

Igor Solovyev

List of Publications by Year in descending order

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109
papers

7,798
citations

87723

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48187

88
g-index

111
all docs

111
docs citations

111
times ranked

7027
citing authors

#	ARTICLE	IF	CITATIONS
1	Density-functional theory and NiO photoemission spectra. Physical Review B, 1993, 48, 16929-16934.	1.1	1,991
2	Intermediate-spin state and properties of LaCoO ₃ . Physical Review B, 1996, 54, 5309-5316.	1.1	774
3	Corrected atomic limit in the local-density approximation and the electronic structure of impurities in Rb. Physical Review B, 1994, 50, 16861-16871.	1.1	656
4	Crucial Role of the Lattice Distortion in the Magnetism of LaMnO ₃ . Physical Review Letters, 1996, 76, 4825-4828.	2.9	344
5	t_{2g} versus all $3d$ localization in LaMO ₃ perovskites (M=Ti-Cu): First-principles study. Physical Review B, 1996, 53, 7158-7170.	1.1	342
6	Phase Diagram of Tetragonal Manganites. Physical Review Letters, 2000, 84, 3169-3172.	2.9	311
7	Origin of orbital magnetization and magnetocrystalline anisotropy in ordered alloys (where T=Fe,Co). Physical Review Letters, 2000, 84, 1078-1081.	1.1	179
8	Is Hund's Second Rule Responsible for the Orbital Magnetism in Solids?. Physical Review Letters, 1998, 80, 5758-5761.	2.9	157
9	Calculation of magneto-optical properties for 4f systems: LSDA + Hubbard U results. Journal of Physics and Chemistry of Solids, 1995, 56, 1521-1524.	1.9	151
10	First-principles study on electronic structures and phase stability of MnO and FeO under high pressure. Physical Review B, 1999, 59, 762-774.	1.1	116
11	Spin-polarized relativistic linear-muffin-tin-orbital method: Volume-dependent electronic structure and magnetic moment of plutonium. Physical Review B, 1991, 43, 14414-14422.	1.1	110
12	Screening of Coulomb interactions in transition metals. Physical Review B, 2005, 71, .	1.1	110
13	Effective single-particle potentials for MnO in light of interatomic magnetic interactions: Existing theories and perspectives. Physical Review B, 1998, 58, 15496-15507.	1.1	99
14	Electronic structure and stability of the ferrimagnetic ordering in double perovskites. Physical Review B, 2002, 65, .	1.1	96
15	Combining DFT and many-body methods to understand correlated materials. Journal of Physics Condensed Matter, 2008, 20, 293201.	0.7	94
16	Singlet Semiconductor to Ferromagnetic Metal Transition in FeSi. Physical Review Letters, 1996, 76, 1735-1738.	2.9	92
17	Magnetic Spin Origin of the Charge-Ordered Phase in Manganites. Physical Review Letters, 1999, 83, 2825-2828.	2.9	92
18	Lattice distortion and magnetism of $3d^4$ t_{2g} perovskite oxides. Physical Review B, 2006, 74, .	1.1	74

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19	Zone Boundary Softening of the Spin-Wave Dispersion in Doped Ferromagnetic Manganites. Physical Review Letters, 1999, 82, 2959-2962.	2.9	70
20	Magnetic and electronic properties of Cr ₂ Ge ₂ Te ₆ monolayer by strain and electric-field engineering. Applied Physics Letters, 2019, 114, .	1.5	69
21	Electronic Structure of Strongly Correlated Systems Emerging from Combining Path-Integral Renormalization Group with the Density-Functional Approach. Physical Review Letters, 2005, 95, 176405.	2.9	66
22	Inverse versus Normal NiAs Structures as High-Pressure Phases of FeO and MnO. Physical Review Letters, 1998, 81, 1027-1030.	2.9	65
23	Effects of crystal structure and on-site Coulomb interactions on the electronic and magnetic structure of A ₂ Mo ₂ O ₇ (A=Y, Gd, and Nd) pyrochlores. Physical Review B, 2003, 67, .	1.1	64
24	Electronic structure of $\text{BiM}_x\text{O}_{3-x}$ and related oxides. Physical Review B, 2010, 81, .	1.1	64
25	Microscopic origin of ferromagnetism in the trihalides CrCl_3 and CrI_3 . Physical Review B, 2012, 86, .	1.1	62
26	Magnetic structure of hexagonal YMnO_3 and LuMnO_3 from a microscopic point of view. Physical Review B, 2012, 86, .	1.1	54
27	Spin canting in three-dimensional perovskite manganites. Physical Review B, 2001, 63, .	1.1	53
28	Lattice distortion and magnetic ground state of YTiO_3 and LaTiO_3 . Physical Review B, 2004, 69, .	1.1	49
29	Magnetic-field control of the electric polarization in BiMnO_3 . Physical Review B, 2010, 82, .	1.1	48
30	Classical and quantum spin dynamics in the fcc antiferromagnet NiS_2 with frustration. Physical Review B, 2003, 68, .	1.1	47
31	First-principles Wannier functions and effective lattice fermion models for narrow-band compounds. Physical Review B, 2006, 73, .	1.1	46
32	Ab initio calculations of Coulomb U parameters for transition-metal impurities. Physical Review B, 1994, 49, 6736-6740.	1.1	44
33	Mechanisms and origins of half-metallic ferromagnetism in CrO_2 . Physical Review B, 2015, 92, .	1.2	43
34	Orbital ordering and magnetic interactions in BiMnO_3 . New Journal of Physics, 2008, 10, 073021.	1.2	41
35	Long-Range Magnetic Interactions Induced by the Lattice Distortions and the Origin of the E-Type Antiferromagnetic Phase in the Undoped Orthorhombic Manganites. Journal of the Physical Society of Japan, 2009, 78, 054710.	0.7	40
36	Orbital Polarization in Itinerant Magnets. Physical Review Letters, 2005, 95, 267205.	2.9	39

