Olle E Eriksson

List of Publications by Year
in descending order

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762 papers	32,754 citations	4120 87 h-index	7931 149 g-index
785 all docs	785 docs citations	785 times ranked	23772 citing authors

#	Article	IF	Citations
1	Density functional theory for calculation of elastic properties of orthorhombic crystals: Application to TiSi2. Journal of Applied Physics, 1998, 84, 4891-4904.	1.1	1,565
2	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
3	First-principles theory of dilute magnetic semiconductors. Reviews of Modern Physics, 2010, 82, 1633-1690.	16.4	959
4	Electronic structure of two-dimensional crystals fromab initiotheory. Physical Review B, 2009, 79, .	1.1	941
5	Theoretical investigation of magnetoelectric behavior inBiFeO3. Physical Review B, 2006, 74, .	1.1	582
6	Elastic constants of hexagonal transition metals: Theory. Physical Review B, 1995, 51, 17431-17438.	1.1	546
7	Substrate-induced magnetic ordering and switching of iron porphyrin molecules. Nature Materials, 2007, 6, 516-520.	13.3	396
8	Giant Magnetic Anisotropy in Tetragonal FeCo Alloys. Physical Review Letters, 2004, 93, 027203.	2.9	331
9	Entropy Driven Stabilization of Energetically Unstable Crystal Structures Explained from First Principles Theory. Physical Review Letters, 2008, 100, 095901.	2.9	331
10	Orbital polarization in narrow-band systems: Application to volume collapses in light lanthanides. Physical Review B, 1990, 41, 7311-7314.	1.1	330
11	Accurate electronic band gap of pure and functionalized graphane from GW calculations. Physical Review B, 2009, 79, .	1.1	279
12	Ultra-low magnetic damping of a metallicÂferromagnet. Nature Physics, 2016, 12, 839-842.	6.5	274
13	Magnetic Percolation in Diluted Magnetic Semiconductors. Physical Review Letters, 2004, 93, 137202.	2.9	263
14	Structural, elastic, and high-pressure properties of cubic TiC, TiN, and TiO. Physical Review B, 1996, 53, 3072-3079.	1.1	259
15	Theory of elastic constants of cubic transition metals and alloys. Physical Review B, 1993, 48, 5844-5851.	1.1	256
16	A method for atomistic spin dynamics simulations: implementation and examples. Journal of Physics Condensed Matter, 2008, 20, 315203.	0.7	249
17	Orbital magnetism in Fe, Co, and Ni. Physical Review B, 1990, 42, 2707-2710.	1.1	244
18	Ultrafast Spin Dynamics in Multisublattice Magnets. Physical Review Letters, 2012, 108, 057202.	2.9	217

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19	Enhancement of Orbital Magnetism at Surfaces: Co on Cu(100). Physical Review Letters, 1995, 75, 1602-1605.	2.9	216
20	Mn+1AXnphases in theTiâˆ'Siâˆ'Csystem studied by thin-film synthesis andab initiocalculations. Physical Review B, 2004, 70, .	1.1	212
21	Deposition and characterization of ternary thin films within the Tiâ€"Alâ€"C system by DC magnetron sputtering. Journal of Crystal Growth, 2006, 291, 290-300.	0.7	212
22	4f-Band Magnetism in CeFe2. Physical Review Letters, 1988, 60, 2523-2526.	2.9	196
23	Two-Dimensional Indium Selenides Compounds: An Ab Initio Study. Journal of Physical Chemistry Letters, 2015, 6, 3098-3103.	2.1	190
24	A unified picture of the crystal structures of metals. Nature, 1995, 374, 524-525.	13.7	189
25	Total Energy Calculation of the Magnetocrystalline Anisotropy Energy in the Ferromagnetic3dMetals. Physical Review Letters, 1995, 75, 2871-2874.	2.9	189
26	Tailoring the Nature of Magnetic Coupling of Fe-Porphyrin Molecules to Ferromagnetic Substrates. Physical Review Letters, 2009, 102, 047202.	2.9	188
27	Large magnetocrystalline anisotropy in bilayer transition metal phases from first-principles full-potential calculations. Physical Review B, 2001, 63, .	1.1	182
28	Two-Dimensional Materials from Data Filtering andAb InitioCalculations. Physical Review X, 2013, 3, .	2.8	180
29	Experimental and theoretical identification of a new high-pressure phase of silica. Nature, 1997, 388, 362-365.	13.7	177
30	Calculated spin and orbital moments in the surfaces of the3dmetals Fe, Co, and Ni and their overlayers on Cu(001). Physical Review B, 1996, 53, 9204-9213.	1.1	172
31	Full-potential optical calculations of lead chalcogenides. International Journal of Quantum Chemistry, 1998, 69, 349-358.	1.0	172
32	Electronic structure, chemical bonding, and optical properties of ferroelectric and antiferroelectricNaNO2. Physical Review B, 1999, 59, 1776-1785.	1.1	160
33	Molecular adsorption in graphene with divacancy defects. Physical Review B, 2009, 79, .	1.1	155
34	Crystal structures of Ti, Zr, and Hf under compression: Theory. Physical Review B, 1993, 48, 16269-16279.	1.1	151
35	Optical properties of the group-IVBrefractory metal compounds. Physical Review B, 1996, 54, 1673-1681.	1.1	147
36	Theory of bulk and surface quasiparticle spectra for Fe, Co, and Ni. Physical Review B, 2007, 76, .	1.1	147

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37	Positron Emission Tomography in Clinical Islet Transplantation. American Journal of Transplantation, 2009, 9, 2816-2824.	2.6	144
38	Magnetic anisotropy and magnetostriction in tetragonal and cubic Ni. Physical Review B, 1997, 55, 15026-15032.	1.1	143
39	Calculated magnetic properties of binary alloys between Fe, Co, Ni, and Cu. Physical Review B, 1999, 59, 419-430.	1.1	143
40	3d-5d band magnetism in rare earth transition metal intermetallics: LuFe2. Journal of Physics Condensed Matter, 1989, 1, 5861-5874.	0.7	138
41	Spin and orbital magnetism in Fe-Co and Co-Ni alloys. Physical Review B, 1992, 45, 12911-12916.	1.1	134
42	Electronic properties off-electron metals using the generalized gradient approximation. Physical Review B, 1994, 50, 7291-7294.	1.1	134
43	Phase stabilities and structural relaxations in substoichiometricTiC1â^'x. Physical Review B, 2001, 63, .	1.1	134
44	Full-Potential Electronic Structure Method. Springer Series in Solid-state Sciences, 2010, , .	0.3	132
45	Pharmacokinetics of tranexamic acid after intravenous administration to normal volunteers. European Journal of Clinical Pharmacology, 1974, 7, 375-380.	0.8	130
46	Prediction of ferromagnetism and metamagnetism in 4dtransition-metal overlayers on the (001) surface of Ag (4d=Tc, Ru, Rh, and Pd). Physical Review Letters, 1991, 66, 1350-1353.	2.9	130
47	Theoretical analysis of the chemical bonding and electronic structure of graphene interacting with Group IA and Group VIIA elements. Physical Review B, 2010, 81, .	1.1	130
48	Analysis of reproducibility of subjective grading systems for breast carcinoma.. Journal of Clinical Pathology, 1979, 32, 979-985.	1.0	128
49	Novel electronic configuration in â^,â^'Pu. Journal of Alloys and Compounds, 1999, 287, 1-5.	2.8	128
50	Ferromagnetic materials in the zinc-blende structure. Physical Review B, 2003, 68, .	1.1	128
51	Magnetic, optical, and magneto-optical properties of MnX(X=As, Sb, or Bi) from full-potential calculations. Physical Review B, 1999, 59, 15680-15693.	1.1	126
52	Influence of Ligand States on the Relationship between Orbital Moment and Magnetocrystalline Anisotropy. Physical Review Letters, 2007, 99, 177207.	2.9	124
53	Theoretical aspects of theFecNi1â^'cInvar alloy. Physical Review B, 1995, 51, 1058-1063.	1.1	123
54	Data mining and accelerated electronic structure theory as a tool in the search for new functional materials. Computational Materials Science, 2009, 44, 1042-1049.	1.4	123

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55	Formation and Structure of Graphene Waves on Fe(110). Physical Review Letters, 2012, 109, 026101.	2.9	122
56	CARDIAC GLYCOSIDES AND BREAST CANCER. Lancet, The, 1979, 313, 563.	6.3	121
57	Perpendicular Magnetocrystalline Anisotropy in Tetragonally Distorted Fe-Co Alloys. Physical Review Letters, 2006, 96, 037205.	2.9	118
58	Surface energies and work functions of the transition metal carbides. Surface Science, 2004, 557, 243-254.	0.8	117
59	Adsorption of Cu, Ag, and Au atoms on graphene including van der Waals interactions. Journal of Physics Condensed Matter, 2011, 23, 395001.	0.7	117
60	Atomistic Spin Dynamics. , 2017, , .		117
61	Fermi Condensation Near van Hove Singularities Within the Hubbard Model on the Triangular Lattice. Physical Review Letters, 2014, 112, 070403.	2.9	116
62	Optical properties of graphite from first-principles calculations. Physical Review B, 1997, 55, 4999-5005.	1.1	115
63	Magnetic anisotropy ofL10FePt andFe1âˆ'xMnxPt. Physical Review B, 2005, 71, .	1.1	113
64	Defect formation in graphene nanosheets by acid treatment: an x-ray absorption spectroscopy and density functional theory study. Journal Physics D: Applied Physics, 2008, 41, 062001.	1.3	112
65	Effects of growth hormone substitution on mental performance in adults with growth hormone deficiency: a pilot study. Psychoneuroendocrinology, 1986, 11, 347-352.	1.3	111
66	Restricting Dislocation Movement in Transition Metal Carbides by Phase Stability Tuning. Science, 2001, 293, 2434-2437.	6.0	110
67	Crystal structure and elastic-constant anomalies in the magnetic 3dtransition metals. Physical Review B, 1994, 50, 5918-5927.	1.1	109
68	Quasiab initiomolecular dynamic study of Cu melting. Physical Review B, 2000, 61, 3838-3844.	1.1	108
69	Ground-state and excited-state properties ofLaMnO3from full-potential calculations. Physical Review B, 2002, 65, .	1.1	108
70	The self-consistent ab initio lattice dynamical method. Computational Materials Science, 2009, 44, 888-894.	1.4	108
71	Defect-Induced Magnetic Structure in(Ga1âˆ'xMnx)As. Physical Review Letters, 2002, 88, 187202.	2.9	107
72	Strength of Correlation Effects in the Electronic Structure of Iron. Physical Review Letters, 2009, 103, 267203.	2.9	107

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73	Meta-magnetism in UCoAl. Journal of Physics Condensed Matter, 1989, 1, 4005-4011.	0.7	105
74	Crystal-structure stabilities and electronic structure for the light actinides Th, Pa, and U. Physical Review B, 1992, 45, 13879-13890.	1.1	105
75	Trends of the elastic constants of cubic transition metals. Physical Review Letters, 1992, 68, 2802-2805.	2.9	101
76	Theory of phase stabilities and bonding mechanisms in stoichiometric and substoichiometric molybdenum carbide. Journal of Applied Physics, 1999, 86, 3758-3767.	1.1	100
77	Theoretical study of the magnetism of Mn-doped ZnO with and without defects. Physical Review B, 2006, 74, .	1.1	99
78	Electronic structure of two-dimensional transition metal dichalcogenide bilayers fromab initiotheory. Physical Review B, 2014, 89, .	1.1	99
79	Theoretical aspects of the magnetism in the ferromagneticAFe2systems (A=U, Np, Pu, and Am). Physical Review B, 1990, 41, 9087-9094.	1.1	98
80	Charge self-consistent dynamical mean-field theory based on the full-potential linear muffin-tin orbital method: Methodology and applications. Computational Materials Science, 2012, 55, 295-302.	1.4	98
81	Exchange parameters of strongly correlated materials: Extraction from spin-polarized density functional theory plus dynamical mean-field theory. Physical Review B, 2015, 91, .	1.1	98
82	First-principles calculations of the ultralow thermal conductivity in two-dimensional group-IV selenides. Physical Review B, 2018, 98, .	1.1	98
83	Structural properties of plutonium from first-principles theory. Physical Review B, 1997, 55, 1997-2004.	1.1	97
84	Elastic and high pressure properties of ZnO. Journal of Applied Physics, 1998, 83, 8065-8067.	1.1	96
85	Theory of ferromagnetism inCeCo5. Physical Review B, 1990, 41, 9111-9120.	1.1	94
86	Photoemission and the Electronic Structure ofPuCoGa5. Physical Review Letters, 2003, 91, 176401.	2.9	94
87	Phase stabilities and homogeneity ranges in4d-transition-metal carbides: A theoretical study. Physical Review B, 2001, 63, .	1.1	93
88	Conductivity engineering of graphene by defect formation. Journal Physics D: Applied Physics, 2010, 43, 045404.	1.3	89
89	Orbital Magnetism and Magnetic Anisotropy Probed with Ferromagnetic Resonance. Physical Review Letters, 1999, 82, 2390-2393.	2.9	87
90	Design of Nanocomposite Low-Friction Coatings. Advanced Functional Materials, 2007, 17, 1611-1616.	7.8	84

