Igor R Shein

List of Publications by Year in Descending Order

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	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	5.1	0
231	Photocatalytic Properties of BiTiO (= 0, 0.5) Pyrochlores: Hybrid DFT Calculations and Experimental Study. *Inorganic Chemistry*, **2020**, 59, 12385-12396	5.1	11
230	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
229	Thermodynamic properties and lattice dynamics investigation of LuBC: experiment and ab initio calculations. *Physical Chemistry Chemical Physics*, **2019**, 21, 24684-24694	3.6	1
228	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	0.9	
227	Bismuth titanate pyrochlores doped by alkaline earth elements: First-principles calculations and experimental study. *Solid State Ionics*, **2018**, 317, 183-189	3.3	11
226	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
225	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
224	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	0.9	1
223	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
222	Mechanical and Dynamic Stability of Complete and Nonstoichiometric 3C-SixCy from Ab Initio Calculations. *Physics of the Solid State*, **2018**, 60, 2012-2018	0.8	
221	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	1.7	
220	Impurity centers and electronic band structure of lithium-doped cadmium oxide. *Ceramics International*, **2018**, 44, 17313-17318	5.1	5
219	Metal-metal bond excitation in colloidal solution of NbS. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2017**, 179, 46-50	4.4	3
218	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
217	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	3.9	5
216	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	0.8	2

215	Structural, elastic and electronic properties of Ir-based carbides-antiperovskites Ir 3 M C (M = Ti, Zr, Nb and Ta) as predicted from first-principles calculations. *Computational Condensed Matter*, **2017**, 11, 60-68	1.7	3
214	Electronic structure of non-stoichiometric ZrCuSiAs-like layered LaZnAsO1 compositions: FLAPW-GGA modeling. *Journal of Structural Chemistry*, **2016**, 57, 805-807	0.9	
213	Pressure-induced zircon to monazite phase transition in Y1 La PO4: First-principles calculations. *Journal of Structural Chemistry*, **2016**, 57, 1513-1518	0.9	4
212	Electronic structure and formation energies of nonstoichiometric dichalcogenides M x X2 (M = Nb, Mo, W; X = Se, Te). *Journal of Structural Chemistry*, **2016**, 57, 281-286	0.9	1
211	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	0.9	2
210	Synthesis, optical properties, and photocatalytic activity of lanthanide-doped anatase. *Russian Journal of Inorganic Chemistry*, **2014**, 59, 29-33	1.5	9
209	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	1.2	
208	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
207	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
206	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
205	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	3.5	4
204	Effect of fluorine, nitrogen, and carbon impurities on the electronic and magnetic properties of WO3. *Semiconductors*, **2013**, 47, 740-744	0.7	2
203	Electronic band structure, optical absorption, and photocatalytic activity of iron-doped anatase. *Physics of the Solid State*, **2013**, 55, 1903-1912	0.8	12
202	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	0.8	3
201	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
200	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	1.5	3
199	Correlated band structure of superconducting NdFeAsO0.9F0.1: Dynamical mean-field study. *JETP Letters*, **2013**, 98, 373-377	1.2	1
198	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	0.8	4

197	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
196	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
195	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
194	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
193	The effect of arsenic vacancies on the electronic and magnetic properties of LaFeAs1□O. *Journal of Magnetism and Magnetic Materials*, **2013**, 335, 21-27	2.8	2
192	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	5.7	3
191	Ab initio Probing of Magnetic and Electronic Properties of Monoclinic □WO3 Doped with 3d Transition Metals Within GGA and GGA+U. *Journal of Superconductivity and Novel Magnetism*, **2013**, 26, 2343-2346	1.5	1
190	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
189	Graphene-like nanocarbides and nanonitrides of d metals (MXenes): synthesis, properties and simulation. *Micro and Nano Letters*, **2013**, 8, 59-62	0.9	66
188	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
187	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
186	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
185	Mechanical properties and electronic structure of zircon: Ab inito FLAPW-GGA calculations. *Inorganic Materials: Applied Research*, **2012**, 3, 7-10	0.6	2
184	The influence of oxygen deficiency on structural and electronic properties of layered superconductor (Fe2As2)(Sr4V2O6□). *Journal of Materials Science*, **2012**, 47, 3663-3668	4.3	2
183	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
182	Electronic band structure of pseudo-binary AlB2-like hexagonal silicides SrNixSi2□ as novel low-TC superconductors. *Physica B: Condensed Matter*, **2012**, 407, 4592-4594	2.8	0
181	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
180	Structural, electronic, elastic properties and chemical bonding in LaNi2P2 and LaNi2Ge2 from first principles. *Intermetallics*, **2012**, 26, 1-7	3.5	9