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37	Disorder effects in half-metallic Sr ₂ FeMoO ₆ single crystals. Applied Physics Letters, 2009, 94, .	1.5	39
38	Spin-orbital superexchange physics emerging from interacting oxygen molecules in KO ₂ . New Journal of Physics, 2008, 10, 013035.	1.2	38
39	Structural and electronic origin of the magnetic structures in hexagonal LuFeO ₃ . Physical Review B, 2014, 90, .	1.1	38
40	Origin of magnetoelectric effect in Co ₄ O ₉ and Co ₄ FeO ₁₁ . Physical Review B, 2016, 94, .	1.1	37
41	Orbital magnetization of insulating perovskite transition-metal oxides with a net ferromagnetic moment in the ground state. Physical Review B, 2014, 89, .	1.1	32
42	Mn ₂ FeSbO ₆ : A ferrimagnetic ilmenite and an antiferromagnetic perovskite. Physical Review B, 2013, 87, .	1.1	31
43	Optical investigations of the charge gap in orbital-ordered La _{1/2} Sr _{3/2} MnO ₄ . Physical Review B, 2000, 61, 6902-6906.	1.1	30
44	Spin-spiral inhomogeneity as the origin of ferroelectric activity in orthorhombic manganites. Physical Review B, 2011, 83, .	1.1	28
45	Origin of multiferroicity in MnWO ₄ . Physical Review B, 2013, 87, .	1.1	28
46	Ferromagnetic zigzag chains and properties of the charge-ordered perovskite manganites. Physical Review B, 2001, 63, .	1.1	26
47	Validity and limitations of the superexchange model for the magnetic properties of Sr ₂ IrO ₄ and Ba ₂ IrO ₄ mediated by the strong spin-orbit coupling. Physical Review B, 2015, 92, .	1.1	26
48	Magneto-optical effect in the weak ferromagnets LaMO ₃ (M= Cr, Mn, and Fe). Physical Review B, 1997, 55, 8060-8063.	1.1	25
49	Magnetic order near 270 K in mineral and synthetic Mn ₂ FeSbO ₆ ilmenite. Applied Physics Letters, 2011, 98, 022505.	1.5	24
50	Magnetism of sodium superoxide. CrystEngComm, 2014, 16, 522-531.	1.3	24
51	Exchange interactions and magnetic force theorem. Physical Review B, 2021, 103, .	1.1	24
52	Self-consistent linear response for the spin-orbit interaction related properties. Physical Review B, 2014, 90, .	1.1	22
53	Exchange interactions of CaMnO ₃ in the bulk and at the surface. Physical Review B, 2017, 95, .	1.1	22
54	Microscopic toy model for magnetoelectric effect in polar Fe ₂ O ₈ . Physical Review Materials, 2019, 3, .	0.9	22