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91	Spin-orbit coupling in the actinide elements:â€ƒA critical evaluation of theoretical equilibrium volumes. Physical Review B, 2000, 63, .	1.1	83
92	Calculation of uniaxial magnetic anisotropy energy of tetragonal and trigonal Fe, Co, and Ni. Physical Review B, 2004, 69, .	1.1	83
93	Predicting breast cancer recurrence. Cancer, 1982, 50, 2884-2893.	2.0	82
94	Theoretical and experimental study of the graphite 1sx-ray absorption edges. Physical Review B, 1996, 54, 14396-14404.	1.1	82
95	Optical properties of monoclinic SnI2from relativistic first-principles theory. Physical Review B, 1997, 56, 6851-6861.	1.1	82
96	Topological excitations in a kagome magnet. Nature Communications, 2014, 5, 4815.	5.8	82
97	Sum rules for electron energy loss near edge spectra. Physical Review B, 2007, 76, .	1.1	80
98	Complex edge effects in zigzag graphene nanoribbons due to hydrogen loading. Physical Review B, 2010, 82, .	1.1	80
99	Interatomic Exchange Interactions for Finite-Temperature Magnetism and Nonequilibrium Spin Dynamics. Physical Review Letters, 2013, 111, 127204.	2.9	79
100	Density functional study of elastic and vibrational properties of the Heusler-type alloys<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub>	1.1	77
101	Computerized nuclear morphometry as an objective method for characterizing human cancer cell populations. Cancer Research, 1978, 38, 4688-97.	0.4	77
102	Spin and orbital contributions to surface magnetism in 3delements. Physical Review B, 1992, 45, 2868-2875.	1.1	76
103	Phase stability diagrams of transition metal carbides, a theoretical study. Chemical Physics Letters, 2001, 333, 444-450.	1.2	76
104	Phonon spectrum, thermodynamic properties, and pressure-temperature phase diagram of uranium dioxide. Physical Review B, 2013, 88, .	1.1	75
105	Magnetic coupling in 3dtransition-metal monolayers and bilayers on bcc (100) iron. Physical Review B, 1995, 52, 15070-15073.	1.1	74
106	Modeling the actinides with disordered local moments. Physical Review B, 2003, 67, .	1.1	74
107	A novel electronic configuration of the 5f states in Î´-plutonium as revealed by the photo-electron spectra. Journal of Electron Spectroscopy and Related Phenomena, 2004, 135, 163-166.	0.8	74
108	Evolving properties of two-dimensional materials: from graphene to graphite. Journal of Physics Condensed Matter, 2009, 21, 335502.	0.7	74

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109	Efficient Spin Injection Through Exchange Coupling at Organic Semiconductor/Ferromagnet Heterojunctions. Advanced Materials, 2010, 22, 1626-1630.	11.1	74
110	Chemical bonding and magnetism in 3d-5f intermetallics. Journal of Physics F: Metal Physics, 1988, 18, L33-L39.	1.6	73
111	Origin of Magnetic Anisotropy of Gd Metal. Physical Review Letters, 2003, 91, 157201.	2.9	73
112	Theoretical Confirmation of the High Pressure Simple Cubic Phase in Calcium. Physical Review Letters, 1995, 75, 3473-3476.	2.9	72
113	AlM₂B₂(Mâ€‰â€‰=â€‰â€‰Cr, Mn, Fe, Co, Ni): a group of nanolaminated materials. Journal of Physics Condensed Matter, 2017, 29, 155402.	0.7	72
114	Bonding mechanism in the nitrides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi mathvariant="normal">Ti</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Al</mml:mi><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>and TiN: An experimental and theoretical investigation. Physical Review B, 2007, 76, .	1.1	69
115	Microscopic Origin of Heisenberg and Non-Heisenberg Exchange Interactions in Ferromagnetic bcc Fe. Physical Review Letters, 2016, 116, 217202.	2.9	69
116	Theoretical Aspects of the Charge Density Wave in Uranium. Physical Review Letters, 1998, 81, 2978-2981.	2.9	68
117	Graphene as a Reversible Spin Manipulator of Molecular Magnets. Physical Review Letters, 2011, 107, 257202.	2.9	68
118	Histopathological systems of breast cancer classification: reproducibility and clinical significance.. Journal of Clinical Pathology, 1983, 36, 392-398.	1.0	67
119	Tuning of dielectric properties and magnetism of SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>by site-specific doping of Mn. Physical Review B, 2011, 84, .	1.1	67
120	Electronic, quasiharmonic, and anharmonic entropies of transition metals. Physical Review B, 1992, 46, 5221-5228.	1.1	66
121	Magnetically induced crystal structure and phase stability inFe1â^'cCoc. Physical Review B, 1996, 54, 3380-3384.	1.1	65
122	Electronic structure of Ti3SiC2. Applied Physics Letters, 2000, 76, 2226-2228.	1.5	65
123	Standard model of the rare earths analyzed from the Hubbard I approximation. Physical Review B, 2016, 94, .	1.1	65
124	Magnetic and electronic structure of(Ga1â^'xMnx)As. Physical Review B, 2003, 67, .	1.1	64
125	Diffusion of Tranexamic Acid to the Joint. Acta Orthopaedica, 1976, 47, 486-488.	1.4	62
126	Balanced crystal orbital overlap populationâ€"a tool for analysing chemical bonds in solids. Journal of Physics Condensed Matter, 2003, 15, 7751-7761.	0.7	62

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127	Magnetic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>Fe</mml:mi><mml:m /><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">B</mml:mi></mml:mrow></mml:math>alloys and the effect of doping by<mml:math xmlns:mml="http://www.w3.org/1998/Mat. Physical Review B, 2015, 92, .	1.1	62
128	Special considerations with regard to the dosage of tranexamic acid in patients with chronic renal diseases. Urological Research, 1978, 6, 83-8.	1.5	61
129	Quantitative Magnetic Information from Reciprocal Space Maps in Transmission Electron Microscopy. Physical Review Letters, 2009, 102, 037201.	2.9	61
130	Theory of spin-polarized scanning tunneling microscopy applied to local spins. Physical Review B, 2010, 81, .	1.1	61
131	Improved gas sensing activity in structurally defected bilayer graphene. Nanotechnology, 2012, 23, 505501.	1.3	61
132	Transition-metal dioxides with a bulk modulus comparable to diamond. Physical Review B, 1998, 57, 4979-4982.	1.1	60
133	Effects of spin-dependent quasiparticle renormalization in Fe, Co, and Ni photoemission spectra:An experimental and theoretical study. Physical Review B, 2012, 85, .	1.1	60
134	Stabilization of the tetragonal distortion of Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>Co<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>alloys by C impurities: A potential new permanent magnet. Physical Review B, 2014, 89, .	1.1	60
135	Electronic structure investigation ofTi3AlC2,Ti3SiC2, andTi3GeC2by soft x-ray emission spectroscopy. Physical Review B, 2005, 72, .	1.1	59
136	Electronic structure and chemical bonding inTi2AlCinvestigated by soft x-ray emission spectroscopy. Physical Review B, 2006, 74, .	1.1	59
137	Electronic Entanglement in Late Transition Metal Oxides. Physical Review Letters, 2012, 109, 186401.	2.9	59
138	High-temperature phonon stabilization of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>-uranium from relativistic first-principles theory. Physical Review B, 2012, 85, .	1.1	59
139	Full-Potential LMTO Total Energy and Force Calculations. , 1999, , 148-167.		58
140	Dynamical stability of body center cubic iron at the Earthâ€™s core conditions. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9962-9964.	3.3	58
141	Electronic structure of graphite: Effect of hydrostatic pressure. Physical Review B, 1995, 51, 4813-4819.	1.1	57
142	Magnetic properties and disorder effects in diluted magnetic semiconductors. Physical Review B, 2005, 72, .	1.1	57
143	Cohesive properties of the lanthanides: Effect of generalized gradient corrections and crystal structure. Physical Review B, 1998, 58, 4345-4351.	1.1	56
144	Disorder-induced metallicity in amorphous graphene. Physical Review B, 2011, 84, .	1.1	56

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145	Enhanced orbital contribution to surface magnetism in Fe, Co, and Ni. Solid State Communications, 1991, 78, 801-806.	0.9	55
146	On the semiconducting state and structural properties of YH3 from first principles theory. Applied Physics Letters, 1997, 71, 3498-3500.	1.5	54
147	Compounds with affinity for serotonergic receptors in the treatment of premenstrual dysphoria: a comparison of buspirone, nefazodone and placebo. Psychopharmacology, 2001, 155, 292-298.	1.5	54
148	Influence of Electron Correlation on the Electronic Structure and Magnetism of Transition-Metal Phthalocyanines. Journal of Chemical Theory and Computation, 2016, 12, 1772-1785.	2.3	54
149	Isomer shifts and hyperfine fields in iron compounds. Journal of Physics Condensed Matter, 1989, 1, 1589-1599.	0.7	53
150	Theoretical studies of the high pressure phases in cerium. Physical Review Letters, 1991, 67, 2215-2218.	2.9	53
151	Chemical vapour deposition of molybdenum carbides: aspects of phase stability. Thin Solid Films, 2000, 370, 203-212.	0.8	53
152	Tailor-Made Electronic and Magnetic Properties in One-Dimensional Pure and Y-SubstitutedCa3Co2O6. Physical Review Letters, 2003, 91, 186404.	2.9	53
153	Magnetic structures of small Fe, Mn, and Cr clusters supported on Cu(111): Noncollinear first-principles calculations. Physical Review B, 2007, 75, .	1.1	53
154	Valence-band electronic structure of iron phthalocyanine: An experimental and theoretical photoelectron spectroscopy study. Journal of Chemical Physics, 2011, 134, 074312.	1.2	53
155	Atomistic spin dynamics of low-dimensional magnets. Physical Review B, 2013, 87, .	1.1	53
156	Mapping the magnetic transition temperatures for medium- and high-entropy alloys. Intermetallics, 2018, 95, 80-84.	1.8	53
157	Bonding of an Isolated K atom to a Surface: Experiment and Theory. Physical Review Letters, 1997, 78, 4994-4997.	2.9	52
158	Method for Calculating Valence Stability in Lanthanide Systems. Physical Review Letters, 1997, 79, 4637-4640.	2.9	52
159	Crystal-field levels and magnetic susceptibility inPuO2. Physical Review B, 2002, 65, .	1.1	52
160	Electronic structure, magnetic, and cohesive properties ofLixMn2O4:Theory. Physical Review B, 2002, 65, .	1.1	52
161	Electronic structure and bulk properties of MB6 and MB12 borides. Low Temperature Physics, 2008, 34, 921-929.	0.2	52
162	Polaron mobility in oxygen-deficient and lithium-doped tungsten trioxide. Physical Review B, 2015, 92, .	1.1	52

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163	AbÂInitioTheory of Dynamical Core-Hole Screening in Graphite from X-Ray Absorption Spectra. Physical Review Letters, 2005, 94, 167401.	2.9	51
164	Electron correlations in MnxGa1â€“xAs as seen by resonant electron spectroscopy and dynamical mean field theory. Nature Communications, 2013, 4, 2645.	5.8	51
165	Conditions for Noncollinear Instabilities of Ferromagnetic Materials. Physical Review Letters, 2004, 93, 107205.	2.9	50
166	Simulation of hydrogenated graphene field-effect transistors through a multiscale approach. Physical Review B, 2010, 82, .	1.1	50
167	Manipulation of spin state of iron porphyrin by chemisorption on magnetic substrates. Physical Review B, 2013, 88, .	1.1	50
168	Bulk and surface magnetism and interplanar spacings in Gd from first-principles calculations. Physical Review B, 1995, 52, 4420-4426.	1.1	48
169	Anomaly inc/aRatio of Zn under Pressure. Physical Review Letters, 1997, 79, 2301-2303.	2.9	48
170	Optical evidence of 4f-band formation in CeN. Physical Review B, 1997, 55, R10173-R10176.	1.1	48
171	Electronic Configuration of Yb Compounds. Physical Review Letters, 1999, 83, 3900-3903.	2.9	48
172	General trend of the mechanical properties of the ternary carbidesM3SiC2(M=transitionmetal). Physical Review B, 2006, 74, .	1.1	48
173	Magneticâ€Instabilityâ€Induced Giant Magnetoelectric Coupling. Advanced Materials, 2008, 20, 1353-1356.	11.1	47
174	Electronic structure and chemical and magnetic interactions in ZnO doped with Co and Al: Experiments andab initiodensity-functional calculations. Physical Review B, 2008, 78, .	1.1	47
175	Direct lightâ€“induced spin transfer between different elements in a spintronic Heusler material via femtosecond laser excitation. Science Advances, 2020, 6, eaaz1100.	4.7	47
176	Relativistic effects in heavy elements. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1986, 144, 1-13.	0.9	46
177	Electronic structure and magnetic properties of selected lanthanide and actinide intermetallic Laves-phase alloys. Physical Review B, 1989, 40, 9519-9528.	1.1	46
178	Novel method of self-interaction corrections in density functional calculations. International Journal of Quantum Chemistry, 2001, 81, 247-252.	1.0	46
179	High-pressure structural study of fluoro-perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CsCdF</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml:mr to 60 GPa: A combined experimental and theoretical study. Physical Review B, 2010, 81, .	1.1	46
180	A new 2D monolayer BiXene, M₂C (M = Mo, Tc, Os). Nanoscale, 2016, 8, 15753-15762.	2.8	46

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181	Magnetic interactions of Mn clusters supported on Cu. Physical Review B, 2006, 73, .	1.1	45
182	First-principles theory for helium and xenon diffusion in uranium dioxide. Journal of Nuclear Materials, 2009, 385, 364-367.	1.3	45
183	Design of carbide-based nanocomposite thin films by selective alloying. Surface and Coatings Technology, 2011, 206, 583-590.	2.2	45
184	Analytic continuation by averaging PadÃ© approximants. Physical Review B, 2016, 93, .	1.1	45
185	Delocalization and new phase in americium:â€ƒDensity-functional electronic structure calculations. Physical Review B, 2000, 61, 8119-8124.	1.1	44
186	Many-Body Approach to Spin-Dependent Transport in Quantum Dot Systems. Physical Review Letters, 2002, 88, 226601.	2.9	44
187	First-principles investigation of two-dimensional trichalcogenide and sesquichalcogenide monolayers. Physical Review B, 2016, 93, .	1.1	44
188	Endotoxemia in Chronic Renal Failure. Nephron, 1987, 45, 93-97.	0.9	43
189	Nature of the magnetic interaction between Fe-porphyrin molecules and ferromagnetic surfaces. Progress in Surface Science, 2009, 84, 18-29.	3.8	43
190	Elucidating the 3d Electronic Configuration in Manganese Phthalocyanine. Journal of Physical Chemistry A, 2014, 118, 927-932.	1.1	43
191	Calculation of elastic constants in UC, US, and UTe. Physical Review B, 1995, 52, 2496-2503.	1.1	42
192	On the sharpness of the interfaces in metallic multilayers. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 4742-4745.	3.3	42
193	Forcing Ferromagnetic Coupling Between Rare-Earth-Metal and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:math>Ferromagnetic Films. Physical Review Letters, 2010, 104, 156402.	2.9	42
194	Small gold clusters on graphene, their mobility and clustering: a DFT study. Journal of Physics Condensed Matter, 2011, 23, 205301.	0.7	42
195	Hexagonal M₂C₃ (M = As, Sb, and Bi) monolayers: new functional materials with desirable band gaps and ultrahigh carrier mobility. Journal of Materials Chemistry C, 2018, 6, 12689-12697.	2.7	42
196	Theoretical predictions of structural phase transitions in Cr, Mo, and W. Physical Review B, 1994, 49, 9365-9371.	1.1	41
197	Electronic and optical properties of redHgI2. Physical Review B, 1996, 54, 10419-10424.	1.1	41
198	Mood changes correlate to changes in brain serotonin precursor trapping in women with premenstrual dysphoria. Psychiatry Research - Neuroimaging, 2006, 146, 107-116.	0.9	41