179	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
178	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 iron□halcogenide superconductors. *Computational Materials Science*, **2012**, 60, 1-6	3.2	2
177	Electronic structure, Fermi surface, and chemical bonding in new layered oxyselenide: HgCuSeO. *Journal of Structural Chemistry*, **2012**, 53, 634-638	0.9	
176	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
175	Electronic, magnetic properties and correlation effects in the layered quaternary iron oxyselenide Na2Fe2Se2O from first principles. *Solid State Communications*, **2012**, 152, 1969-1972	1.6	2
174	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	4.3	4
173	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	1.5	1
172	Impurity-Induced Magnetization of Layered Semiconductor LaCuSeO as Predicted from First-Principles Calculations. *Journal of Superconductivity and Novel Magnetism*, **2012**, 25, 1509-1513	1.5	2
171	Nanotubes of layered iron-based superconductors: Simulations of atomic structure and electronic properties. *Computational Materials Science*, **2011**, 50, 824-827	3.2	3
170	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
169	Structure-induced semiconductor -> metal transition in lead monosulfide PbS: Ab initio calculations. *Doklady Physical Chemistry*, **2011**, 437, 50-53	0.8	
168	Magnetization of zircon induced by 3d impurities: Ab initio calculations. *Doklady Physical Chemistry*, **2011**, 438, 90-93	0.8	2
167	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	3.4	1
166	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
165	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
164	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	1.3	5
163	23Na NMR in binary lithium-sodium cobaltite. *Bulletin of the Russian Academy of Sciences: Physics*, **2011**, 75, 1157-1159	0.4	1
162	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	1.5	4

161	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
160	Composition of beryllium oxide ceramics. *Refractories and Industrial Ceramics*, **2011**, 51, 377-381	1.1	11
159	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
158	Elastic properties of superconducting MAX phases from first-principles calculations. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 228-232	1.3	56
157	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
156	Elastic properties and inter-atomic bonding in layered Fe□u arsenide oxide Sr2Fe2CuAs2O2. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 2165-2169	1.3	
155	Structural, electronic, and magnetic properties of tungsten oxycarbides WC1□Ox and WO3□Cx from first principles calculations. *Physica Status Solidi (B): Basic Research*, **2011**, 248, 2884-2892	1.3	6
154	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	2.8	3
153	Stability, structural, elastic, and electronic properties of polymorphs of the superconducting disilicide YIr2Si2. *Physica B: Condensed Matter*, **2011**, 406, 3525-3530	2.8	14
152	Electronic band structure and Fermi surface of new 3.7 K superconductor LiCu2P2 from first-principles calculations. *Physica C: Superconductivity and Its Applications*, **2011**, 471, 226-228	1.3	5
151	Structural, electronic properties and inter-atomic bonding in layered iron□nictide oxides (Fe2As2)(Sr4O6), where M are Mg and Ti. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2011**, 375, 2075-2078	2.3	2
150	Elastic properties and inter-atomic bonding in new superconductor KFe2Se2 from first principles calculations. *Solid State Communications*, **2011**, 151, 671-673	1.6	10
149	Structural, elastic, electronic and magnetic properties of ThCr2Si2 from first-principles calculations. *Solid State Communications*, **2011**, 151, 1165-1168	1.6	8
148	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
147	Fermi surface, structural and electronic properties of ThCr2Si2-type charge-balanced KFe2AsSe: A parent system for the group of mixed pnictide-chalcogenide superconductors. *Physical Review B*, **2011**, 84,	3.3	1
146	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
145	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
144	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

