Igor R Shein

List of Publications by Citations

232 papers	4,048 citations	32 h-index	52 g-index
235 ext. papers	4,439 ext. citations	1.9 avg, IF	5.81 L-index

#	Paper	IF	Citations
232	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	3.2	201
231	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	1.8	190
230	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	2.5	184
229	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	2.8	108
228	Elastic properties of quaternary oxypnictides LaOFeAs and LaOFeP as basic phases for new 26–52K superconducting materials from first principles. *Scripta Materialia*, **2008**, 59, 1099-1102	5.6	80
227	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	3.4	74
226	Structural, electronic and magnetic properties of ternary carbides (Fe3W3C, Fe6W6C, Co3W3C and Co6W6C) from first principles calculations. *Physica B: Condensed Matter*, **2009**, 404, 3544-3549	2.8	72
225	Graphene-like nanocarbides and nanonitrides of d metals (MXenes): synthesis, properties and simulation. *Micro and Nano Letters*, **2013**, 8, 59-62	0.9	66
224	Elastic and electronic properties of hexagonal and cubic polymorphs of tungsten monocarbide WC and mononitride WN from first-principles calculations. *Physica Status Solidi (B): Basic Research*, **2008**, 245, 1590-1597	1.3	63
223	Structural, electronic properties and stability of tungsten mono- and semi-carbides: A first principles investigation. *Journal of Physics and Chemistry of Solids*, **2009**, 70, 64-71	3.9	62
222	Band structure of ZrB2, VB2, NbB2, and TaB2 hexagonal diborides: Comparison with superconducting MgB2. *Physics of the Solid State*, **2002**, 44, 1833-1839	0.8	62
221	Band structure and the magnetic and elastic properties of SrFeO3 and LaFeO3 perovskites. *Physics of the Solid State*, **2005**, 47, 2082	0.8	62
220	Electronic and structural properties of low-temperature superconductors and ternary pnictides ANi2Pn2 (A=Sr,Ba and Pn=P,As). *Physical Review B*, **2009**, 79,	3.3	60
219	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	2.3	57
218	Elastic properties of superconducting MAX phases from first-principles calculations. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 228-232	1.3	56
217	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	2.3	51
216	Elastic and electronic properties and stability of SrThO3, SrZrO3 and ThO2 from first principles. *Journal of Nuclear Materials*, **2007**, 361, 69-77	3.3	49

215	Magnetism without magnetic ions in non-magnetic perovskites SrTiO3, SrZrO3 and SrSnO3. *Journal of Magnetism and Magnetic Materials*, **2008**, 320, 936-942	2.8	49
214	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	2.8	48
213	Elastic properties of antiperovskite-type Ni-rich nitrides MNNi3 (M=Zn, Cd, Mg, Al, Ga, In, Sn, Sb, Pd, Cu, Ag and Pt) as predicted from first-principles calculations. *Physica B: Condensed Matter*, **2010**, 405, 4615-4619	2.8	48
212	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	3	47
211	First-principle study of B1-like thorium carbide, nitride and oxide. *Journal of Nuclear Materials*, **2006** , 353, 19-26	3.3	47
210	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	1.3	46
209	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	0.8	45
208	Electronic structure of new oxygen-free 38-K superconductor Ba1 K x Fe2As2 in comparison with BaFe2As2 from the first principles. *JETP Letters*, **2008**, 88, 107-110	1.2	44
207	Electronic band structure, Fermi surface, and elastic properties of polymorphs of the 5.2 K iron-free superconductor SrPt2As2 from first-principles calculations. *Physical Review B*, **2011**, 83,	3.3	39
206	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,	3.3	39
205	Elastic and electronic properties of hexagonal rhenium sub-nitrides Re3N and Re2N in comparison with hcp-Re and wurtzite-like rhenium mononitride ReN. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 1369-1374	1.3	35
204	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	1.3	35
203	Structural and electronic properties of the 17 K superconductor Sr2ScFePO3 in comparison to Sr2ScFeAsO3 from first principles calculations. *Physical Review B*, **2009**, 79,	3.3	32
202	Elastic properties and chemical bonding in ternary arsenide SrFe2As2 and quaternary oxyarsenide LaFeAsO Basic phases for new 38 5K superconductors from first principles. *Physica C: Superconductivity and Its Applications*, **2009**, 469, 15-19	1.3	32
201	Magnetization of carbon-doped MgO nanotubes. *Physical Review B*, **2007**, 75,	3.3	32
200	Effect of Co doping on the electronic structure of MgCNi3. *Physical Review B*, **2002**, 66,	3.3	32
199	Band structure of new superconducting AlB2-like ternary silicides M(Al0.5Si0.5)2and M(Ga0.5Si0.5)2(where M Ca, Sr and Ba). *Journal of Physics Condensed Matter*, **2003**, 15, L541-L545	1.8	31
198	Band structure of superconducting dodecaborides YB12 and ZrB12. *Physics of the Solid State*, **2003**, 45, 1429-1434	0.8	31