#	Article	IF	Citations
199	Lattice dynamics and elastic properties of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml:math>electron system: CeN. Physical Review B, 2011, 84, .	1.1	41
200	Oxygen-tuned magnetic coupling of Fe-phthalocyanine molecules to ferromagnetic Co films. Physical Review B, 2013, 88, .	1.1	41
201	All-thermal switching of amorphous Gd-Fe alloys: Analysis of structural properties and magnetization dynamics. Physical Review B, 2015, 92, .	1.1	41
202	Database of novel magnetic materials for high-performance permanent magnet development. Computational Materials Science, 2019, 168, 188-202.	1.4	41
203	Elastic constants of cubicf-electron elements: Theory. Physical Review B, 1993, 48, 9306-9312.	1.1	40
204	Electronic structure and chemical bonding inTi4SiC3investigated by soft x-ray emission spectroscopy and first-principles theory. Physical Review B, 2006, 74, .	1.1	40
205	Multiplet effects in the electronic structure of intermediate-valence compounds. Physical Review B, 2009, 79, .	1.1	40
206	Theory of He trapping, diffusion, and clustering in UO2. Journal of Nuclear Materials, 2009, 385, 510-516.	1.3	40
207	Quantitative determination of spin-dependent quasiparticle lifetimes and electronic correlations in hcp cobalt. Physical Review B, 2010, 82, .	1.1	40
208	Transition between direct and indirect band gap in silicon nanocrystals. Physical Review B, 2013, 87, .	1.1	40
209	Stability of the Anomalous Large-Void CoSn Structure. Physical Review Letters, 1997, 79, 1333-1336.	2.9	39
210	Electronic-structure calculations of praseodymium metal by means of modified density-functional theory. Physical Review B, 1997, 56, 7143-7148.	1.1	39
211	Electronic structure, chemical bonding, phase stability, and ground-state properties ofYNi2â^'x(Co/Cu)xB2C. Physical Review B, 1998, 58, 3381-3393.	1.1	39
212	Electronic and optical properties of BaTiO3 and SrTiO3. Journal of Applied Physics, 2001, 90, 1854-1859.	1.1	39
213	Current-voltage asymmetries and negative differential conductance due to strong electron correlations in double quantum dots. Physical Review B, 2004, 70, .	1.1	39
214	Ab initiocalculations of the phonon spectra and the thermal expansion coefficients of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>4</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math>metals. Physical Review B, 2008, 77, .	1.1	39
215	Magnon softening in a ferromagnetic monolayer: A first-principles spin dynamics study. Physical Review B, 2010, 81, .	1.1	39
216	Itinerant ferromagnetism in Fe2P. Journal of Magnetism and Magnetic Materials, 1988, 74, 347-358.	1.0	38

#	Article	IF	Citations
217	Calculated magneto-optical properties of cubic and tetragonal Fe, Co, and Ni. Physical Review B, 1999, 60, 14105-14114.	1.1	38
218	Uniaxial Magnetocrystalline Anisotropy of Metal/Semiconductor Interfaces:Fe/ZnSe(001). Physical Review Letters, 2002, 89, 267203.	2.9	38
219	Reciprocal and real space maps for EMCD experiments. Ultramicroscopy, 2010, 110, 1380-1389.	0.8	38
220	Microscopic Model for Ultrafast Remagnetization Dynamics. Physical Review Letters, 2012, 109, 157201.	2.9	38
221	Comparison of van der Waals corrected and sparse-matter density functionals for the metal-free phthalocyanine/gold interface. Physical Review B, 2014, 89, .	1.1	38
222	Magnetization and domain structure of bccFe81Ni19/Co(001) superlattices. Physical Review B, 2004, 69, .	1.1	37
223	Anomalous Thermal Expansion in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Titanium. Physical Review Letters, 2007, 99, 015901.	2.9	37
224	General method for atomistic spin-lattice dynamics with first-principles accuracy. Physical Review B, 2019, 99, .	1.1	37
225	Electronic structure of the (111) and (100) surfaces of Î´-Pu. Physical Review B, 1991, 43, 9467-9474.	1.1	36
226	Local electronic structure information contained in energy-filtered diffraction patterns. Physical Review B, 2011, 84, .	1.1	36
227	Identifying the Electronic Character and Role of the Mn States in the Valence Band of (Ga,Mn)As. Physical Review Letters, 2013, 111, 097201.	2.9	36
228	Site-selective local fluorination of graphene induced by focused ion beam irradiation. Scientific Reports, 2016, 6, 19719.	1.6	36
229	Prediction of the new efficient permanent magnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SmCoNiFe</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2017, 96, .	1.1	36
230	Structural, electronic, and thermodynamic properties of curium dioxide: Density functional theory calculations. Physical Review B, 2017, 96, .	1.1	36
231	Spin and orbital magnetism in 3dsystems. Physical Review B, 1990, 41, 11807-11812.	1.1	35
232	fccâ†'bct phase transition in Th at extreme compressions: Theory. Physical Review B, 1992, 45, 12588-12591.	1.1	35
233	Anomalous fcc Crystal Structure of Thorium Metal. Physical Review Letters, 1995, 75, 280-283.	2.9	35
234	Sign reversal of the orbital moment via ligand states. Physical Review B, 2001, 63, .	1.1	35

#	Article	IF	Citations
235	Effect of spin orbit coupling and Hubbard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math>on the electronic structure of IrO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 89, .	1.1	35
236	The Bethe-Slater curve revisited; new insights from electronic structure theory. Scientific Reports, 2017, 7, 4058.	1.6	35
237	Surface electronic structure of Ce in the Î± and Î³ phase. Physical Review B, 1991, 43, 3137-3142.	1.1	34
238	Break-down of Hundâ€™s third rule for induced magnetism in U metal. Physical Review Letters, 1993, 71, 1459-1461.	2.9	34
239	Density Functional Theory of Crystal Field Quasiparticle Excitations and theAb InitioCalculation of Spin Hamiltonian Parameters. Physical Review Letters, 1997, 79, 2546-2549.	2.9	34
240	Serotonin transporter gene polymorphisms and platelet [3H] paroxetine binding in premenstrual dysphoria. Psychoneuroendocrinology, 2003, 28, 446-458.	1.3	34
241	Layered compound Nb3SiC2 predicted from first-principles theory. Applied Physics Letters, 2004, 85, 3071-3073.	1.5	34
242	Influence of defects on the magnetism of Mn-doped ZnO. Journal of Applied Physics, 2007, 101, 09H101.	1.1	34
243	Electronic structure, bulk and magnetic properties of MB6 and MB12 borides. Journal of Alloys and Compounds, 2007, 442, 228-230.	2.8	34
244	Toward Rare-Earth-Free Permanent Magnets: A Combinatorial Approach Exploiting the Possibilities of Modeling, Shape Anisotropy in Elongated Nanoparticles, and Combinatorial Thin-Film Approach. Jom, 2015, 67, 1318-1328.	0.9	34
245	High-throughput and data-mining approach to predict new rare-earth free permanent magnets. Physical Review B, 2020, 101, .	1.1	34
246	Electronic structure and spectroscopic properties of thulium monochalcogenides. Physical Review B, 2005, 72, .	1.1	33
247	Competing Exchange Interactions in Magnetic Multilayers. Physical Review Letters, 2006, 96, 057205.	2.9	33
248	Design of the lattice parameter of embedded nanoparticles. Chemical Physics Letters, 2010, 496, 95-99.	1.2	33
249	Ab initiostudy of interacting lattice vibrations and stabilization of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î²</mml:mi></mml:math>phase in Ni-Ti shape-memory alloy. Physical Review B, 2010, 81, .	1.1	33
250	Magnetic exchange interactions in B-, Si-, and As-doped Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>P from first-principles theory. Physical Review B, 2012, 85, .	1.1	33
251	Iron porphyrin molecules on Cu(001): Influence of adlayers and ligands on the magnetic properties. Physical Review B, 2013, 87, .	1.1	33
252	Theoretical investigation of the high-pressure crystal structures of Ce and Th. Physical Review B, 1995, 52, 13169-13176.	1.1	32

#	Article	IF	Citations
253	Effects of non-orthogonality and electron correlations on the time-dependent current through quantum dots. Physical Review B, 2002, 66, .	1.1	32
254	Ultrafast switching in a synthetic antiferromagnetic magnetic random-access memory device. Physical Review B, 2011, 83, .	1.1	32
255	Treatment of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:math>states of the rare earths: The case study of TbN. Physical Review B, 2014, 89, .	1.1	32
256	Atomistic spin dynamics and surface magnons. Journal of Physics Condensed Matter, 2015, 27, 243202.	0.7	32
257	Calculated cohesive properties of lanthanide and lanthanide-like actinide elements. Journal of the Less Common Metals, 1990, 158, 207-220.	0.9	31
258	Electronic structure of hydrogen and oxygen chemisorbed on plutonium: Theoretical studies. Physical Review B, 1991, 43, 4590-4597.	1.1	31
259	Defect controlled magnetism in FeP/graphene/Ni(111). Scientific Reports, 2013, 3, 3405.	1.6	31
260	Amorphous Wâ€“Sâ€“N thin films: The atomic structure behind ultra-low friction. Acta Materialia, 2015, 82, 84-93.	3.8	31
261	Correlation between cytometric features and mitotic frequency in human breast carcinoma. Cytometry, 1981, 1, 287-291.	1.8	30
262	Electronic structure of the strongly hybridized ferromagnetCeFe2. Physical Review B, 2000, 62, 14304-14312.	1.1	30
263	Ab initiostudy of structural and magnetic properties of Si-doped<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2010, 82, .	1.1	30
264	Possibility of a Î´-like surface for Î±-Pu: Theory. Physical Review B, 1992, 46, 13576-13583.	1.1	29
265	Theoretical zero-temperature phase diagram for neptunium metal. Physical Review B, 1995, 52, 1631-1639.	1.1	29
266	Orbital polarization in metallicf-electron systems. Physical Review B, 1995, 51, 13987-14000.	1.1	29
267	Theoretical search for the CrB-type high-pressure phase in LiH, NaH, KH and RbH. Physica B: Condensed Matter, 1999, 265, 87-91.	1.3	29
268	First-principles prediction of superplastic transition-metal alloys. Physical Review B, 2004, 70, .	1.1	29
269	Multiplet effects in the electronic structure of light rare-earth metals. Physical Review B, 2006, 74, .	1.1	29
270	Correlated electronic structure and chemical bonding of cerium pnictides and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î³</mml:mi></mml:math>-Ce. Physical Review B, 2012, 86, .	1.1	29

#	Article	IF	Citations
271	Electronic structure and magnetic properties of Mn, Co, and Ni substitution of Fe in Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>4</mml:mn></mml:msub></mml:math>N. Physical Review B, 2013, 88, .	1.1	29
272	Hubbard parameters for metallic Ce. Physical Review Letters, 1992, 68, 2652-2655.	2.9	28
273	Theoretical aspects of the 5fdelocalization of americium under pressure. Physical Review B, 1992, 45, 3198-3203.	1.1	28
274	Non-collinear states in magnetic sensors. Nature, 2000, 406, 280-282.	13.7	28
275	Calculated trends of the magnetostriction coefficient of 3d alloys from first principles. Applied Physics Letters, 2000, 76, 915-917.	1.5	28
276	Magnetism of Fe/V and Fe/Co multilayers. Journal of Physics Condensed Matter, 2003, 15, S599-S615.	0.7	28
277	Dynamical core-hole screening in the x-ray absorption spectra of graphite,C60, and carbon nanotubes: A first-principles electronic structure study. Physical Review B, 2006, 73, .	1.1	28
278	Anisotropy in the electronic structure of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>V</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>GeC</mml:m by soft x-ray emission spectroscopy and first-principles theory. Physical Review B, 2008, 78, .	1.1	28
279	Electronic Structure of Actinide Intermetallic Compounds: Systems with Properties varying from Paramagnetism, Itinerant Magnetism, Heavy Fermion Behaviour to 5f Localization. Physica Scripta, 1986, T13, 65-72.	1.2	27
280	Magnetism and bonding in light actinide and rare earth systems (invited). Journal of Applied Physics, 1991, 69, 5897-5902.	1.1	27
281	Core Hole Effects in Resonant Inelastic X-Ray Scattering of Graphite. Physical Review Letters, 1996, 76, 1761-1761.	2.9	27
282	Magnetic susceptibility of hcp iron and the seismic anisotropy of Earthâ€™s inner core. Physical Review B, 2003, 68, .	1.1	27
283	Crystal and magnetic structure ofMn3IrSi. Physical Review B, 2004, 69, .	1.1	27
284	Dynamical effects in x-ray absorption spectra of graphene and monolayered<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>h</mml:mi></mml:math>-BN on Ni(111). Physical Review B, 2010, 81, .	1.1	27
285	Temperature-driven Î±-to-Î² phase transformation in Ti, Zr and Hf from first-principles theory combined with lattice dynamics. Europhysics Letters, 2011, 96, 66006.	0.7	27
286	Order-disorder induced magnetic structures of FeMnP0.75Si0.25. Physical Review B, 2011, 83, .	1.1	27
287	Wake downstream of the Lillgrund wind farm - A Comparison between LES using the actuator disc method and a Wind farm Parametrization in WRF. Journal of Physics: Conference Series, 2015, 625, 012028.	0.3	27
288	Magnetic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>1 its alloys with P, S, and Co. Physical Review B, 2016, 93, .	1.1	27