143	Band structure of new layered arsenides SrRu2As2 and BaRu2As2. *Physics of the Solid State*, **2010**, 52, 6-11	0.8	3
142	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
141	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	0.8	1
140	Electronic structure of Ti-doped Sr4Sc2Fe2As2O6 as a possible parent phase for the new FeAs superconductors. *Open Physics*, **2010**, 8,	1.3	5
139	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
138	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
137	Structural, electronic, and magnetic properties of CaCNi3, SrCNi3, and BaCNi3 antiperovskites in comparison to superconducting MgCNi3. *Journal of Structural Chemistry*, **2010**, 51, 170-172	0.9	6
136	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
135	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	0.9	3
134	Effect of Li and Na impurities on the electronic and magnetic properties of beryllium oxide. *Journal of Structural Chemistry*, **2010**, 51, 960-963	0.9	1
133	Single crystals and light-transmitting BeO-ceramic for electronic technology. *Refractories and Industrial Ceramics*, **2010**, 51, 167-171	1.1	5
132	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
131	The influence of carbon non-stoichiometry on the electronic properties of thorium monocarbide ThC. *Solid State Sciences*, **2010**, 12, 1580-1584	3.4	6
130	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
129	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
128	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
127	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
126	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

125	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
124	Stability, structural, elastic and electronic properties of RuN polymorphs from first-principles calculations. *Solid State Communications*, **2010**, 150, 953-956	1.6	6
123	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
122	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
121	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
120	Specific features of steady-state implantation of crystalline silicon with a molecular oxygen-nitrogen beam: Si L 2, 3 x-ray emission spectra **2010**, 50, 146		
119	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
118	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
117	Electronic properties and chemical bonding in quaternary arsenide oxides LaZnAsO and YZnAsO. *Materials Chemistry and Physics*, **2009**, 116, 129-133	4.4	21
116	Hydrogen-induced enhancement of ductility of fcc iridium: A first-principles study. *Materials Letters* , **2009**, 63, 2413-2415	3.3	9
115	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
114	Electronic structure of tungsten carbonitrides WC1− N x. *Journal of Structural Chemistry*, **2009**, 50, 1-9	0.9	5
113	Chemical bonding in LaFeAsO, SrFe2As2, and LiFeAs: Basic phases of new 18–26 K superconductors. *Journal of Structural Chemistry*, **2009**, 50, 552-555	0.9	4
112	Electronic and Magnetic Properties of Superconducting Sr4V2Fe2As2O6 Versus Sr4Sc2Fe2As2O6. *Journal of Superconductivity and Novel Magnetism*, **2009**, 22, 613-617	1.5	28
111	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
110	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
109	Influence of carbon vacancies on the electronic properties of solid solutions in the W-Al-C system from first principles calculations. *Doklady Physical Chemistry*, **2009**, 424, 14-16	0.8	3
108	Electronic structure and properties of beryllium oxide. *Inorganic Materials*, **2009**, 45, 223-234	0.9	30

107	Band structure of (Sr3Sc2O5)Fe2As2 as a possible basis phase of new FeAs superconductors. *JETP Letters*, **2009**, 89, 41-45	1.2	6
106	Band structure of a new layered La3Ni4P4O2 superconductor. *JETP Letters*, **2009**, 89, 285-289	1.2	4
105	Band structure of new layered superconductors BaRh2P2 and BaIr2P2. *JETP Letters*, **2009**, 89, 357-361	1.2	7
104	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
103	Structural, electronic and magnetic properties of □tarbides (Fe3W3C, Fe6W6C, Co3W3C and Co6W6C) from first principles calculations. *Physica B: Condensed Matter*, **2009**, 404, 3544-3549	2.8	72
102	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
101	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
100	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
99	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
98	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
97	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
96	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
95	Electronic structure of tungsten aluminum carbides W2AlC and WAlC2. *Russian Journal of Inorganic Chemistry*, **2009**, 54, 1433-1439	1.5	7
94	Electronic and elastic properties of the superconducting nanolaminate Ti2InC. *Physics of the Solid State*, **2009**, 51, 1608-1612	0.8	12
93	First principles calculations of structural states of nonstoichiometric (B/Mg > 2) magnesium diboride. *Doklady Physical Chemistry*, **2008**, 420, 140-143	0.8	
92	New superconductor with a layered crystal structure: Nickel oxybismuthide LaO1□NiBi. *JETP Letters*, **2008**, 87, 649-651	1.2	25
91	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
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