197	Electronic structure and properties of beryllium oxide. *Inorganic Materials*, **2009**, 45, 223-234	0.9	30
196	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	3.3	28
195	Electronic and Magnetic Properties of Superconducting Sr4V2Fe2As2O6 Versus Sr4Sc2Fe2As2O6. *Journal of Superconductivity and Novel Magnetism*, **2009**, 22, 613-617	1.5	28
194	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	1.2	27
193	Electronic band structure of new 122 pnictogen-free superconductor SrPd2Ge2 as compared with SrNi2Ge2 and SrNi2As2 from first principles calculations. *Physica B: Condensed Matter*, **2010**, 405, 3213-3216	2.8	27
192	Electronic and elastic properties of non-oxide anti-perovskites from first principles: Superconducting CdCNi3 in comparison with magnetic InCNi3. *Physical Review B*, **2008**, 77,	3.3	26
191	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	2.8	26
190	New superconductor with a layered crystal structure: Nickel oxybismuthide LaO1−xNiBi. *JETP Letters*, **2008**, 87, 649-651	1.2	25
189	Electronic band structure and chemical bonding in the new antiperovskites AsNMg3 and SbNMg3. *Journal of Solid State Chemistry*, **2004**, 177, 61-64	3.3	25
188	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	1.6	24
187	Electronic structure and thermoelectric properties of skutterudite compounds. *Journal of Physics Condensed Matter*, **2004**, 16, 979-987	1.8	24
186	Electronic properties of hexagonal tungsten monocarbide (h-WC) with 3d impurities from first-principles calculations. *Physica B: Condensed Matter*, **2009**, 404, 1887-1891	2.8	23
185	Electronic structure and magnetic properties of Fe3C with 3d and 4d impurities. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 1971-1981	1.3	23
184	Thorium compounds with non-metals: Electronic structure, chemical bond, and physicochemical properties. *Journal of Structural Chemistry*, **2008**, 49, 348-370	0.9	23
183	Electronic properties of new Ca(AlxSi1−x)2 and Sr(GaxSi1−x)2 superconductors in crystalline and nanotubular states. *JETP Letters*, **2002**, 76, 189-193	1.2	23
182	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	1.5	22
181	Electronic properties of novel 6 K superconductor LiFeP in comparison with LiFeAs from first principles calculations. *Solid State Communications*, **2010**, 150, 152-156	1.6	22
180	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	1.3	22