#	Article	IF	Citations
289	Electronic structure of the actinide-Rh3systems and the 5flocalization inUPd3. Physical Review B, 1989, 40, 9508-9518.	1.1	26
290	Calculated optical properties of a solar energy material: CuGaS2. Solar Energy Materials and Solar Cells, 1998, 53, 357-366.	3.0	26
291	Theory of strongly correlated electron systems: Hubbard-Anderson models from an exact Hamiltonian, and perturbation theory near the atomic limit within a nonorthogonal basis set. International Journal of Quantum Chemistry, 2003, 94, 113-143.	1.0	26
292	Inhomogeneity in Co doped ZnO diluted magnetic semiconductor. Journal of Applied Physics, 2008, 103, .	1.1	26
293	Complex magnetic structure of clusters and chains of Ni and Fe on Pt(111). Scientific Reports, 2013, 3, 3054.	1.6	26
294	Microscopic description of the evolution of the local structure and an evaluation of the chemical pressure concept in a solid solution. Physical Review B, 2014, 89, .	1.1	26
295	First-principles study of the magnetization density inCeFe2. Physical Review B, 1994, 50, 4200-4203.	1.1	25
296	Influence of pseudocore valence-band hybridization on the crystal-structure phase stabilities of transition metals under extreme compressions. Physical Review B, 1994, 50, 14690-14693.	1.1	25
297	Structural and magnetic properties of (Fe1â^'xCox)3P compounds: experiment and theory. Journal of Magnetism and Magnetic Materials, 1998, 189, 69-82.	1.0	25
298	Theoretical study of structural and electronic properties ofVHx. Physical Review B, 1998, 58, 5230-5235.	1.1	25
299	Reflectance anisotropy spectra of Cu and Ag (110) surfaces fromab initiotheory. Physical Review B, 2001, 64, .	1.1	25
300	Calculation of the equation of state of fcc Au from first principles. Physical Review B, 2006, 73, .	1.1	25
301	Dimensionality crossover in the induced magnetization of Pd layers. Journal of Physics Condensed Matter, 2007, 19, 246213.	0.7	25
302	Experimental and theoretical studies on stainless steel transfer onto a TiN-coated cutting tool. Acta Materialia, 2011, 59, 68-74.	3.8	25
303	Quasiâ€2D Cu₂S Crystals on Graphene: Inâ€situ Growth and abâ€initio Calculations. Small, 2015, 11, 1253-1257.	5.2	25
304	Orbital magnetism in energy bands. Physica B: Condensed Matter, 1991, 172, 101-116.	1.3	24
305	Surface electronic structure of Î³-uranium. Physical Review B, 1993, 47, 6680-6684.	1.1	24
306	Field-induced magnetism in itinerantf-electron systems: U, Pu, and Ce. Physical Review B, 1994, 50, 4332-4340.	1.1	24

#	Article	IF	Citations
307	Density-functional calculations for cerium metal. Physical Review B, 1995, 51, 4618-4621.	1.1	24
308	Pressure-induced phase transitions in Pa metal from first-principles theory. Physical Review B, 1997, 56, 10719-10721.	1.1	24
309	In-plane magnetic anisotropy of Fe/V (001) superlattices. Journal of Magnetism and Magnetic Materials, 2002, 241, 260-270.	1.0	24
310	Microscopic picture of Co clustering in ZnO. Physical Review B, 2009, 79, .	1.1	24
311	Influence of plural scattering on the quantitative determination of spin and orbital moments in electron magnetic chiral dichroism measurements. Physical Review B, 2011, 83, .	1.1	24
312	Possible high-temperature superconductors predicted from electronic structure and data-filtering algorithms. Computational Materials Science, 2013, 67, 282-286.	1.4	24
313	Fe phthalocyanine on Co(001): Influence of surface oxidation on structural and electronic properties. Physical Review B, 2014, 89, .	1.1	24
314	Thermally driven domain-wall motion in Fe on W(110). Physical Review B, 2014, 90, .	1.1	24
315	The influence of oxygen adsorption on the NEXAFS and core-level XPS spectra of the C60 derivative PCBM. Journal of Chemical Physics, 2015, 142, 054306.	1.2	24
316	The electronic characterization of biphenyleneâ€"Experimental and theoretical insights from core and valence level spectroscopy. Journal of Chemical Physics, 2015, 142, 074305.	1.2	24
317	Coexistence of Superconductivity and Charge Density Waves in Tantalum Disulfide: Experiment and Theory. Physical Review Letters, 2020, 125, 186401.	2.9	24
318	Self-induced spin glass state in elemental and crystalline neodymium. Science, 2020, 368, .	6.0	24
319	Multifocal breast carcinoma. American Journal of Surgery, 1981, 142, 255-257.	0.9	23
320	Itinerant magnetism inCeRh3B2. Physical Review B, 1989, 40, 5270-5273.	1.1	23
321	Relativistic Stoner theory applied toPuSn3. Physical Review B, 1989, 39, 13115-13119.	1.1	23
322	Electronic structure of the LaS surface and LaS/CdS interface. Physical Review B, 1998, 57, 4067-4072.	1.1	23
323	Theoretical high-pressure studies of silicon VI. Physical Review B, 1999, 60, 14475-14477.	1.1	23
324	Geometry of the Valence Transition Induced Surface Reconstruction of Sm(0001). Physical Review Letters, 2002, 88, 136102.	2.9	23

#	Article	IF	Citations
325	Ab initiostudy of the electronic properties and Fermi surface of the uranium dipnictides. Physical Review B, 2006, 73, .	1.1	23
326	Noncollinear magnetism in the high-pressure hcp phase of iron. Physical Review B, 2008, 78, .	1.1	23
327	Defect-controlled electronic transport in single, bilayer, and N-doped graphene: Theory. Physical Review B, 2010, 81, .	1.1	23
328	Large magnetic anisotropy of Fe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>P investigated viaab initiodensity functional theory calculations. Physical Review B, 2012, 86, .	1.1	23
329	Polar Order and Frustrated Antiferromagnetism in Perovskite Pb₂MnWO₆ Single Crystals. Inorganic Chemistry, 2016, 55, 2791-2805.	1.9	23
330	The Role of Endotoxins in Induced Ruminal Acidosis in Calves. Acta Veterinaria Scandinavica, 1992, 33, 117-127.	0.5	23
331	Electron-phonon coupling in the actinides. Physical Review B, 1988, 37, 1706-1710.	1.1	22
332	Theoretical investigation of the high-pressure phases of Ce. Physical Review B, 1998, 57, 2091-2101.	1.1	22
333	Simple model for complex structures. Physical Review B, 1998, 57, 1320-1323.	1.1	22
334	Magnetovolume effect in UGa3. Journal of Magnetism and Magnetic Materials, 1999, 192, 137-147.	1.0	22
335	Magnetism of Fe clusters embedded in a Co matrix from first-principles theory. Physical Review B, 2004, 70, .	1.1	22
336	Electronic and optical properties of Î±, Î³, and Î² phases of MgH2: A first-principles GW investigation. Journal of Applied Physics, 2005, 98, 096106.	1.1	22
337	Crystal and magnetic structure investigation ofTbNi5â^'xCux(x=0,0.5,1.0,1.5,2.0): Experiment and theory. Physical Review B, 2006, 74, .	1.1	22
338	Electronic structure of Co-phthalocyanine calculated by GGA+U and hybrid functional methods. Chemical Physics, 2010, 377, 96-99.	0.9	22
339	Correlated Electrons Step by Step: Itinerant-to-Localized Transition of Fe Impurities in Free-Electron Metal Hosts. Physical Review Letters, 2010, 104, 117601.	2.9	22
340	Suppression of Standing Spin Waves in Low-Dimensional Ferromagnets. Physical Review Letters, 2011, 107, 037202.	2.9	22
341	Lattice dynamics and chemical bonding in Sb2Te3 from first-principles calculations. Journal of Chemical Physics, 2015, 142, 174702.	1.2	22
342	Magnetism and exchange interaction of small rare-earth clusters; Tb as a representative. Scientific Reports, 2016, 6, 19676.	1.6	22

#	Article	IF	Citations
343	High photon energy spectroscopy of NiO: Experiment and theory. Physical Review B, 2016, 93, .	1.1	22
344	Exchange interactions of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub></ in the bulk and at the surface. Physical Review B, 2017, 95, .	1.1	22
345	Theory of noncollinear interactions beyond Heisenberg exchange: Applications to bcc Fe. Physical Review B, 2017, 96, .	1.1	22
346	Density Functional Theory description of the order-disorder transformation in Fe-Ni. Scientific Reports, 2019, 9, 8172.	1.6	22
347	Segmentation of cervical cells: Detection of overlapping cell nuclei. Computer Graphics and Image Processing, 1981, 16, 382-394.	0.9	21
348	Electronic structure of the uranium-3d transition metal laves phases. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1986, 144, 32-40.	0.9	21
349	Systematic behavior of the hexagonal axial ratio for thedtransition metals. Physical Review B, 1999, 59, 6131-6138.	1.1	21
350	Initial and final state effects in the x-ray absorption process ofLa1âˆ'xSrxMnO3. Physical Review B, 2003, 68, .	1.1	21
351	Theoretical and experimental study of the magnetic structure ofTlCo2Se2. Physical Review B, 2004, 70, .	1.1	21
352	Cycloidal magnetic order in the compound IrMnSi. Physical Review B, 2005, 71, .	1.1	21
353	First-principles studies of the Gilbert damping and exchange interactions for half-metallic Heuslers alloys. Physical Review B, 2016, 93, .	1.1	21
354	Theory of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>L</mml:mi></mml:math>-edge spectroscopy of strongly correlated systems. Physical Review B, 2017, 96, .	1.1	21
355	Electronic structure of the pseudobinary U(Rh1âˆ'yPdy)3alloys. Physical Review B, 1988, 38, 12858-12863.	1.1	20
356	Calculations of valence stabilities for the lanthanide metals. Journal of Alloys and Compounds, 1994, 209, 15-24.	2.8	20
357	Theoretical studies of substitutional impurities in molybdenum carbide. Physical Review B, 1999, 60, 15123-15130.	1.1	20
358	Theory of spin filtering through quantum dots. Physical Review B, 2003, 67, .	1.1	20
359	Defect structure ofGa1âˆ'xMnxAs: A cross-sectional scanning tunneling microscopy study. Physical Review B, 2004, 70, .	1.1	20
360	Dual nature of the 5f electrons in plutonium materials. Physica B: Condensed Matter, 2006, 378-380, 920-924.	1.3	20

#	Article	IF	Citations
361	Differential response to estrogen challenge test in women with and without premenstrual dysphoria. Psychoneuroendocrinology, 2006, 31, 415-427.	1.3	20
362	Dynamics of diluted magnetic semiconductors from atomistic spin-dynamics simulations: Mn-doped GaAs. Physical Review B, 2008, 78, .	1.1	20
363	Strongly enhanced magnetic moments in ferromagnetic FeMnP0.5Si0.5. Applied Physics Letters, 2011, 99, 152502.	1.5	20
364	Ferrimagnetism, antiferromagnetism, and magnetic frustration in La<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>Sr<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>CuRuO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:	1.1	20
365	Electronic structure, cohesive properties, and magnetism of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrRuO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	20
366	Dynamics of quasiparticles in graphene under intense circularly polarized light. Physical Review B, 2015, 91, .	1.1	20
367	Electronic topological transition and noncollinear magnetism in compressed hcp Co. Physical Review B, 2015, 92, .	1.1	20
368	First-principles study of the influence of different interfaces and core types on the properties of CdSe/CdS core-shell nanocrystals. Scientific Reports, 2015, 5, 10865.	1.6	20
369	The dipole moment of the spin density as a local indicator for phase transitions. Scientific Reports, 2014, 4, 5760.	1.6	20
370	A spin dynamics approach to solitonics. Scientific Reports, 2016, 6, 25685.	1.6	20
371	First-principles Dzyaloshinskiiâ€“Moriya interaction in a non-collinear framework. Scientific Reports, 2020, 10, 20339.	1.6	20
372	Heavy-mass magnetic modes in pyrochlore iridates due to dominant Dzyaloshinskii-Moriya interaction. Physical Review Materials, 2018, 2, .	0.9	20
373	High resolution segmentation of cervical cells.. Journal of Histochemistry and Cytochemistry, 1979, 27, 621-628.	1.3	19
374	Experiment and Theory of Actinide Intermetallic Magnetism: A Test Case of NpCo ₂. Europhysics Letters, 1990, 11, 269-274.	0.7	19
375	Magnetism in Rare-Earth Metals and Rare-Earth Intermetallic Compounds. Physica Scripta, 1991, T39, 100-109.	1.2	19
376	Variable-takeoff-angle x-ray-photoelectron-spectroscopy evidence for an electronically modified surface in Î±-Pu. Physical Review B, 1992, 46, 13571-13575.	1.1	19
377	Calculated bond properties of K adsorbed on graphite. Physical Review B, 1998, 58, 13191-13196.	1.1	19
378	Electronic structure and magnetism of diluted magnetic semiconductors. Journal of Physics Condensed Matter, 2004, 16, S5481-S5489.	0.7	19

#	Article	IF	Citations
379	Ferromagnetism in Mn doped half-Heusler NiTiSn: Theory and experiment. Applied Physics Letters, 2006, 89, 212502.	1.5	19
380	Non-collinear magnetisation of V clusters supported on a Cu (111) surface: Theory. Surface Science, 2006, 600, 4838-4842.	0.8	19
381	Dynamical core-hole screening in the x-ray absorption spectra of hydrogenated carbon nanotubes and graphene. Physical Review B, 2007, 76, .	1.1	19
382	A new material for hydrogen storage; ScAl0.8Mg0.2. Journal of Solid State Chemistry, 2009, 182, 3113-3117.	1.4	19
383	Structural properties of amorphous metal carbides: Theory and experiment. Acta Materialia, 2012, 60, 4720-4728.	3.8	19
384	Magnetic and electronic structure of Mn nanostructures on Ag(111) and Au(111). Physical Review B, 2016, 93, .	1.1	19
385	Self-organizing maps as a method for detecting phase transitions and phase identification. Physical Review B, 2019, 99, .	1.1	19
386	Heisenberg and anisotropic exchange interactions in magnetic materials with correlated electronic structure and significant spin-orbit coupling. Physical Review B, 2021, 103, .	1.1	19
387	Nonlocal Gilbert damping tensor within the torque-torque correlation model. Physical Review Materials, 2018, 2, .	0.9	19
388	Magnon-magnon entanglement and its quantification via a microwave cavity. Physical Review B, 2021, 104, .	1.1	19
389	Shiga-like Toxin Production and Connective Tissue Protein Binding of Escherichia coli Isolated from a Patient with Ulcerative Colitis. Scandinavian Journal of Infectious Diseases, 1988, 20, 443-446.	1.5	18
390	Spin and orbital magnetization densities in itinerant magnets. Physica B: Condensed Matter, 1993, 192, 39-49.	1.3	18
391	First principles studies of crystal structures of f elements. Physica B: Condensed Matter, 1993, 190, 5-11.	1.3	18
392	Structural and magnetic characterization of Mn3IrGe and Mn3Ir(Si1âˆ'xGex): experiments and theory. Journal of Solid State Chemistry, 2004, 177, 4058-4066.	1.4	18
393	Thermodynamics of a two-dimensional Heisenberg ferromagnet with dipolar interaction. Physical Review B, 2005, 71, .	1.1	18
394	Theory of the temperature dependence of the easy axis of magnetization in hcp Gd. Physical Review B, 2005, 72, .	1.1	18
395	Multiplet effects in the electronic structure of heavy rare-earth metals. Journal of Physics Condensed Matter, 2006, 18, 6329-6335.	0.7	18
396	Î³-Mn at the border between weak and strong correlations. European Physical Journal B, 2009, 72, 473-478.	0.6	18