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55	Charge Ordering due to Magnetic Symmetry Breaking. Physical Review Letters, 2003, 91, 177201. Magnetic structure of the noncentrosymmetric perovskites PbVO_3	2.9	21
56	Magnetic structure of the noncentrosymmetric perovskites PbVO_3 and BiCoO_3	1.1	21
57	Spin dependence of ferroelectric polarization in the double exchange model for manganites. Physical Review B, 2014, 90, .	1.1	21
58	Pressure dependence of the structure and electronic properties of $\text{Sr}_3\text{Mn}_7\text{O}_{10}$. Physical Review B, 2016, 93, .	1.1	21
59	Electronic band structure and lattice distortion in perovskite transition-metal oxides. Physica B: Condensed Matter, 1997, 237-238, 11-13.	1.3	19
60	On the competition between ferromagnetic and antiferromagnetic states in $\text{Sr}_2\text{MnMoO}_6$. Journal of Magnetism and Magnetic Materials, 2004, 268, 194-197.	1.0	19
61	Construction of Wannier functions from localized atomiclike orbitals. Physical Review B, 2007, 75, .	1.1	19
62	Defects of the crystal structure and Jahn-Teller distortion in BiMnO_3 . Physical Review B, 2010, 82, .	1.1	18
63	Magnetic structure and ferroelectric activity in orthorhombic YMnO_3 : Relative roles of magnetic symmetry breaking and atomic displacements. Physical Review B, 2012, 86, .	1.1	18
64	Microscopic theory of electric polarization induced by skyrmionic order in GaV_4S_8 . Physical Review B, 2019, 99, .	1.1	18
65	Superexchange interactions in orthorhombically distorted titanates R_3TiO_3 ($\text{R} = \text{Y, Gd, Sm and La}$). New Journal of Physics, 2009, 11, 093003.	1.2	17
66	Orbital magnetism in FeO . Journal of Magnetism and Magnetic Materials, 1998, 185, 118-120.	1.0	16
67	Magnetic ground state and multiferroicity in BiMnO_3 . JETP Letters, 2009, 89, 597-602.	0.4	16
68	Low-temperature spin dynamics of doped manganites: Roles of Mn ^{2g} , Mn ^{eg} , and O _{2p} states. Physical Review B, 1999, 60, 11439-11443.	1.1	14
69	GW study of half-metallic electronic structure of $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$. Physica B: Condensed Matter, 2003, 329-333, 858-859. Realization of the anisotropic compass model on the diamond lattice of CuAlO_2	1.3	14
70	Realization of the anisotropic compass model on the diamond lattice of CuAlO_2 and CuAl_2O_4	1.1	14
71	Giant contribution of the ligand states to the magnetic properties of the $\text{Cr}_2\text{Ge}_2\text{Te}_6$ monolayer. Physical Chemistry Chemical Physics, 2019, 21, 9597-9604.	1.3	13
72	Quantum spin liquid and cluster Mott insulator phases in the Mo_3O_8 magnets. Npj Quantum Materials, 2021, 6, .	1.8	13

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73	vanadium silicate BaVSi_2O_7 : A noncollinear ferrimagnetic ground state in $\text{Ni}(\text{NO}_3)_2$. Physical Review B, 2014, 90, .	1.1	12
74	Noncollinear ferrimagnetic ground state in $\text{Ni}(\text{NO}_3)_2$. Physical Review B, 2014, 90, .	1.1	12
75	Skyrmionic order and magnetically induced polarization change in lacunar spinel compounds GaV_4S_8 and GaMo_4S_8 . Physical Review B, 2015, 91, .	1.1	11
76	Cluster size dependence of double ionization energy spectra of spin-polarized aluminum and sodium clusters: All-electron spin-polarized GW+T-matrix method. Physical Review B, 2010, 81, .	1.1	10
77	Magnetization-induced local electric dipoles and multiferroic properties of Ba_2O_7 . Physical Review B, 2015, 91, .	1.1	10
78	Covalency effects reflected in the magnetic form factor of low-dimensional cuprates. Physical Review B, 2015, 92, .	1.1	10
79	Hybridization and spin-orbit coupling effects in the quasi-one-dimensional spin-1 magnet $\text{Ba}_3\text{Cu}_3\text{Sc}_4\text{O}_{12}$. Physical Review B, 2016, 94, .	1.1	10
80	Ordering of Fe and Zn Ions and the Magnetic Properties of $\text{FeZnMo}_3\text{O}_8$. JETP Letters, 2019, 109, 786-789.	0.4	10
81	Modeling of complex oxide materials from the first principles: systematic applications to vanadates RVO_3 with distorted perovskite structure. Journal of Computational Electronics, 2011, 10, 21-34.	1.3	9
82	Superexchange theory of electronic polarization driven by relativistic spin-orbit interaction at half filling. Physical Review B, 2017, 95, .	1.1	9
83	The X-ray emission spectra and electronic structure of the misfit layer compounds $(\text{BiS})_{1.08}\text{NbS}_2$ and $(\text{PbS})_{1.14}\text{TaS}_2$. Journal of Physics Condensed Matter, 1994, 6, 3993-3998.	0.7	8
84	First principles T-matrix calculations for Auger spectra of hydrocarbon systems. Physical Review B, 2008, 77, .	1.1	8
85	Double-exchange theory of ferroelectric polarization in orthorhombic manganites with twofold periodic magnetic texture. Physical Review B, 2013, 87, .	1.1	8
86	Unconventional magnetism and electronic state in the frustrated layered system PdCrO_2 . Physical Review B, 2020, 102, .	1.1	8
87	Excitation energy dependence of X-ray emission spectra and electronic structure of $\text{Eu}_{1-x}\text{Ca}_x\text{MnO}_3$. Journal of Electron Spectroscopy and Related Phenomena, 1998, 96, 187-194.	0.8	7
88	Optimized effective potential for the extended Hubbard model. Physical Review B, 1999, 60, 8550-8558.	1.1	7
89	Magnetism of NaFePO_4 and related polyanionic compounds. Physical Chemistry Chemical Physics, 2018, 20, 13497-13507.	1.3	7
90	Can the Highly Symmetric $\text{SU}(4)$ Spin-Orbital Model Be Realized in ZrCl_3 ? JETP Letters, 2020, 112, 642-646.	0.4	7