179	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	0.7	22
178	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	0.9	22
177	Structural, luminescence, and electronic properties of the alkaline metal-strontium cyclotetravanadates M2Sr(VO3)4, (M=Na, K, Rb, Cs). *Physical Review B*, **2005**, 72,	3.3	22
176	Electronic properties and chemical bonding in quaternary arsenide oxides LaZnAsO and YZnAsO. *Materials Chemistry and Physics*, **2009**, 116, 129-133	4.4	21
175	Electronic structure and Fermi surface of the superconductors LaNiBiO and LaCuBiO from first principles. *Physical Review B*, **2008**, 78,	3.3	21
174	Non-stoichiometric s-, p- and d-metal diborides: synthesis, properties and simulation. *Russian Chemical Reviews*, **2008**, 77, 467-486	6.8	21
173	Structural, electronic, magnetic and elastic properties of tetragonal layered diselenide KCo2Se2 from first principles calculations. *Physica B: Condensed Matter*, **2012**, 407, 271-275	2.8	20
172	Band structure, elastic and magnetic properties, and stability of antiperovskites MCNi3(M = Y Ag) according to FLAPW-GGA calculations. *Physics of the Solid State*, **2007**, 49, 1704-1714	0.8	20
171	Electronic band structure of thorium hydrides: ThH2 and Th4H15. *Physica B: Condensed Matter*, **2007**, 389, 296-301	2.8	19
170	Ab initio calculations of the electronic properties of new superconducting nanolaminates: Nb2SnC and Nb2SC1. *Doklady Physical Chemistry*, **2006**, 411, 317-321	0.8	19
169	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	3.9	19
168	Structural, electronic properties and inter-atomic bonding in layered chalcogenide oxides LaMChO (where M = Cu, Ag, and Ch = S, Se) from FLAPW-GGA calculations. *Solid State Sciences*, **2012**, 14, 89-93	3.4	18
167	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	3.2	18
166	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	1.6	18
165	Electronic structure of the new MgCNi3 superconductor and related intermetallic compounds. *JETP Letters*, **2001**, 74, 122-127	1.2	18
164	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	1.6	17
163	Elastic properties of single- and polycrystalline LaFeAsO, SrFe2As2, and LiFeAs basic phases for new FeAs superconductors. *Technical Physics Letters*, **2009**, 35, 961-963	0.7	17
162	Structural, elastic, electronic and magnetic properties of perovskite-like Co3WC, Rh3WC and Ir3WC from first principles calculations. *Solid State Sciences*, **2010**, 12, 814-817	3.4	17

161	Design of novel magnetic materials based on ZrCuSiAs-like semiconducting pnictide-oxides from first-principles calculations. *Solid State Communications*, **2010**, 150, 2069-2071	1.6	17
160	Structural, vibrational, electronic, and luminescence properties of the cyclotetravanadates A2M(VO3)4 (A=Na,Ag; M=Ca,Sr). *Physical Review B*, **2008**, 77,	3.3	17
159	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	2.8	17
158	Energy-band structure of the A(Sn1− Mx)O3 (A = Ca, Sr, Ba; M = Mn, Fe, Co) perovskite-type phases: A search for new magnetic semimetals. *Semiconductors*, **2006**, 40, 1261-1265	0.7	17
157	Magnetization of beryllium oxide in the presence of nonmagnetic impurities: Boron, carbon, and nitrogen. *JETP Letters*, **2007**, 85, 246-250	1.2	16
156	Band structure and properties of polymorphic modifications of lower tungsten carbide W2C. *Physics of the Solid State*, **2008**, 50, 1420-1426	0.8	16
155	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	0.8	16
154	Structural, elastic, and electronic properties of new 211 MAX phase Nb2GeC from first-principles calculations. *Physica B: Condensed Matter*, **2013**, 410, 42-48	2.8	15
153	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	1.2	15
152	Electronic and elastic properties of perovskite-like W3NiC, W3NiN and Co3WC from first-principles calculations. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1646-1651	1.3	15
151	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	3.9	15
150	Effect of metal vacancies on the band structure of Nb, Zr, and Y diborides. *Physics of the Solid State*, **2003**, 45, 1617-1621	0.8	15
149	Stability, structural, elastic, and electronic properties of polymorphs of the superconducting disilicide YIr2Si2. *Physica B: Condensed Matter*, **2011**, 406, 3525-3530	2.8	14
148	Band structure of SrFeAsF and CaFeAsF the base phases of a new group of oxygen-free FeAs superconductors. *JETP Letters*, **2008**, 88, 683-687	1.2	14
147	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	5.7	13
146	Electronic structure of cubic tungsten subnitride W2N in comparison to hexagonal and cubic tungsten mononitrides WN. *Journal of Structural Chemistry*, **2010**, 51, 199-203	0.9	13
145	Electronic and magnetic properties of beryllium oxide with 3d impurities from first-principles calculations. *Physica B: Condensed Matter*, **2007**, 400, 47-52	2.8	13
144	Thorite versus huttonite: stability, electronic properties and X-ray emission spectra from first-principle calculations. *Physics and Chemistry of Minerals*, **2006**, 33, 545-552	1.6	13