#	Article	IF	Citations
397	Europium Cyclooctatetraene Nanowire Carpets: A Low-Dimensional, Organometallic, and Ferromagnetic Insulator. Journal of Physical Chemistry Letters, 2019, 10, 911-917.	2.1	18
398	Direct writing of lateral fluorographene nanopatterns with tunable bandgaps and its application in new generation of moirÃ© superlattice. Applied Physics Reviews, 2020, 7, .	5.5	18
399	A morphometric expression of differentiation in fine-needle biopsies of breast cancer. Cytometry, 1981, 1, 292-295.	1.8	17
400	Calculations of crystal-structure stabilities of Ce under pressure. Physical Review B, 1992, 46, 12981-12989.	1.1	17
401	Prediction of a bcc structure in compressed yttrium. Physical Review B, 1993, 48, 15574-15577.	1.1	17
402	First-principles calculations of the magnetic anisotropy energy of Fe-V multilayers. Physical Review B, 2002, 65, .	1.1	17
403	Stabilization of potential superhardRuO2phases: A theoretical study. Physical Review B, 2002, 66, .	1.1	17
404	First-Principles Theory of Intermediate-Valencef-electron Systems. Physical Review Letters, 2004, 93, 096403.	2.9	17
405	Electronic and magnetic properties of disordered Feâ€“Cr alloys using different electronic structure methods. Journal of Physics Condensed Matter, 2008, 20, 445201.	0.7	17
406	Effects of strain on ferroelectric polarization and magnetism in orthorhombic HoMnO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2013, 87, .	1.1	17
407	Photoelectron and Absorption Spectroscopy Studies of Metal-Free Phthalocyanine on Au(111): Experiment and Theory. Journal of Physical Chemistry C, 2013, 117, 7018-7025.	1.5	17
408	Origin of the magnetostructural coupling in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">FeMnP</mml:mi><mml:mrow><mml:mn>0.75</mml:mn></mml:mrow></mml:msub><mml:msub><mml:mi mathvariant="normal">Si</mml:mi><mml:mrow><mml:mn>0.25</mml:mn></mml:mrow></mml:msub></mml:math>. Physical Review B, 2014, 90, .	1.1	17
409	Field-regulated switching of the magnetization of Co-porphyrin on graphene. Physical Review B, 2014, 89, .	1.1	17
410	Tuning order-by-disorder multiferroicity in CuO by doping. Physical Review B, 2014, 90, .	1.1	17
411	Controlling Electronic Structure and Transport Properties of Zigzag Graphene Nanoribbons by Edge Functionalization with Fluorine. Journal of Physical Chemistry C, 2015, 119, 21227-21233.	1.5	17
412	Theoretical study of the metamagnetism inThCo5. Physical Review B, 1990, 42, 8367-8374.	1.1	16
413	Occurrence of endotoxin in dialysis fluid from 39 dialysis units. Journal of Hospital Infection, 1993, 24, 29-37.	1.4	16
414	Beneficial effects of preâ€treatment with vitamin A on cardiac and pulmonary functions in endotoxaemic pigs. Acta Anaesthesiologica Scandinavica, 1996, 40, 538-548.	0.7	16

#	Article	IF	Citations
415	A Theoretical Study of the Pressure-Induced Structural Phase Transition in CdTe. Physica Status Solidi (B): Basic Research, 1997, 199, 75-79.	0.7	16
416	Comment on â€œStability and the equation of state of Î±-manganese under ultrahigh pressureâ€• Physical Review B, 1998, 57, 10989-10992.	1.1	16
417	Probing the local electronic structure in the H induced metal - insulator transition of Y. Journal of Physics Condensed Matter, 1999, 11, L119-L125.	0.7	16
418	Magnetic properties of selected Mn-based transition metal compounds withÎ²â˜Mnstructure: Experiments and theory. Physical Review B, 2005, 72, .	1.1	16
419	Experimental and theoretical study of annealed Ni-Pt alloys. Physical Review B, 2006, 74, .	1.1	16
420	Understanding mixed valent materials: Effects of dynamical core-hole screening in high-pressure x-ray spectroscopy. Physical Review B, 2006, 74, .	1.1	16
421	Prediction of MAX phases, VN+1SiCN (N=1,2), from first-principles theory. Journal of Applied Physics, 2007, 101, 013511.	1.1	16
422	First-principles modeling of He-clusters in UO2. Journal of Nuclear Materials, 2009, 385, 72-74.	1.3	16
423	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>Fe</mml:mi><mml:mi>n</mml:mi></mml:msub></mml clusters chemisorbed on vacancy defects in graphene: Stability, spin-dipole moment, and magnetic anisotropy. Physical Review B, 2014, 89, .	1.1	16
424	Effect of uniaxial strain on the site occupancy of hydrogen in vanadium from density-functional calculations. Scientific Reports, 2015, 5, 10301.	1.6	16
425	Combining electronic structure and many-body theory with large databases: A method for predicting the nature of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>4</mml:mn><mml:mi>f</mml:mi></mml:mrow></mml states in Ce compounds. Physical Review Materials, 2017, 1, .	0.9	16
426	Analysis of the linear relationship between asymmetry and magnetic moment at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>M</mml:mi></mml:math> edge of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r transition metals. Physical Review Research, 2020, 2, .	1.3	16
427	Orbital magnetism in the itinerant ferromagnetNpOs2. Physical Review B, 1990, 41, 9095-9100.	1.1	15
428	Electronic structure of the RBiPt compounds (Rî—¼Y and Yb). Journal of Alloys and Compounds, 1992, 185, 145-149.	2.8	15
429	First-principles calculations of the magnetic properties of and its hydrides. Journal of Physics Condensed Matter, 1996, 8, 3373-3384.	0.7	15
430	Surface segregation of transition metal impurities on the TiC(100) surface. Surface Science, 2005, 585, 101-107.	0.8	15
431	Phase separation and charge localization in UHV-lithiated anataseTiO2nanoparticles. Physical Review B, 2005, 71, .	1.1	15
432	Carbon release by selective alloying of transition metal carbides. Journal of Physics Condensed Matter, 2011, 23, 355401.	0.7	15

#	Article	IF	Citations
433	Atomistic theory of magnetism in the magnetocaloric material<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>P<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>T<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow />	1.1	15
434	Experimental and theoretical study of electronic structure of lutetium bi-phthalocyanine. Journal of Chemical Physics, 2013, 138, 234701.	1.2	15
435	Correlated electron behavior of metal-organic molecules: Insights from density functional theory combined with many-body effects using exact diagonalization. Physical Review B, 2016, 93, .	1.1	15
436	Towards sub-nanometer real-space observation of spin and orbital magnetism at the Fe/MgO interface. Scientific Reports, 2017, 7, 44802.	1.6	15
437	Peculiar magnetic states in the double perovskite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Nd</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2019, 100, .	1.1	15
438	Theory of orbital splittings applied to NpAl2. Journal of Physics Condensed Matter, 1990, 2, 1529-1535.	0.7	14
439	Local-moment collapse in compressed samarium metal. Physical Review B, 1993, 48, 9212-9215.	1.1	14
440	Effect of generalized gradient corrections on lanthanide cohesive properties. Journal of Alloys and Compounds, 1998, 275-277, 472-475.	2.8	14
441	Structural and magnetic properties of(Fe1â^’xMnx)3Pâ€,(x<0.25). Physical Review B, 2000, 61, 413-421.	1.1	14
442	Unusual magnetism and magnetocrystalline anisotropy of CrPt3. Journal of Magnetism and Magnetic Materials, 2002, 240, 371-373.	1.0	14
443	Ab initiocalculation of depth-resolved optical anisotropy of the Cu(110) surface. Physical Review B, 2003, 68, .	1.1	14
444	Many-body effects and excitonic features in 2D biphenylene carbon. Journal of Chemical Physics, 2016, 144, 024702.	1.2	14
445	Electronic and magnetic properties of single Fe atoms on a CuN surface: Effects of electron correlations. Physical Review B, 2016, 93, .	1.1	14
446	Quantitative determination of endotoxins on surgical gloves. Journal of Hospital Infection, 1990, 16, 167-172.	1.4	13
447	Theoretical high-pressure studies of Cs metal. Physical Review B, 2000, 63, .	1.1	13
448	Absence of a pressure-induced structural phase transition inTi3Alup to 25 GPa. Physical Review B, 2000, 63, .	1.1	13
449	Magnetic moments and exchange interactions inFe0.82Ni0.18â^•Vbcc (001) multilayers. Physical Review B, 2004, 70, .	1.1	13
450	Electronic structure and transport properties ofCrAsâ^•GaAsâ^•CrAstrilayers from first principles theory. Physical Review B, 2004, 70, .	1.1	13

#	Article	IF	Citations
451	Ab initiocalculation of the magnetocrystalline anisotropy and spin and orbital moments of a bcc Co(001) surface. Physical Review B, 2005, 72, .	1.1	13
452	Investigation of transcription factor AP-2beta genotype in women with premenstrual dysphoric disorder. Neuroscience Letters, 2005, 377, 49-52.	1.0	13
453	Role of defects on the magnetic interactions in Mn-doped ZnO. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 53-60.	0.8	13
454	Electronic structure and exchange interactions of insulating double perovskite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>La</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> Physical Review B, 2016, 94, .	1.1	13
455	Magnetic properties of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> system. Physical Review B, 2017, 96, .	1.1	13
456	Magnetism and ultrafast magnetization dynamics of Co and CoMn alloys at finite temperature. Physical Review B, 2017, 95, .	1.1	13
457	Measuring the Intra-Atomic Exchange Energy in Rare-Earth Adatoms. Physical Review X, 2020, 10, .	2.8	13
458	Pressure effect on the orderâ€“disorder transformation in L10 FeNi. Scientific Reports, 2020, 10, 14766.	1.6	13
459	Nonreciprocal spin pumping damping in asymmetric magnetic trilayers. Physical Review B, 2020, 101, .	1.1	13
460	Theoretical studies of actinide intermetallic compounds. Inorganica Chimica Acta, 1987, 140, 59-66.	1.2	12
461	Electronic structure, cohesive, and magnetic properties of the actinide-iridium Laves phases. Physical Review B, 1989, 39, 5647-5654.	1.1	12
462	Crystallographic phase transitions in actinide metals as a function of pressure. Journal of Alloys and Compounds, 1994, 213-214, 268-277.	2.8	12
463	Modification of the standard model for the lanthanides. Solid State Communications, 2000, 115, 7-12.	0.9	12
464	Exchange interactions and critical temperatures in diluted magnetic semiconductors. Journal of Physics Condensed Matter, 2004, 16, S5571-S5578.	0.7	12
465	Asymmetric negative differential conductance in double quantum dots. Journal of Physics Condensed Matter, 2004, 16, L85-L91.	0.7	12
466	Vanishing Magnetic Interactions in Ferromagnetic Thin Films. Physical Review Letters, 2005, 94, 217202.	2.9	12
467	Phenomenological model of the magnetic states of ferromagnetic film with competing surface and bulk anisotropies. Physical Review B, 2008, 77, .	1.1	12
468	Dynamical stabilization of the body centered cubic phase in lanthanum and thorium by phononâ€“phonon interaction. Journal of Physics Condensed Matter, 2009, 21, 175402.	0.7	12

#	Article	IF	Citations
469	Quantitative magnetic measurements with transmission electron microscope. Journal of Magnetism and Magnetic Materials, 2010, 322, 1478-1480.	1.0	12
470	Metastable noncollinear canted states from a phenomenological model of a symmetric ferromagnetic film. Physical Review B, 2010, 81, .	1.1	12
471	Kinetic arrest induced antiferromagnetic order in hexagonal FeMnP0.75Si0.25 alloy. Applied Physics Letters, 2014, 105, .	1.5	12
472	Gilbert-like damping caused by time retardation in atomistic magnetization dynamics. Physical Review B, 2015, 92, .	1.1	12
473	Layer-resolved magnetic exchange interactions of surfaces of late<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math> Effects of electronic correlations. Physical Review B, 2015, 92, .	1.1	12
474	Correlation effects and orbital magnetism of Co clusters. Physical Review B, 2016, 93, .	1.1	12
475	Magnetic anisotropy in permalloy: Hidden quantum mechanical features. Physical Review B, 2018, 97, .	1.1	12
476	Plastic deformation transition in FeCrCoNiAl_x high-entropy alloys. Materials Research Letters, 2019, 7, 439-445.	4.1	12
477	Charge disproportionate antiferromagnetism at the verge of the insulator-metal transition in doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>LaFeO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> Physical Review B, 2019, 99, .	1.1	12
478	Exotic magnetic and electronic properties of layered <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CrI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> single crystals under high pressure. Physical Review B, 2022, 105, .	1.1	12
479	Exchange scaling of ultrafast angular momentum transfer in 4f antiferromagnets. Nature Materials, 2022, 21, 514-517.	13.3	12
480	Endotoxin concentrations in the blood following intravenous injection and effect on prostaglandin F2Î± release, calcium and bile acids in goats. Research in Veterinary Science, 1990, 48, 190-195.	0.9	11
481	Field-induced magnetism in uranium compounds:UGe3andURh3. Physical Review B, 1994, 50, 9226-9234.	1.1	11
482	Vitamin A exerts potential therapeutic effects in the endotoxaemic pig. Acta Anaesthesiologica Scandinavica, 1997, 41, 824-829.	0.7	11
483	Negative electron affinity material: LaS on InP. Physical Review B, 2001, 65, .	1.1	11
484	Effect of pressure on the magnetic susceptibility of CeCo2. Physica B: Condensed Matter, 2002, 319, 268-276.	1.3	11
485	Origin of the negative giant magnetoresistance effect inCo1âˆ’xCrx/Cu/Co(111) trilayers. Physical Review B, 2004, 69, .	1.1	11
486	Volume-dependent exchange interactions and noncollinear magnetism in zinc-blende MnAs. Physical Review B, 2006, 74, .	1.1	11

