Igor R Shein

List of Publications by Year
in descending order

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233 papers	4,756 citations	136950 32 h-index	149698 56 g-index
235 all docs	235 docs citations	235 times ranked	4371 citing authors

#	Article	IF	Citations
1	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.	3.0	286
2	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	234
3	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.	2.4	218
4	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.	2.7	130
5	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.	2.7	96
6	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.	5.2	87
7	Grapheneâ€like nanocarbides and nanonitrides of d metals (MXenes): synthesis, properties and simulation. Micro and Nano Letters, 2013, 8, 59-62.	1.3	84
8	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.	3.2	83
9	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.	0.6	74
10	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.	1.5	73
11	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.	4.0	73
12	Band structure of ZrB2, VB2, NbB2, and TaB2 hexagonal diborides: Comparison with superconducting MgB2. Physics of the Solid State, 2002, 44, 1833-1839.	0.6	68
13	Elastic properties of superconducting MAX phases from firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2011, 248, 228-232.	1.5	68
14	Electronic and structural properties of low-temperature superconductors and ternary pnictides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		

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19	Elastic and electronic properties and stability of SrThO3, SrZrO3 and ThO2 from first principles. Journal of Nuclear Materials, 2007, 361, 69-77.	2.7	56
20	Magnetism without magnetic ions in non-magnetic perovskites SrTiO3, SrZrO3 and SrSnO3. Journal of Magnetism and Magnetic Materials, 2008, 320, 936-942.	2.3	55
21	First-principle study of B1-like thorium carbide, nitride and oxide. Journal of Nuclear Materials, 2006, 353, 19-26.	2.7	53
22	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.	2.7	53
23	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.	1.2	50
24	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.	0.6	49
25	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, .	3.2	47
26	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.	1.4	44
27	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.	1.2	43
28	Elastic and electronic properties of hexagonal rhenium subâ€nitrides Re₃N and Re₂N in comparison withhcpâ€Re and wurtziteâ€like rhenium mononitride ReN. Physica Status Solidi (B): Basic Research, 2011, 248, 1369-1374.	1.5	41
29	Electronic, magnetic, structural, 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, 83, .	3.2	40
30	Electronic structure and properties of beryllium oxide. Inorganic Materials, 2009, 45, 223-234.	0.8	36
31	Band structure of superconducting dodecaborides YB12 and ZrB12. Physics of the Solid State, 2003, 45, 1429-1434.	0.6	35
32	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.	1.2	35
33	Magnetization of carbon-doped MgO nanotubes. Physical Review B, 2007, 75, .	3.2	34
34	Effect of Co doping on the electronic structure ofMgCNi3. Physical Review B, 2002, 66, .	3.2	32
35	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.	1.8	32
36	Structural and electronic properties of the 17 K superconductor<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sr</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> comparison to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Sr</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub> Physical Review B, 2009, 79, .	3.2	32

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37	Electronic and Magnetic Properties of Superconducting Sr4V2Fe2As2O6 Versus Sr4Sc2Fe2As2O6. Journal of Superconductivity and Novel Magnetism, 2009, 22, 613-617.	1.8	30
38	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.	2.9	30
39	Electronic band structure and chemical bonding in the new antiperovskites AsNMg3 and SbNMg3. Journal of Solid State Chemistry, 2004, 177, 61-64.	2.9	29
40	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.	1.4	29
41	Structural, luminescence, and electronic properties of the alkaline metal-strontium cyclotetravanadatesM2Sr(VO3)4, (M=Na, K, Rb, Cs). Physical Review B, 2005, 72, .	3.2	28
42	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.	2.7	28
43	Structural, elastic, and electronic properties of new 211 MAX phase Nb2GeC from first-principles calculations. Physica B: Condensed Matter, 2013, 410, 42-48.	2.7	28
44	Electronic properties of hexagonal tungsten monocarbide (h-WC) with 3d impurities from first-principles calculations. Physica B: Condensed Matter, 2009, 404, 1887-1891.	2.7	27
45	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.	3.2	27
46	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.	1.9	26
47	Electronic structure and thermoelectric properties of skutterudite compounds. Journal of Physics Condensed Matter, 2004, 16, 979-987.	1.8	26
48	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.	2.7	26
49	Structural, elastic and electronic properties of cubic 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	3.2	26
50	Structural, elastic, electronic and magnetic properties of perovskite-like Co3WC, Rh3WC and Ir3WC from first principles calculations. Solid State Sciences, 2010, 12, 814-817.	3.2	26
51	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	25
52	Thorium compounds with non-metals: Electronic structure, chemical bond, and physicochemical properties. Journal of Structural Chemistry, 2008, 49, 348-370.	1.0	25
53	New superconductor with a layered crystal structure: Nickel oxybismuthide LaO1â^ÎNiBi. JETP Letters, 2008, 87, 649-651.	1.4	25
54	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.	1.5	25