143	Electronic band structure, optical absorption, and photocatalytic activity of iron-doped anatase. *Physics of the Solid State*, **2013**, 55, 1903-1912	0.8	12
142	Structural, electronic properties and chemical bonding in protonated lithium metallates Li2 H x MO3 (M = Ti, Zr, Sn). *Journal of Structural Chemistry*, **2011**, 52, 1043-1050	0.9	12
141	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	1.5	12
140	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	1.2	12
139	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	2.8	12
138	Electronic and elastic properties of the superconducting nanolaminate Ti2InC. *Physics of the Solid State*, **2009**, 51, 1608-1612	0.8	12
137	Tungsten carbides and nitrides and ternary systems based on them: the electronic structure, chemical bonding and properties. *Russian Chemical Reviews*, **2010**, 79, 611-634	6.8	12
136	MAGNETIZATION OF BERYLLIUM MONOXIDE (BeO) WITHOUT MAGNETIC IMPURITIES: A FIRST-PRINCIPLES STUDY. *International Journal of Modern Physics B*, **2008**, 22, 4987-4992	1.1	12
135	Electronic structure and stability of thorium carbonitrides. *Physica Status Solidi (B): Basic Research*, **2007**, 244, 3198-3205	1.3	12
134	Elastic properties of thorium ceramics ThX (X = C, N, O, P, As, Sb, S, Se). *Technical Physics Letters*, **2007**, 33, 128-131	0.7	12
133	Magnetic properties and electronic structure of the LaGaO3 perovskite doped with nickel. *Physics of the Solid State*, **2008**, 50, 2121-2126	0.8	12
132	Effects of atomic relaxation and the electronic structure of niobium (100) and (110) surfaces. *Physics of Metals and Metallography*, **2006**, 102, 604-610	1.2	12
131	Bismuth titanate pyrochlores doped by alkaline earth elements: First-principles calculations and experimental study. *Solid State Ionics*, **2018**, 317, 183-189	3.3	11
130	Electronic Structure, Mechanical and Dynamical Stability of Hexagonal Subcarbides M2C (M = Tc, Ru, Rh, Pd, Re, Os, Ir, and Pt): Ab Initio Calculations. *Physics of the Solid State*, **2018**, 60, 213-224	0.8	11
129	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	1.3	11
128	Composition of beryllium oxide ceramics. *Refractories and Industrial Ceramics*, **2011**, 51, 377-381	1.1	11
127	Electronic structure and magnetic properties of Fe3C with 2p and 3p impurities. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 2167-2171	1.3	11
126	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	1.6	11