#	Article	IF	Citations
487	Electronic structure and magnetic properties of RNi5â^'xCux alloys (R=Y, La, Ce). Low Temperature Physics, 2006, 32, 1140-1146.	0.2	11
488	Ordering in diluted magnetic semiconductors: A magnetic percolation phenomenon (invited). Journal of Applied Physics, 2007, 101, 09H114.	1.1	11
489	Electronic structure of Co doped ZnO: Theory and experiment. Journal of Applied Physics, 2008, 103, .	1.1	11
490	Atomistic spin dynamics of the Cu-Mn spin-glass alloy. Physical Review B, 2009, 79, .	1.1	11
491	From collinear to vortex magnetic structures in Mn corrals on Pt(111). Physical Review B, 2011, 83, .	1.1	11
492	Revisiting the adsorption of copper-phthalocyanine on Au(111) including van der Waals corrections. Journal of Chemical Physics, 2014, 140, 124711.	1.2	11
493	Enhanced spinâ€“orbit coupling in tetragonally strained Feâ€“Coâ€“B films. Journal of Physics Condensed Matter, 2017, 29, 275802.	0.7	11
494	Evolution of the structural and multiferroic properties of PbFe2/3W1/3O3 ceramics upon Mn-doping. Materials Chemistry and Physics, 2017, 187, 218-232.	2.0	11
495	Topological edge-state engineering with high-frequency electromagnetic radiation. Physical Review B, 2017, 96, .	1.1	11
496	A majority gate with chiral magnetic solitons. Journal of Physics Condensed Matter, 2018, 30, 375801.	0.7	11
497	High-throughput compatible approach for entropy estimation in magnetocaloric materials: FeRh as a test case. Journal of Alloys and Compounds, 2021, 857, 157811.	2.8	11
498	The cohesive energy and band structure of black phosphorus. Journal of Physics and Chemistry of Solids, 1990, 51, 1025-1032.	1.9	10
499	Photoelectron spectra and magnetic moments in UPdSn: Theory. Physical Review B, 1994, 49, 7165-7169.	1.1	10
500	Electronic and optical properties of InP. Solid State Communications, 1997, 104, 249-252.	0.9	10
501	Calculated electronic and transport properties of Fe/GaAs/Fe(001) tunnel junctions. Surface Science, 2004, 566-568, 303-308.	0.8	10
502	Fermiology of PuCoGa5 and of related Pu-115 compounds. Journal of Alloys and Compounds, 2007, 444-445, 109-113.	2.8	10
503	Quasiparticle and optical properties of BeH2. Journal of Physics Condensed Matter, 2007, 19, 036223.	0.7	10
504	Textured growth of the high moment material Gd(0â€‰0â€‰0â€‰1)/Cr(0â€‰0â€‰0â€‰1)/Fe(0â€‰0â€‰0â€‰1). Journal Physics D: Applied Physics, 2011, 44, 265004.	1.3	10

#	Article	IF	Citations
505	Route towards finding large magnetic anisotropy in nanocomposites: Application to a W<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>1</mml:mn><mml:mo>â’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mathRe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>/Fe multilayer. Physical Review B, 2011, 84, .	1.1	10
506	Electronic structure and optical properties of ordered compounds potassium tantalate and potassium niobate and their disordered alloys. Physica B: Condensed Matter, 2012, 407, 4615-4621.	1.3	10
507	Size dependence of the stability, electronic structure, and optical properties of silicon nanocrystals with various surface impurities. Physical Review B, 2015, 91, .	1.1	10
508	Women with Premenstrual Dysphoria Lack the Seemingly Normal Premenstrual Right-Sided Relative Dominance of 5-HTP-Derived Serotonergic Activity in the Dorsolateral Prefrontal Cortices - A Possible Cause of Disabling Mood Symptoms. PLoS ONE, 2016, 11, e0159538.	1.1	10
509	Finite-temperature interatomic exchange and magnon softening in Fe overlayers on Ir(001). Physical Review B, 2016, 94, .	1.1	10
510	Mechanisms behind large Gilbert damping anisotropies. Physical Review B, 2021, 103, .	1.1	10
511	Ultrafast magnetization dynamics in the half-metallic Heusler alloy <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">Co</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi>FeAl</mml:mi></mml:math>. Physical Review B, 2021, 104, .	1.1	10
512	The Full-Potential Electronic Structure Problem and RSPt. Springer Series in Solid-state Sciences, 2010, , 47-73.	0.3	10
513	Quantifying Spin-Mixed States in Ferromagnets. Physical Review Letters, 2021, 127, 207201.	2.9	10
514	Electronic structure of actinide intermetallic compounds. Journal of the Less Common Metals, 1987, 133, 25-29.	0.9	9
515	Calculated magnetic properties of the antiferromagnetic UNiSn compound. Physical Review B, 1991, 43, 5649-5652.	1.1	9
516	A theoretical study of the crystallographic structures in neptunium. Journal of Physics Condensed Matter, 1994, 6, 6573-6580.	0.7	9
517	ORBITAL PARAMAGNETISM IN METALLIC SYSTEMS WITH LARGE ANGULAR MOMENTA. International Journal of Modern Physics B, 1995, 09, 2735-2751.	1.0	9
518	Correlation mechanism off-electron delocalization. Physical Review B, 2000, 62, 16370-16377.	1.1	9
519	On the structural polymorphism of CePt2Sn2: experiment and theory. Journal of Alloys and Compounds, 2000, 306, 30-39.	2.8	9
520	Effects of melagatran, a novel direct thrombin inhibitor, during experimental septic shock. Expert Opinion on Investigational Drugs, 2000, 9, 1129-1137.	1.9	9
521	Probing surface states of Cu/Ni thin films using x-ray absorption spectroscopy. Physical Review B, 2001, 63, .	1.1	9
522	Effects of nonorthogonality in the time-dependent current through tunnel junctions. Physical Review B, 2001, 64, .	1.1	9

#	Article	IF	Citations
523	Electronic structure and magnetic properties of GdM2 compounds. Journal of Magnetism and Magnetic Materials, 2003, 258-259, 520-522.	1.0	9
524	The antiferromagnetism of (Fe1â^'xMnx)3P, xâ©¾0.67, compounds. Journal of Magnetism and Magnetic Materials, 2003, 256, 117-128.	1.0	9
525	Highly anisotropic sliding at TiN/Fe interfaces: A first principles study. Journal of Applied Physics, 2010, 108, 113511.	1.1	9
526	Magnetocrystalline anisotropy and uniaxiality of MnAs/GaAs(100) films. Physical Review B, 2011, 83, .	1.1	9
527	Magnetic ordering in Ni-rich NiMn alloys around the multicritical point: Experiment and theory. Physical Review B, 2012, 85, .	1.1	9
528	Tribochemically Active Tiâ€“Câ€“S Nanocomposite Coatings. Materials Research Letters, 2013, 1, 148-155.	4.1	9
529	Valence and spectral properties of rare-earth clusters. Physical Review B, 2015, 92, .	1.1	9
530	Atomic contributions to the valence band photoelectron spectra of metal-free, iron and manganese phthalocyanines. Journal of Electron Spectroscopy and Related Phenomena, 2015, 205, 92-97.	0.8	9
531	Mapping of Defects in Individual Silicon Nanocrystals Using Real-Space Spectroscopy. Journal of Physical Chemistry Letters, 2016, 7, 1047-1054.	2.1	9
532	On the origin of perpendicular magnetic anisotropy in strained Feâ€“Co(â€“X) films. Journal Physics D: Applied Physics, 2017, 50, 045003.	1.3	9
533	Coupling atomistic and continuum modelling of magnetism. Computer Methods in Applied Mechanics and Engineering, 2018, 329, 219-253.	3.4	9
534	Data-driven design of a new class of rare-earth free permanent magnets. Acta Materialia, 2021, 212, 116913.	3.8	9
535	A program system for interactive measurements on digitized cell images.. Journal of Histochemistry and Cytochemistry, 1977, 25, 641-654.	1.3	8
536	Conduction-electron Zeeman splitting in the noble metals. Physical Review B, 1989, 40, 5961-5966.	1.1	8
537	Electronic structure of platinum at ultrahigh pressure. High Pressure Research, 1994, 12, 161-170.	0.4	8
538	Calculated electronic and optical properties of a graphite intercalation compound:. Journal of Physics Condensed Matter, 1997, 9, 9845-9852.	0.7	8
539	Theoretical confirmation of the high-pressure orthorhombic phase in strontium. Physical Review B, 1998, 58, 8152-8154.	1.1	8
540	Effect of hydrogenation on the magnetic state in cubicPd3Mn. Physical Review B, 1999, 60, 6765-6769.	1.1	8

#	Article	IF	Citations
541	Tuning the orbital moment in transition metal compounds using ligand states. Journal of Physics Condensed Matter, 2001, 13, 4553-4566.	0.7	8
542	Fe/V and Fe/Co (001) superlattices: growth, anisotropy, magnetisation and magnetoresistance. Physica B: Condensed Matter, 2003, 327, 344-348.	1.3	8
543	Phase relations in the Ti3Snâ€“D system. Journal of Alloys and Compounds, 2004, 364, 127-131.	2.8	8
544	Simulation of a spin-wave instability from atomistic spin dynamics. Physical Review B, 2009, 79, .	1.1	8
545	Wear-resistant magnetic thin film material based on aTi1âˆ'xFexC1âˆ'ynanocomposite alloy. Physical Review B, 2010, 81, .	1.1	8
546	Augmented space recursion formulation of the study of disordered alloys with noncollinear magnetism and spin-orbit coupling: Application to MnPt and Mn3Rh. Physical Review B, 2011, 83, .	1.1	8
547	Hole bipolaron formation at (100) MgO/CaO epitaxial interface. Physical Review B, 2014, 89, .	1.1	8
548	Searching for materials with reduced dimension. Nature Nanotechnology, 2018, 13, 180-181.	15.6	8
549	Investigation of the spectral properties and magnetism of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiFeO</mml:mi><mml:mn>3</mml:mn></mml:msub> by dynamical mean-field theory. Physical Review B, 2018, 97, .	1.1	8
550	Equation of motion and the constraining field in ab initio spin dynamics. Physical Review B, 2020, 102, .	1.1	8
551	Exchange constants for local spin Hamiltonians from tight-binding models. Physical Review B, 2021, 103, .	1.1	8
552	Fermi surface of noble metals: Full-potential generalized-gradient-approximation calculations. Physical Review B, 1994, 50, 11183-11186.	1.1	7
553	Electronic structure and x-ray photoelectron spectroscopy of the Î±, Î², and Î³ phases of Np. Physical Review B, 1996, 54, 14405-14412.	1.1	7
554	Theoretical high-pressure studies of caesium hydride. Journal of Physics Condensed Matter, 1998, 10, L153-L158.	0.7	7
555	Theoretical study of the pressure-concentration diagram for the Ce-Th alloy system. Physical Review B, 1999, 60, 9372-9376.	1.1	7
556	Observation of short- and long-range hybridization of a buried Cu monolayer in Ni. Physical Review B, 2000, 62, R16239-R16242.	1.1	7
557	A first-principles study of the magnetism and electronic structure of Cr clusters supported on a Au(111) surface. Journal of Physics Condensed Matter, 2007, 19, 156226.	0.7	7
558	Effect of diffusion and alloying on the magnetic and transport properties ofFeâ•Vâ•Fetrilayers. Physical Review B, 2007, 75, .	1.1	7

#	Article	IF	Citations
559	Coupling between the4fcore binding energy and the5fvalence band occupation of elemental Pu and Pu-based compounds. Physical Review B, 2008, 78, .	1.1	7
560	Role of magnetic impurities in Fe/V multilayers. Physical Review B, 2008, 77, .	1.1	7
561	Increasing the Equilibrium Solubility of Dopants in Semiconductor Multilayers and Alloys. Physical Review Letters, 2008, 100, 105501.	2.9	7
562	Density functional study of the electronic structure and lattice dynamics of SrCl2. Journal of Physics Condensed Matter, 2010, 22, 445402.	0.7	7
563	Designing Fe Nanostructures at Graphene/h-BN Interfaces. Journal of Physical Chemistry C, 2013, 117, 21763-21771.	1.5	7
564	Electronic structure of In₃Se₄ and In₃Te₄ monolayers from abâ€initio calculations. Annalen Der Physik, 2014, 526, 402-407.	0.9	7
565	Influence of dimensionality and interface type on optical and electronic properties of CdS/ZnS core-shell nanocrystalsâ€”A first-principles study. Journal of Chemical Physics, 2015, 143, 164701.	1.2	7
566	Thermodynamic-state and kinetic-process dependent dual ferromagnetic states in high-Si content FeMn(PSi) alloys. Journal of Applied Physics, 2015, 118, .	1.1	7
567	Scale Transitions in Magnetisation Dynamics. Communications in Computational Physics, 2016, 20, 969-988.	0.7	7
568	Another view on Gilbert damping in two-dimensional ferromagnets. Scientific Reports, 2018, 8, 17148.	1.6	7
569	Local structure in amorphous Sm$$_x$$Co$$_{1-x}$$: a combined experimental and theoretical study. Journal of Materials Science, 2020, 55, 12488-12498.	1.7	7
570	Antichiral ferromagnetism. Physical Review B, 2021, 104, .	1.1	7
571	Localized surface electromagnetic waves in CrI₃-based magnetophotonic structures. Optics Express, 2020, 28, 29155.	1.7	7
572	Pressure effects on intermetallic actinide compounds. High Pressure Research, 1990, 2, 303-313.	0.4	6
573	Spin and orbital magnetism in Feî—¸Co and Coî—¸Ni alloys. Journal of Magnetism and Magnetic Materials, 1992, 104-107, 2037-2039.	1.0	6
574	Anomalous fcc Crystal Structure of Thorium Metal. Physical Review Letters, 1995, 75, 3968-3968.	2.9	6
575	From the transition metals to the rare earths â€” via the actinides. Journal of Alloys and Compounds, 1995, 223, 204-210.	2.8	6
576	Repetitive dosing of artemisinin and quinine against Plasmodium falciparum in vitro: a simulation of the in vivo pharmacokinetics. Acta Tropica, 1997, 65, 11-22.	0.9	6