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55	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.	1.4	24
56	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.	1.0	24
57	Non-stoichiometric s-, p- and d-metal diborides: synthesis, properties and simulation. Russian Chemical Reviews, 2008, 77, 467-486.	6.5	24
58	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	24
59	Electronic properties of novel 6 K superconductor LiFeP in comparison with LiFeAs from first principles calculations. Solid State Communications, 2010, 150, 152-156.	1.9	24
60	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.	4.0	23
61	Electronic structure and magnetic properties of Fe3C with 3d and 4d impurities. Physica Status Solidi (B): Basic Research, 2007, 244, 1971-1981.	1.5	23
62	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.	1.8	23
63	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.	0.6	22
64	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.	0.6	22
65	Electronic band structure of thorium hydrides: ThH2 and Th4H15. Physica B: Condensed Matter, 2007, 389, 296-301.	2.7	22
66	Electronic properties and chemical bonding in quaternary arsenide oxides LaZnAsO and YZnAsO. Materials Chemistry and Physics, 2009, 116, 129-133.	4.0	22
67	Structural, electronic, magnetic and elastic properties of tetragonal layered diselenide KCo2Se2 from first principles calculations. Physica B: Condensed Matter, 2012, 407, 271-275.	2.7	22
68	Ab initio calculations of the electronic properties of new superconducting nanolaminates: Nb2SnC and Nb2SC1â^'x. Doklady Physical Chemistry, 2006, 411, 317-321.	0.9	21
69	Band structure and properties of polymorphic modifications of lower tungsten carbide W2C. Physics of the Solid State, 2008, 50, 1420-1426.	0.6	21
70	Electronic structure and Fermi surface of the superconductors LaNiBiO and LaCuBiO from first principles. Physical Review B, 2008, 78, .	3.2	21
71	Structural, vibrational, electronic, and luminescence properties of the cyclotetravanadatesA2M(VO3)4(A=Na,Ag;M=Ca,Sr). Physical Review B, 2008, 77, .	3.2	21
72	Stability, structural, elastic, and electronic properties of polymorphs of the superconducting disilicide YIr2Si2. Physica B: Condensed Matter, 2011, 406, 3525-3530.	2.7	21