125	Ab initio calculations of the stability and structural defects of the B2 CuxFe1 Al phases. *Physics of the Solid State*, **2007**, 49, 1253-1258	0.8	11
124	Bending of MgO tubes: Mechanically induced hexagonal phase of magnesium oxide. *Physical Review B*, **2007**, 75,	3.3	11
123	Photocatalytic Properties of BiTiO (= 0, 0.5) Pyrochlores: Hybrid DFT Calculations and Experimental Study. *Inorganic Chemistry*, **2020**, 59, 12385-12396	5.1	11
122	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	0.8	10
121	Synthesis and characterisation of new MO(OH)2 (M = Zr, Hf) oxyhydroxides and related Li2MO3 salts. *Dalton Transactions*, **2014**, 43, 2755-63	4.3	10
120	Charge distribution and mobility of lithium ions in Li2TiO3 from 6,7Li NMR data. *Journal of Structural Chemistry*, **2013**, 54, 111-118	0.9	10
119	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	5.7	10
118	First-principles study of structural, elastic and electronic properties of thorium dicarbide (ThC2) polymorphs. *Journal of Nuclear Materials*, **2009**, 393, 192-196	3.3	10
117	Elastic properties and inter-atomic bonding in new superconductor KFe2Se2 from first principles calculations. *Solid State Communications*, **2011**, 151, 671-673	1.6	10
116	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	0.8	10
115	Electronic and magnetic properties of new quaternary oxybismuthides LaOMBi (where M = V, Cr, Ni, Cu) from first principles. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2008**, 372, 5838-5840	2.3	10
114	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	1.5	10
113	Ab Initio and Experimental Insights on Structural, Electronic, Optical, and Magnetic Properties of Cr-Doped BiTiO. *Inorganic Chemistry*, **2019**, 58, 9904-9915	5.1	9
112	Synthesis, optical properties, and photocatalytic activity of lanthanide-doped anatase. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 29-33	1.5	9
111	Electronic band structure, optical absorption and photocatalytic activity of anatase doped with bismuth or carbon. *Journal of Alloys and Compounds*, **2013**, 548, 46-51	5.7	9
110	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	1.5	9
109	Structural, electronic, elastic properties and chemical bonding in LaNi2P2 and LaNi2Ge2 from first principles. *Intermetallics*, **2012**, 26, 1-7	3.5	9
108	Hydrogen-induced enhancement of ductility of fcc iridium: A first-principles study. *Materials Letters* , **2009**, 63, 2413-2415	3.3	9

107	Ab initio study of elastic and electronic properties of cubic thorium pnictides ThPn and Th3Pn4 (Pn = P, As, and Sb). *Solid State Sciences*, **2010**, 12, 2106-2112	3.4	9
106	Origin of incompressibility and hardness from electronic and mechanical properties of hard material ruthenium diboride. *Solid State Communications*, **2010**, 150, 1095-1098	1.6	9
105	Cesium adsorption on the □-GaAs(001) surface. *Journal of Experimental and Theoretical Physics*, **2007**, 104, 590-601	1	9
104	Effect of chromium on the electronic structure and magnetic properties of cementite. *Physics of Metals and Metallography*, **2008**, 105, 568-573	1.2	9
103	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	0.8	8
102	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	3.3	8
101	Ab initio predictions of stability and electronic properties of cubic rhodium carbides RhCx as dependent on carbon content. *Physica Status Solidi - Rapid Research Letters*, **2009**, 3, 218-220	2.5	8
100	Structural, elastic, electronic and magnetic properties of ThCr2Si2 from first-principles calculations. *Solid State Communications*, **2011**, 151, 1165-1168	1.6	8
99	Quinate:NAP(P)+-oxidoreductase from Larix sibirica: purification, characterization and function. *Trees - Structure and Function*, **1995**, 10, 46	2.6	8
98	Band structure of new layered superconductors BaRh2P2 and BaIr2P2. *JETP Letters*, **2009**, 89, 357-361	1.2	7
97	Electronic structure of tungsten aluminum carbides W2AlC and WAlC2. *Russian Journal of Inorganic Chemistry*, **2009**, 54, 1433-1439	1.5	7
96	Band structure of a new (16□8 K) superconductor LiFeAs compared to Li0.5FeAs and LiCoAs. *JETP Letters*, **2008**, 88, 329-333	1.2	7
95	Short-range atomic order in Fe2B powders. *Physics of Metals and Metallography*, **2007**, 103, 470-480	1.2	7
94	Atomic models of non-stoichiometric layered diborides M1□B2 (M = Mg, Al, Zr and Nb) from first principles. *Physica C: Superconductivity and Its Applications*, **2008**, 468, 2224-2228	1.3	7
93	Elastic properties of carbide, nitride, and boride ceramics with WC-type structures. *Technical Physics Letters*, **2008**, 34, 841-844	0.7	7
92	New half-metallic ferromagnets: Double perovskites SR(FeM)O3 (M = Sn, Ti, Zr). *JETP Letters*, **2005**, 82, 220-223	1.2	7
91	Elastic properties and chemical bonding in fluoritelike Be2B, AlBeB, MgBeB, and NaBeB. *Journal of Structural Chemistry*, **2005**, 46, 535-537	0.9	7
90	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	1.2	6

89	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	3.2	6
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