#	Article	IF	Citations
577	Retinyl palmitate injections reduce serum levels and effects of endotoxin on systemic haemodynamics and oxygen transport in the pig. Acta Anaesthesiologica Scandinavica, 1998, 42, 406-413.	0.7	6
578	Photoemission and inverse-photoemission study of ferromagnetic valence fluctuating system CeFe2. Journal of Electron Spectroscopy and Related Phenomena, 1998, 88-91, 303-307.	0.8	6
579	On the non-orthogonality problem in the description of quantum devices. Physica B: Condensed Matter, 1999, 272, 28-30.	1.3	6
580	Effect of pressure on the Fermi surface and electronic structure of ErGa3. Low Temperature Physics, 1999, 25, 670-676.	0.2	6
581	Comment on â€œMystery of the Alkali Metals: Giant Moments of Fe and Co on and in Cs Filmsâ€• Physical Review Letters, 2000, 85, 1583-1583.	2.9	6
582	First principles calculations of the magnetic profiles of the Fe-V multilayers. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 1722-1724.	1.0	6
583	Theoretical investigation of a pressure-induced phase transition inEuCo2P2. Physical Review B, 2002, 65, .	1.1	6
584	On the magnetic structure of TlCo2Se2. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 557-558.	1.0	6
585	Pressure effect on the Fermi surface and electronic structure of LuGa3 and TmGa3. Low Temperature Physics, 2005, 31, 313-320.	0.2	6
586	Magnetic properties ofFeâˆ•Co(001)superlattices from first-principles theory. Physical Review B, 2006, 74, .	1.1	6
587	Theory of weakly coupled two-dimensional magnets. Journal of Physics Condensed Matter, 2006, 18, 4853-4860.	0.7	6
588	Cobalt-dopedÎ²-peptide nanotubes: A class of spintronic materials. Physical Review B, 2008, 77, .	1.1	6
589	Magnetic anisotropy and evolution of ground-state domain structures in bcc<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Fe</mml:mtext></mml:mrow><mml:mrow><mml:mn>81</mml:mn> Physical Review B, 2008, 78, .	1.1	6
590	Theoretical Analysis of Inertia-like Switching in Magnets: Applications to a Synthetic Antiferromagnet. Physical Review X, 2012, 2, .	2.8	6
591	Accelerating the switching of magnetic nanoclusters by anisotropy-driven magnetization dynamics. Physical Review B, 2012, 86, .	1.1	6
592	Functionalization of edge reconstructed graphene nanoribbons by H and Fe: A density functional study. Solid State Communications, 2012, 152, 1719-1724.	0.9	6
593	Spin-polaron formation and magnetic state diagram in La-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>CaMnO</mml:mtext><mml:mn>3</mml:mn> Physical Review B, 2017, 95, .	1.1	6
594	Suppression of the Verwey Transition by Charge Trapping. Annalen Der Physik, 2018, 530, 1700363.	0.9	6

#	Article	IF	Citations
595	Cation ordering, ferrimagnetism and ferroelectric relaxor behavior in Pb(Fe1â^'xScx)2â^•3W1â^•3O3 solid solutions. European Physical Journal B, 2019, 92, 1.	0.6	6
596	Ligand Effects on the Linear Response Hubbard U: The Case of Transition Metal Phthalocyanines. Journal of Physical Chemistry A, 2019, 123, 3214-3222.	1.1	6
597	Interlayer charge transfer in tin disulphide: Orbital anisotropy and temporal aspects. Physical Review B, 2020, 102, .	1.1	6
598	Alloying effect on the orderâ€“disorder transformation in tetragonal FeNi. Scientific Reports, 2021, 11, 5253.	1.6	6
599	Ab-initio study of the electronic structure and magnetic properties of Ce2Fe17. Journal of Alloys and Compounds, 2021, 888, 161521.	2.8	6
600	Magnetic two-dimensional electron liquid at the surface of Heusler semiconductors. Physical Review Materials, 2020, 4, .	0.9	6
601	Hierarchy of magnon mode entanglement in antiferromagnets. Physical Review B, 2020, 102, .	1.1	6
602	Comment on â€œProper and improper chiral magnetic interactionsâ€• Physical Review B, 2022, 105, .	1.1	6
603	Surface layer relaxation for Be(101Ì„0): theory. Surface Science, 1996, 355, 214-220.	0.8	5
604	Enhancement of Orbital Magnetism at Surfaces: Co on Cu(100). Physical Review Letters, 1996, 76, 1403-1403.	2.9	5
605	Periodical Anderson model for Pr metal. Physica B: Condensed Matter, 1997, 230-232, 445-447.	1.3	5
606	Theory of the Anisotropic Magneto-Optical Kerr Effect in Artificial FeAu and MnAu and in XAu₄ (X=V, Cr, Mn) Compounds. Journal of the Magnetics Society of Japan, 1999, 23, S1_21-26.	0.4	5
607	The relationship between interlayer spacing and magnetic ordering in gadolinium. Journal of Physics Condensed Matter, 2000, 12, 10441-10456.	0.7	5
608	Hyperfine interaction study of(Fe1â^'xCox)3Pcompounds. Physical Review B, 2000, 61, 6798-6804.	1.1	5
609	Band structure calculations of cerium activated inorganic scintillators. Radiation Effects and Defects in Solids, 2001, 154, 231-235.	0.4	5
610	H-H interaction and structural phase transition inTi3SnHx. Physical Review B, 2002, 66, .	1.1	5
611	Electronic structure and magnetic properties of lithium manganese spinels. Journal of Magnetism and Magnetic Materials, 2003, 258-259, 287-289.	1.0	5
612	Doping-induced bandgap narrowing in Si rich n- and p-type Si1ÂxGex. Journal of Physics Condensed Matter, 2003, 15, 489-502.	0.7	5

#	Article	IF	Citations
613	Many-body projector orbitals for electronic structure theory of strongly correlated electrons. International Journal of Quantum Chemistry, 2005, 105, 160-165.	1.0	5
614	Magnetic moments of Fe clusters embedded in an Fe-Co alloy. Physical Review B, 2006, 74, .	1.1	5
615	Volume dependent magnetism in zinc-blende MnXâ€ˆ(X=N,P,As,Sb,Bi) compounds. Journal of Applied Physics, 2008, 103, .	1.1	5
616	Spin and orbital moments of Fe clusters supported on Ni(001). Journal of Physics Condensed Matter, 2008, 20, 015001.	0.7	5
617	Competing anisotropies in bcc Fe81Ni19/Co(001) superlattices. Applied Physics Letters, 2009, 94, .	1.5	5
618	First principles calculations of magnetism, dielectric properties and spinâ€“phonon coupling in double perovskite Bi2CoMnO6. Journal of Physics Condensed Matter, 2012, 24, 295901.	0.7	5
619	Ovarian morphology in premenstrual dysphoria. Psychoneuroendocrinology, 2012, 37, 742-751.	1.3	5
620	X-ray absorption spectra: Graphene,<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>h</mml:mi></mml:mrow></mml:math>-BN, and their alloy. Physical Review B, 2013, 87, .	1.1	5
621	Hydrogen storage properties of the pseudo binary laves phase (Sc1â^'xZrx)(Co1â^'yNiy)2 system. International Journal of Hydrogen Energy, 2013, 38, 9772-9778.	3.8	5
622	Photoelectron Spectroscopy of Molecules Beyond the Electric Dipole Approximation. Journal of Chemical Theory and Computation, 2019, 15, 5483-5494.	2.3	5
623	Atomic photoionization cross sections beyond the electric dipole approximation. Journal of Chemical Physics, 2019, 150, 044306.	1.2	5
624	Localized versus itinerant character of 4f-states in cerium oxides. Journal of Physics Condensed Matter, 2020, 32, 215502.	0.7	5
625	Vibrational entropy-enhanced magnetocaloric effect in Mn-rich high-entropy alloys. Applied Physics Letters, 2021, 119, 084102.	1.5	5
626	Novel method of self-interaction corrections in density functional calculations. , 2001, 81, 247.		5
627	Exchange Coupling and Exchange Bias in FM/AFM Bilayers for a Fully Compensated AFM Interface. Acta Physica Polonica A, 2009, 115, 25-29.	0.2	5
628	Element-selective ultrafast magnetization dynamics of hybrid Stoner-Heisenberg magnets. Physical Review B, 2022, 105, .	1.1	5
629	A software system to record and analyze digitized cell images. Computer Programs in Biomedicine, 1977, 7, 233-246.	0.8	4
630	Electronically driven volume collapses of bantam-heavy actinide elements at high pressure. Physica B: Condensed Matter, 1993, 190, 12-20.	1.3	4

#	Article	IF	Citations
631	Fermi surface of alkali metals using the full-potential linear muffin-tin orbital method and the generalized gradient approximation. Physical Review B, 1994, 50, 18003-18006.	1.1	4
632	Theoretical aspects of the 4f-localization at the surface of Î±-Ce. Surface Science, 1997, 382, 93-99.	0.8	4
633	Electronic and optical properties of FeS₂ and CoS₂. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1998, 78, 475-480.	0.6	4
634	Are there two types of f-electrons in Pr-metal?. Physica B: Condensed Matter, 1999, 259-261, 231-232.	1.3	4
635	Precise solution for H-point oscillation: Mo, Na, and Fe. Journal of Physics Condensed Matter, 2002, 14, L453-L459.	0.7	4
636	A perfect spin-filter quantum dot system. Journal of Physics Condensed Matter, 2004, 16, L249-L254.	0.7	4
637	Theory of the magnetic anisotropy of Gd metal. Journal of Magnetism and Magnetic Materials, 2004, 272-276, E201-E202.	1.0	4
638	Polar magneto-optical Kerr effect for low-symmetric ferromagnets. Physical Review B, 2005, 72, .	1.1	4
639	Noncollinear spin states inTlCo2Se2â^'xSxalloys from first principles. Physical Review B, 2007, 75, .	1.1	4
640	Theoretical studies of the incommensurate magnetic structure of a heavy fermion system:CeRhIn5. Physical Review B, 2010, 81, .	1.1	4
641	Fe_{3.3}Ni_{83.2}Mo_{13.5}: a likely candidate to show spin-glass behaviour at low temperatures. Journal of Physics Condensed Matter, 2011, 23, 106002.	0.7	4
642	Lattice dynamics of cubic AuZn from first principles. Physical Review B, 2014, 89, .	1.1	4
643	Analysis of long distance wakes of Horns Rev I using actuator disc approach. Journal of Physics: Conference Series, 2014, 555, 012032.	0.3	4
644	Monovacancy formation energies and Fermi surface topological transitions in Pd-Ag alloys. Physical Review B, 2015, 92, .	1.1	4
645	Spin polaronics: Static and dynamic properties of spin polarons in La-doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>CaMnO</mml:mi><mml:mn>3</mml:mn></mml:msub> Physical Review B, 2019, 100, .	1.1	4
646	Realistic first-principles calculations of the magnetocaloric effect: applications to hcp Gd. Materials Research Letters, 2022, 10, 156-162.	4.1	4
647	Adiabatic spin dynamics and effective exchange interactions from constrained tight-binding electronic structure theory: Beyond the Heisenberg regime. Physical Review B, 2022, 105, .	1.1	4
648	<title>Object Oriented Cell Image Segmentation</title>. Proceedings of SPIE, 1982, , .	0.8	3

#	Article	IF	Citations
649	Orbital polarization in narrow band systems: Application to the volume collapse in Ce. Physica B: Condensed Matter, 1990, 163, 337-339.	1.3	3
650	The band structure, electron density, and heat of formation of scandium monophosphide. Journal of Physics and Chemistry of Solids, 1990, 51, 1033-1046.	1.9	3
651	The band structure, heat of formation, and atomic interactions in titanium monophosphide. Journal of Solid State Chemistry, 1990, 86, 300-309.	1.4	3
652	First Principles Theory of Magnetoâ€"Crystalline Anisotropy. , 1999, , 247-285.		3
653	The effect of hydrogenation on the crystal structure and magnetic state in Pd3Mn. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 1040-1041.	1.0	3
654	Crystal structure and magnetic properties of the new phase Mn3IrSi. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 823-825.	1.0	3
655	Intrinsic defects and transition metal impurities in GaAs. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 1961-1962.	1.0	3
656	Transport through quasi-degenerate states in coupled quantum dots. Photonics and Nanostructures - Fundamentals and Applications, 2004, 2, 11-21.	1.0	3
657	Electronic spectra and magnetic properties of RB6, RB12 and RB2C2 borides. Physica Status Solidi C: Current Topics in Solid State Physics, 2006, 3, 229-232.	0.8	3
658	Magnetism of Co overlayers and nanostructures on W(001): A first-principles study. Journal of Magnetism and Magnetic Materials, 2008, 320, 1173-1179.	1.0	3
659	Study of phase stability in a class of binary alloys using augmented space recursion based orbital peeling technique. Physica B: Condensed Matter, 2008, 403, 4111-4119.	1.3	3
660	EMCD in the TEM â€“ Optimization of signal acquisition and data evaluation. Microscopy and Microanalysis, 2008, 14, 1148-1149.	0.2	3
661	Magnetism-driven anomalous surface alloying between Cu and Cr. Applied Physics Letters, 2009, 94, .	1.5	3
662	Electronic structure and optical properties of solid C60. Physica B: Condensed Matter, 2009, 404, 1776-1780.	1.3	3
663	Magnetic properties of FexCo1â^'xnanochains on Pt(1â€‰1â€‰1) surfaces. Journal of Physics Condensed Matter, 2014, 26, 206003.	0.7	3
664	Analysis of long distance wakes behind a row of turbines â€“ a parameter study. Journal of Physics: Conference Series, 2014, 524, 012152.	0.3	3
665	Communication: Visualization and spectroscopy of defects induced by dehydrogenation in individual silicon nanocrystals. Journal of Chemical Physics, 2016, 144, 241102.	1.2	3
666	Low temperature magneto-structural transitions in Mn3Ni20P6. Journal of Solid State Chemistry, 2016, 237, 343-348.	1.4	3