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73	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.	3.0	20
74	Electronic structure of the new MgCNi3 superconductor and related intermetallic compounds. JETP Letters, 2001, 74, 122-127.	1.4	19
75	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.	1.9	19
76	Effect of metal vacancies on the band structure of Nb, Zr, and Y diborides. Physics of the Solid State, 2003, 45, 1617-1621.	0.6	18
77	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.	2.7	18
78	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.	1.9	18
79	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.	4.0	18
80	Design of novel magnetic materials based on ZrCuSiAs-like semiconducting pnictide-oxides from first-principles calculations. Solid State Communications, 2010, 150, 2069-2071.	1.9	18
81	Electronic Structure, Mechanical and Dynamical Stability of Hexagonal Subcarbides M2C (M = Tc, Ru,) Tj ETQq1 1 0.784314 rgBT /Ove	0.6	18
82	Ab Initio and Experimental Insights on Structural, Electronic, Optical, and Magnetic Properties of Cr-Doped Bi₂Ti₂O₇. Inorganic Chemistry, 2019, 58, 9904-9915.	4.0	18
83	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.	4.0	18
84	Energy-band structure of the A(Sn1âˆ'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.	0.5	17
85	Bismuth titanate pyrochlores doped by alkaline earth elements: First-principles calculations and experimental study. Solid State Ionics, 2018, 317, 183-189.	2.7	17
86	Magnetization of beryllium oxide in the presence of nonmagnetic impurities: Boron, carbon, and nitrogen. JETP Letters, 2007, 85, 246-250.	1.4	16
87	Electronic and elastic properties of perovskiteâ€like W₃NiC, W₃NiN and Co₃WC from firstâ€principles calculations. Physica Status Solidi (B): Basic Research, 2009, 246, 1646-1651.	1.5	16
88	Electronic and elastic properties of the superconducting nanolaminate Ti2InC. Physics of the Solid State, 2009, 51, 1608-1612.	0.6	16
89	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.	1.4	16
90	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.	5.5	16

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91	Thorite versus huttonite: stability, electronic properties and X-ray emission spectra from first-principle calculations. Physics and Chemistry of Minerals, 2006, 33, 545-552.	0.8	15
92	Electronic structure of cubic tungsten subnitride W2N in comparison to hexagonal and cubic tungsten mononitrides WN. Journal of Structural Chemistry, 2010, 51, 199-203.	1.0	15
93	Electronic band structure, optical absorption, and photocatalytic activity of iron-doped anatase. Physics of the Solid State, 2013, 55, 1903-1912.	0.6	15
94	Effects of atomic relaxation and the electronic structure of niobium (100) and (110) surfaces. Physics of Metals and Metallography, 2006, 102, 604-610.	1.0	14
95	Bending of MgO tubes: Mechanically induced hexagonal phase of magnesium oxide. Physical Review B, 2007, 75, .	3.2	14
96	Band structure of SrFeAsF and CaFeAsFâ€"the base phases of a new group of oxygen-free FeAs superconductors. JETP Letters, 2008, 88, 683-687.	1.4	14
97	MAGNETIZATION OF BERYLLIUM MONOXIDE (BeO) WITHOUT MAGNETIC IMPURITIES: A FIRST-PRINCIPLES STUDY. International Journal of Modern Physics B, 2008, 22, 4987-4992.	2.0	14
98	Tungsten carbides and nitrides and ternary systems based on them: the electronic structure, chemical bonding and properties. Russian Chemical Reviews, 2010, 79, 611-634.	6.5	14
99	Ab initio study of elastic and electronic properties of cubic thorium pnictides ThPnÂand Th3Pn4 (PnÂ=ÂP,) Tj ETQq1 1 0.784314 rgBT	3.2	14
100	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.	1.8	14
101	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.	0.6	14
102	Electronic and magnetic properties of beryllium oxide with 3d impurities from first-principles calculations. Physica B: Condensed Matter, 2007, 400, 47-52.	2.7	13
103	Electronic structure and stability of thorium carbonitrides. Physica Status Solidi (B): Basic Research, 2007, 244, 3198-3205.	1.5	13
104	Elastic properties of thorium ceramics ThX (X = C, N, O, P, As, Sb, S, Se). Technical Physics Letters, 2007, 33, 128-131.	0.7	13
105	First-principles study of structural, elastic and electronic properties of thorium dicarbide (ThC2) polymorphs. Journal of Nuclear Materials, 2009, 393, 192-196.	2.7	13
106	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.	1.4	13
107	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.	1.0	13
108	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.	5.5	13

