacancies and electronic properties of zirconium hydrides. Journal of the Less Common Metals, 1990, 167, 1-9.	0.9	1