#	Article	IF	Citations
667	First-principles theory of electronic structure and magnetism of Cr nano-islands on Pd(1â€‰1â€‰1). Journal of Physics Condensed Matter, 2017, 29, 025807.	0.7	3
668	Photoelectron dispersion in metallic and insulating <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>VO</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math> thin films. Physical Review Research, 2021, 3, .	1.3	3
669	Full-potential optical calculations of lead chalcogenides. , 1998, 69, 349.		3
670	Structural Stability in Fe-Based Alloys. , 1997, , 57-62.		3
671	Pressure Effect on Magnetic Properties of UGa3. Acta Physica Polonica A, 1997, 92, 331-333.	0.2	3
672	Multiscale approach for magnetization dynamics: unraveling exotic magnetic states of matter. Physical Review Research, 2020, 2, .	1.3	3
673	Connection between magnetic interactions and the spin-wave gap of the insulating phase of NaOsO3. Physical Review B, 2021, 104, .	1.1	3
674	Effects of vitamin A on endotoxaemia in rats. The European Journal of Surgery, 1991, 157, 565-9.	1.0	3
675	Density functional theory of spin and orbital magnetization densities in actinide magnets. Journal of Alloys and Compounds, 1994, 213-214, 238-242.	2.8	2
676	Field-induced magnetism in actinide systems. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 1353-1354.	1.0	2
677	Brookset al.Reply:. Physical Review Letters, 1998, 80, 4108-4108.	2.9	2
678	From local-density approximation to strong electron correlations. Physica B: Condensed Matter, 1999, 259-261, 229-230.	1.3	2
679	Electronic Structure Calculations of Phase Stability: Cohesive and Elastic Properties. , 2003, , 1-11.		2
680	Pressure Effect on Magnetic Properties of UX 3 (X=Al, Ga, In, Si, Ge) Compounds. European Physical Journal D, 2004, 54, 359-362.	0.4	2
681	Ab InitioElectronic Structure Calculations of Pu-115 Compounds. Journal of the Physical Society of Japan, 2006, 75, 215-219.	0.7	2
682	Ab-initio modeling of spintronic materials. Physica Status Solidi (A) Applications and Materials Science, 2007, 204, 33-43.	0.8	2
683	Spin and orbital moment sum-rules for the electron energy loss chiral magnetic dichroism. Physica B: Condensed Matter, 2008, 403, 1614-1615.	1.3	2
684	Elasticity model for the evaluation of structural parameters in multilayer systems with applications to transition metal and Si-based multilayers. Physical Review B, 2011, 84, .	1.1	2

#	Article	IF	Citations
685	Theoretical prediction of the elastic properties of body-centered cubic Fe-Ni-Mg alloys under extreme conditions. Philosophical Magazine, 2012, 92, 888-898.	0.7	2
686	Formation of 2D transition metal dichalcogenides on TiC_{1â^'x}A_x surfaces (A = S, Se, Te): A theoretical study. Journal of Materials Research, 2014, 29, 207-214.	1.2	2
687	A charge self-consistent LDA+DMFT study of the spectral properties of hexagonal NiS. New Journal of Physics, 2014, 16, 093049.	1.2	2
688	Anisotropy of magnetic properties of Fe_{1+y}Te. Journal of Physics Condensed Matter, 2014, 26, 436003.	0.7	2
689	Ab initioinvestigation of competing antiferromagnetic structures in low Si-content FeMn(PSi) alloy. Journal of Physics Condensed Matter, 2016, 28, 216002.	0.7	2
690	Correlated electronic structure of CeN. Journal of Electron Spectroscopy and Related Phenomena, 2016, 208, 111-115.	0.8	2
691	Electronic specific heat coefficient and magnetic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">Y</mml:mi><mml:msub><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>Fe</mml:mi><mml:mrow> Laves phases: A combined experimental and first-. Physical Review B, 2019, 100, .	1.1	2
692	Soft Xâ€Ray Magnetic Circular Dichroism of Vanadium in the Metalâ€“Insulator Twoâ€Phase Region of Paramagnetic V₂O₃ Doped with 1.1% Chromium. Physica Status Solidi (B): Basic Research, 2020, 257, 1900456.	0.7	2
693	Giant anisotropy of Gilbert damping in a Rashba honeycomb antiferromagnet. Physical Review B, 2020, 101, .	1.1	2
694	In Situ Pseudopotentials for Electronic Structure Theory. Journal of Physical Chemistry C, 2021, 125, 15103-15111.	1.5	2
695	Novel method of self-interaction corrections in density functional calculations. , 2001, 81, 247.		2
696	First Principles Theory of Magnetism for Materials with Reduced Dimensionality. Lecture Notes in Physics, 2001, , 243-266.	0.3	2
697	ELECTRONIC STRUCTURE AND MAGNETIC PROPERTIES OF THE Y (Fe_{1-x}C_{ox})₂ ALLOYS. Journal De Physique Colloque, 1988, 49, C8-295-C8-296.	0.2	2
698	Local structural evolution in the anionic solid solution ZnSexS1â^'x. Physical Review B, 2021, 104, .	1.1	2
699	Structural and electronic properties of the random alloy <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>ZnSe</mml:mi><mml:mi>x</mml:mi></m mathvariant="normal">S</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow> Physical Review B, 2022, 105, .	1.1	2
700	A program for logistic prediction modelling. Computer Programs in Biomedicine, 1985, 19, 235-237.	0.8	1
701	Magnetic instabilities of light rare earth impurities in 5dtransition metals. Physica Scripta, 1989, 39, 394-396.	1.2	1
702	Calculated magnetic behaviour for the (Fe1-xNix)2P pseudo-binary alloys. Journal of Physics Condensed Matter, 1989, 1, 7329-7334.	0.7	1

#	Article	IF	Citations
703	The relativistic equation of state of actinide metals and compounds. High Pressure Research, 1990, 2, 265-271.	0.4	1
704	Ground state properties of the AnFe2 systems (An = U, Np and Pu). Physica B: Condensed Matter, 1990, 163, 710-712.	1.3	1
705	ELASTIC CONSTANTS OF d TRANSITION ELEMENTS AND d TRANSITION ALLOYS. International Journal of Modern Physics B, 1993, 07, 203-206.	1.0	1
706	Poisson equation and a self-consistent periodical Anderson model. Physical Review B, 2001, 64, .	1.1	1
707	Theoretical study of the high-pressure orthorhombic TlI-type phase in NaBr and NaI. Physical Review B, 2001, 63, .	1.1	1
708	Elastic properties of Mg(1Âx)AlxB2from first principles theory. Journal of Physics Condensed Matter, 2004, 16, 5241-5250.	0.7	1
709	<title>Electronic structure and optical spectra of novel rechargeable lithium batteries</title>. , 2004, , .		1
710	Theory of strongly correlated electron systems. I. Intersite Coulomb interaction and the approximation of renormalized fermions in total energy calculations. International Journal of Quantum Chemistry, 2005, 102, 1019-1045.	1.0	1
711	Theory of strongly correlated electron systems. II. Including correlation effects into electronic structure calculations. International Journal of Quantum Chemistry, 2005, 102, 1046-1055.	1.0	1
712	Localized and Itinerant States in Pu Materials. Materials Research Society Symposia Proceedings, 2005, 893, 1.	0.1	1
713	Exchange Interactions and Magnetic Percolation in Diluted Magnetic Semiconductors. , 0, , 131-145.		1
714	Comment on â€œNature of non-magnetic strongly-correlated state in Î´-plutoniumâ€•by L. V. Pourovskii et al.. Europhysics Letters, 2006, 76, 170-171.	0.7	1
715	Controlling dopant solubility in semiconductor alloys. Journal of Physics: Conference Series, 2010, 242, 012014.	0.3	1
716	Thermo-physical properties of body-centered cubic ironâ€“magnesium alloys under extreme conditions. Solid State Communications, 2011, 151, 203-207.	0.9	1
717	Ab initioPhonons in Magnetic Ni2MnAl. Japanese Journal of Applied Physics, 2011, 50, 05FE07.	0.8	1
718	Theory of diluted magnetic semiconductors. Science and Technology of Atomic, Molecular, Condensed Matter and Biological Systems, 2012, 2, 1-19.	0.6	1
719	Correlated electronic structure of Fe in bulk Cs and on a Cs surface. Physical Review B, 2013, 87, .	1.1	1
720	Band alignment switching and the interaction between neighboring silicon nanocrystals embedded in a SiC matrix. Physical Review B, 2015, 91, .	1.1	1

#	Article	IF	Citations
721	Large-eddy simulations of wind farm production and long distance wakes. Journal of Physics: Conference Series, 2015, 625, 012022.	0.3	1
722	An ab initio perspective on scanning tunneling microscopy measurements of the tunable Kondo resonance of the TbPc2 molecule on a gold substrate. Physical Review B, 2020, 101, .	1.1	1
723	Dynamical Mean Field Theory. Springer Series in Solid-state Sciences, 2010, , 75-87.	0.3	1
724	Electronic Structure of Isolated Molecules. SpringerBriefs in Applied Sciences and Technology, 2020, , 25-34.	0.2	1
725	Interaction with Substrates. SpringerBriefs in Applied Sciences and Technology, 2020, , 45-64.	0.2	1
726	Electronic and optical properties of FeS2 and CoS2. , 0, .		1
727	Influence of antiphase boundary of the MnAl Ï„ -phase on the energy product. Physical Review Materials, 2019, 3, .	0.9	1
728	Introduction to Electronic Structure Theory. Springer Series in Solid-state Sciences, 2010, , 25-34.	0.3	1
729	‹title›Computer Assisted Scanning Microscopy In Cytology‹/title›. , 1982, , .		0
730	MAGNETISM IN ACTINIDE TRANSITION METAL INTERMETALLICS. Journal De Physique Colloque, 1988, 49, C8-695-C8-696.	0.2	0
731	Actinide metals and intermetallic compounds: Electronic structure and magnetic properties. Journal of Radioanalytical and Nuclear Chemistry, 1990, 143, 21-34.	0.7	0
732	Giant surface layer relaxation for Be (10 0). Journal of Magnetism and Magnetic Materials, 1996, 156, 85-86.	1.0	0
733	Crystal field levels in lanthanide systems. Journal of Magnetism and Magnetic Materials, 2001, 226-230, 1027-1028.	1.0	0
734	Noncollinear magnetization density in VAu4. International Journal of Quantum Chemistry, 2002, 90, 1610-1613.	1.0	0
735	Fe/V and Fe/Co (001) Superlattices. Growth, Anisotropy, Magnetisation and Magnetoresistance. ChemInform, 2003, 34, no.	0.1	0
736	Electronic Structure of Î´-Pu and PuCoGa5 from Photoemission and the Mixed Level Model. Materials Research Society Symposia Proceedings, 2003, 802, 221.	0.1	0
737	Phase Relations in the Ti3Snâ€”D System.. ChemInform, 2004, 35, no.	0.1	0
738	Structural and magnetic aspects of multilayer interfaces. Journal of Magnetism and Magnetic Materials, 2004, 272-276, E941-E942.	1.0	0

#	Article	IF	Citations
739	Electronic structure and magnetism of diluted magnetic semiconductors and derivatives. Journal of Magnetism and Magnetic Materials, 2004, 272-276, E1581-E1582.	1.0	0
740	Final state effects in the X-ray absorption spectra of La0.7Sr0.3MnO3. Journal of Magnetism and Magnetic Materials, 2004, 272-276, 1780-1781.	1.0	0
741	Electronic Structure Calculations of Electronic and Structural Properties of Plutonium 115 Compounds. Materials Research Society Symposia Proceedings, 2005, 893, 1.	0.1	0
742	Role of asymmetries for EMCD sum rules. , 2008, , 423-424.		0
743	Ab-initio Computational Modeling Of Complex Magnetism In Spintronic Materials. AIP Conference Proceedings, 2008, , .	0.3	0
744	Publisherâ€™s Note: Correlated Electrons Step by Step: Itinerant-to-Localized Transition of Fe Impurities in Free-Electron Metal Hosts [Phys. Rev. Lett.104, 117601 (2010)]. Physical Review Letters, 2010, 104, .	2.9	0
745	A multi-scale approach for performance assessment of hydrogenated graphene Field-Effect Transistors. , 2010, , .		0
746	On the icosahedral metalâ€“phosphorus coordination in melliniite: a gift from the sky for materials chemistry. Journal of Materials Chemistry, 2012, 22, 14741.	6.7	0
747	Dynamic Stabilization of Cubic AuZn. Materials Today: Proceedings, 2015, 2, S569-S572.	0.9	0
748	Universal distribution of magnetic anisotropy of impurities in ordered and disordered nanograins. Physical Review B, 2015, 91, .	1.1	0
749	Partial cation ordering, relaxor ferroelectricity, and ferrimagnetism in Pb(Fe1â€‰â^'â€‰xYbx)2/3W1/3O3 solid solutions. Journal of Applied Physics, 2020, 128, 134102.	1.1	0
750	Majority gate for two-dimensional ferromagnets lacking inversion symmetry. Physical Review Research, 2021, 3, .	1.3	0
751	Chemical Bonding of Solids. Springer Series in Solid-state Sciences, 2010, , 111-131.	0.3	0
752	Density Functional Theory and the Kohnâ€“Sham Equation. Springer Series in Solid-state Sciences, 2010, , 7-19.	0.3	0
753	Total Energy and Forces: Some Numerical Examples. Springer Series in Solid-state Sciences, 2010, , 101-109.	0.3	0
754	Excitated State Properties. Springer Series in Solid-state Sciences, 2010, , 145-178.	0.3	0
755	Ab Initio Studies on the Hydrogenation at the Edges and Bulk of Graphene. Carbon Nanostructures, 2012, , 203-208.	0.1	0
756	Calculated moments for the pseudo-binary alloys Ce(Fe1-xCox)2 AND Ce (Fe1-xNix)2. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1989, 86, 927-931.	0.2	0

#	Article	IF	Citations
757	Crystal Structure and Phase Stability in Fe1-xCox from AB Initio Theory. , 1997, , 13-17.		0
758	Atomic Volume Effect on Electronic Structure and Magnetic Properties of UGa3 Compound. , 1998, , 323-335.		0
759	Magnetic properties of Ruddlesden-Popper phases <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="bold">Sr</mml:mi><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></		