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109	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.	0.6	12
110	Effect of chromium on the electronic structure and magnetic properties of cementite. Physics of Metals and Metallography, 2008, 105, 568-573.	1.0	12
111	Magnetic properties and electronic structure of the LaGaO3 perovskite doped with nickel. Physics of the Solid State, 2008, 50, 2121-2126.	0.6	12
112	Electronic structure and magnetic properties of Fe₃C with 2p and 3p impurities. Physica Status Solidi (B): Basic Research, 2009, 246, 2167-2171.	1.5	12
113	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.	2.3	12
114	Composition of beryllium oxide ceramics. Refractories and Industrial Ceramics, 2011, 51, 377-381.	0.6	12
115	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.	2.9	12
116	Structural, electronic, elastic properties and chemical bonding in LaNi2P2 and LaNi2Ge2 from first principles. Intermetallics, 2012, 26, 1-7.	3.9	12
117	Synthesis and characterisation of new MO(OH)₂(M = Zr, Hf) oxyhydroxides and related Li₂MO₃salts. Dalton Transactions, 2014, 43, 2755-2763.	3.3	12
118	Quinate:NAP(P)+-oxidoreductase from Larix sibirica: purification, characterization and function. Trees - Structure and Function, 1995, 10, 46.	1.9	11
119	Short-range atomic order in Fe2B powders. Physics of Metals and Metallography, 2007, 103, 470-480.	1.0	11
120	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.	1.9	11
121	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.	0.6	11
122	Origin of incompressibility and hardness from electronic and mechanical properties of hard material ruthenium diboride. Solid State Communications, 2010, 150, 1095-1098.	1.9	11
123	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.	1.2	11
124	Elastic properties and inter-atomic bonding in new superconductor from first principles calculations. Solid State Communications, 2011, 151, 671-673.	1.9	11
125	Charge distribution and mobility of lithium ions in Li2TiO3 from 6,7Li NMR data. Journal of Structural Chemistry, 2013, 54, 111-118.	1.0	11
126	Synthesis, optical properties, and photocatalytic activity of lanthanide-doped anatase. Russian Journal of Inorganic Chemistry, 2014, 59, 29-33.	1.3	11

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127	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.	1.8	11
128	Electronic and magnetic properties of new quaternary oxybismuthides LaOMBi (where M=V, Cr, â€¦, Ni,) Tj ETQq0 0 0 rgBT /Overlock 10 5838-5840.	2.1	10
129	Structural, elastic, electronic and magnetic properties of ThCr2Si2 from first-principles calculations. Solid State Communications, 2011, 151, 1165-1168.	1.9	10
130	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.	1.8	10
131	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.	0.6	10
132	Cesium adsorption on the Î²2-GaAs(001) surface. Journal of Experimental and Theoretical Physics, 2007, 104, 590-601.	0.9	9
133	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.	1.2	9
134	Elastic properties of carbide, nitride, and boride ceramics with WC-type structures. Technical Physics Letters, 2008, 34, 841-844.	0.7	9
135	Hydrogen-induced enhancement of ductility of fcc iridium: A first-principles study. Materials Letters, 2009, 63, 2413-2415.	2.6	9
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.	2.4	9
137	Electronic band structure, optical absorption and photocatalytic activity of anatase doped with bismuth or carbon. Journal of Alloys and Compounds, 2013, 548, 46-51.	5.5	9
138	New half-metallic ferromagnets: Double perovskites SR(FeM)O3 (M = Sn, Ti, Zr). JETP Letters, 2005, 82, 220-223.	1.4	8
139	Electronic structure of tungsten aluminum carbides W2AlC and WAlC2. Russian Journal of Inorganic Chemistry, 2009, 54, 1433-1439.	1.3	8
140	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.	4.0	8
141	Elastic properties and chemical bonding in fluoritelike Be2B, AlBeB, MgBeB, and NaBeB. Journal of Structural Chemistry, 2005, 46, 535-537.	1.0	7
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