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91	Microscopic origins and stability of ferromagnetism in $Sr_{2-x}Y_xV_6O_{26}$ and $Sr_{2-x}Y_xV_6O_{26}$. Physical Review B, 2022, 105, .	1.1	6
92	Nonlocal coherent potential approximation for the paramagnetic state of the degenerate double-exchange model. Physical Review B, 2003, 67, .	1.1	5
93	Co(NO ₃) ₂ as an inverted umbrella-type chiral noncoplanar ferrimagnet. Physical Review B, 2020, 102, .	1.1	5
94	Effect of the orthorhombic distortion on the magneto-optical properties of SrRuO ₃ . Journal of Magnetism and Magnetic Materials, 1998, 177-181, 811-812.	1.0	4
95	Correlation energies in distorted 3d-t 2g perovskite oxides. Journal of Experimental and Theoretical Physics, 2007, 105, 46-54.	0.2	4
96	Optimized effective potential model for the double perovskites Sr ₂ â ^x Y _x V ₆ O ₂₆ and Sr ₂ â ^x Y _x V ₆ O ₂₆ . Journal of Physics Condensed Matter, 2011, 23, 326002.	0.7	4
97	Fingerprints of spin-current physics on magnetoelectric response in the spin-12 magnet Ba ₂ CuGe ₂ O ₇ . Physical Review B, 2020, 102, .	1.1	4
98	Publisher's Note: Structural and electronic origin of the magnetic structures in hexagonal $LuFeO_3$ [Phys. Rev. B 90 , 014436 (2014)]. Physical Review B, 2014, 90, .	1.1	3
99	First-principles investigation of exchange interactions in quasi-one-dimensional antiferromagnet CaV ₂ O ₄ . Journal of Physics Condensed Matter, 2015, 27, 026001.	0.7	3
100	Band filling dependence of the Curie temperature in CrO ₂ . Journal of Physics Condensed Matter, 2016, 28, 216001.	0.7	3
101	LMTO-ASA band structure calculations of BaVS ₃ , BaTiS ₃ and their solid solutions. Physica Scripta, 1994, 50, 90-92.	1.2	2
102	Ni ₆ Cr ₅ Mo ₁₈ : A compensated half metal predicted from first-principles. Journal of Applied Physics, 2013, 113, 043718.	1.1	2
103	Magnetically Induced Polarization in Centrosymmetric Bonds. Physical Review Letters, 2021, 127, 187601.	2.9	2
104	Theoretical analysis of electronic and magnetic properties of NaV ₂ O ₄ : Crucial role of the orbital degrees of freedom. Physical Review B, 2012, 86, .	1.1	1
105	Magnetic Interactions in Transition-Metal Oxides. ChemInform, 2005, 36, no.	0.1	0
106	Realistic Modeling of Complex Oxide Materials from the First Principles. , 2009, , .		0
107	Realistic modeling of complex oxide materials. Computer Physics Communications, 2011, 182, 43-45.	3.0	0
108	Publisher's Note: Exchange interactions of $CaMnO_3$ in the bulk and at the surface [Phys. Rev. B 95 , 115120 (2017)]. Physical Review B, 2018, 97, .		

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109	Present Status of the First-Principles Electronic Structure Calculations for the Strongly Correlated Transition-Metal Oxides. Springer Series in Solid-state Sciences, 1999, , 34-44.	0.3	0